# LINKING BIOPHYSICAL MODELS AND LIFE CYCLE ASSESSMENT TO EVALUATE ENVIRONMENTAL TRADEOFFS OF URBAN WATER INFRASTRUCTURE DESIGN

BY

SASKIA HERMINA VERSTEEG

THESIS

Submitted in partial fulfillment of the requirements
for the degree of Master of Science in Civil Engineering
in the Graduate College of the
University of Illinois at Urbana-Champaign, 2016

Urbana, Illinois

Adviser:

Assistant Professor Jeremy S. Guest

# ABSTRACT

Water, a limited resource even on our hydrous planet, has always been inextricably tied to the rise and fall of cities and human infrastructure. Clean, plentiful water drives our food and energy production, provides transport, and keeps humans and the environment healthy. Integrated urban water modelling and improved geospatial databases are allowing water management researchers to analyze the effects of process decisions in the water management sector on a broader scale and with higher spatiotemporal resolution than ever before. Research is driven by the desire to optimize limited resources, respond to changing user patterns, characterize the robustness of the system to climate change pressures, and define the downstream effects of new technologies. Water management decisions today not only require hydraulic and hydrologic knowledge, but also an understanding of energy production systems, environmental biochemistry, economics, and regulatory policy. Although integrated urban water models started by expanding on simple physical urban drainage models, they are now incorporating mechanisms for environmental change, social agents, and economic feedback.

Although originally built to protect public health and the local aquatic environment, wastewater treatment utilities have in recent years taken on additional objectives including greenhouse gas mitigation, reducing chemical use, and reducing long-term environmental impacts due to effluent nutrients and disinfection byproducts. National policies on water quality (EU Water Framework Directive, US Clean Water Act) and electricity demand (GHG emissions targets) both cover utilities, with the goal of improving their environmental sustainability. These multiple objectives may call for

conflicting operational decisions, which presents a direct tradeoff to utility decision makers—increase electricity use for treatment, or allow worse effluent quality to flow into the local environment.

This thesis seeks to characterize the scale of impacts stemming from energy-water tradeoffs and identify sources of uncertainty in making this decision, by placing the operational tradeoff in a larger water-energy-environmental system context. The case study in Eindhoven, the Netherlands is selected for several reasons. The local water management authority has created a well-researched integrated urban water model, comprising the urban water system from raindrop through domestic use, sewer collection, wastewater treatment, and to the receiving river. The national water and energy policies are providing stricter standards for utilities, presenting this tradeoff decision previously mentioned. Finally, the local and national datasets for LCA inventory, meteorology, energy generation, and ecological response are well documented, allowing us to analyze the system from a holistic perspective.

The analysis of the energy-water quality tradeoff is completed by different modeling methods employed by water managers and regulators, to see if the different methods yield improved or conflicting results. First, we use traditional LCA inventory accounting which is the current standard for new capital investments in wastewater treatment. The LCA considers the impacts of kilowatt hours of electricity and ammonia released to the environment in wastewater effluent for four different standards of effluent quality. This analysis demonstrated a clear tradeoff between eutrophication and global warming (energy production emissions) impacts. Second, the spatiotemporal variation of these eutrophication and air emissions impacts is explored using biophysical models. The models include the calibrated integrated urban water system model developed for Eindhoven and the Dommel in conjunction with a generalized atmospheric dispersion model for emission byproducts of electricity generation. We study the downstream transport of ammonium in the river and particulate matter from the power plant emissions. The air emissions modeling found that even a single day of electricity demand associated with wastewater treatment could affect particulate matter concentrations hundreds of kilometers away, crossing international borders. The water quality modelling found that marginal improvements in the effluent quality (of 1 mg/L ammonium) could improve the worst-case ammonia concentrations downstream by up to 20%. Third, the biophysical model results are evaluated using literature-based characterization factors for human health exposure and ecosystem tolerances to the aforementioned ammonium and particulate matter emissions. These calculations framed our physical models in the context of local systems. On the air emissions side, the electricity generated for wastewater treatment was found to contribute less than 0.1% of the background particulate matter concentration in the region modelled. On the water quality side, the wastewater treatment plant significantly reduced the number of ecological exceedances compared to a no-treatment control scenario, on the order of about 50%. However, this control scenario does not account for the influence of other sources of ammonium in the river, such as other wastewater treatment plants or agricultural runoff.

The outcomes of this work show that energy investment in wastewater treatment creates a significant tension in environmental impacts. Our multi-tiered evaluation sought to explore the dimensions of these impacts on higher resolution spatial scales, to better understand how they fit into environmental systems. Ultimately, the physical modeling showed that energy impacts could cross international borders which might have some implication for international policymaking. However, through systems analysis these impacts were shown to be negligible in comparison to the water quality consequences for local ecosystems.

# ACKNOWLEDGEMENTS

I sincerely thank the Graduate College at the University of Illinois for granting me the opportunity to pursue creative and entirely independent research through the Illinois Distinguished Fellowship. The chance to design and manage my own thesis project was a great challenge and capstone to my master's coursework at UIUC and would not have been possible without the university's investment in my education.

My greatest thanks also go to my advisor, Professor Jeremy Guest, for his support of me as a student and friend. I truly appreciated having an open-door advisor who I could count on for ideas and advice. You have become a role model to me in terms of your professionalism, support, and energy for exploration.

I also want to recognize Dr. Lorenzo  Benedetti, who became my personal mentor in teaching me how to use integrated water systems modelling software and provided a lot of background resources for this thesis. I very much appreciate you taking the extra time and energy to screencast with me to show me specific tools within the model. Furthermore, Peter Bach, Andrew Henderson, and Mathew Eckelman have provided valuable high-level insight for the structure and potential impacts of this research paper. Tony Flameling, Stefan Weijer, and Antonia Hadjimichael, from the KALLISTO project itself were generous in sharing resources and background information to make this study possible. The Danish Hydraulics Institute generously provided a research license for the WEST software used to complete this master's thesis.

Finally, I am thankful for the support of my family and friends in Champaign-Urbana, Texas, and beyond. You always help to make the journey fun, and celebrating the prize even more exciting.

# TABLE OF CONTENTS

# CHAPTER 1: INTRODUCTION

Wastewater treatment utilities, originally established to protect local public and environmental health, have in recent years come under additional scrutiny for regional and global environmental impacts stemming from electricity consumption, fugitive greenhouse gas emissions, chemical use, and long-term societal impacts due to nutrient loading and contaminants of emerging concern (Bach et al., 2014). As capital investments reach their lifespan limits, operators and designers are looking for novel ways to meet these multiple objectives. Among the many other goals, operators want to upgrade plants to meet increasingly stringent effluent nutrient requirements. An integrated approach is necessary for decision-making as the policymakers behind the EU Water Framework Directive and the US Clean Water Act are calling for water management on a river-basin wide scale (EPA 1972; European Council 2000).

In specific cases, these design and operational decisions may introduce a tradeoff between two conflicting sustainability objectives. A common example is investing additional electricity to improve effluent quality. Often, operators and policymakers will turn to life cycle assessment (LCA) to summarize information from all energy and material flows into and out of the system boundary and to better understand a decision's impact on different environmental metrics (Pasqualino et al., 2009). Life cycle assessment typically aims to present global and long-term consequences of decision making, focusing on large spatial and temporal scales (Gallego et al., 2008). This may be problematic in the case of wastewater treatment plants, which as point sources of effluent pollution to receiving rivers have high potential for acute, local human health and eutrophication impacts (Fu and Butler, 2012).

Wastewater process decisions can have a significant effect on local urban metabolism, which is difficult to evaluate without physical models specific to the local environment. While a new suite of modeling tools have been developed to explain these mechanisms, scientists are still exploring how to link these results with the more generalized models used in LCA. More LCA software is incorporating sophisticated environmental fate and transport models (ranging from TRACI to IMPACT World+) for key pollutants (Renou et al., 2008). Several life cycle impact assessment (LCIA) methods are seeking to integrate geospatial databases and LCA calculations (Mutel et al., 2012). Examples of some innovative approaches coupling local model resources with LCA metrics include human health analysis through quantitative microbial risk assessment (Harder et al., 2015; Kobayashi et al., 2015), land use analysis through water footprinting (Gasparatos et al., 2009; Mekonnen and Hoekstra, 2015), and emergy analysis (Pizzigallo et al., 2008).

However, when using LCA to support decision-making, the scope, resolution, and uncertainty of the environmental assessment must be clearly communicated in both directions between scientists and decision makers. For example, aggregating impacts using LCA from different categories or locations may obscure the actual system influence of the process in question by underemphasizing local acute impacts or overemphasizing low, distributed impacts (Gasparatos et al., 2009; Mutel et al., 2012; Renou et al., 2008). Since the composition of wastewater effluent depends greatly on diurnal patterns and hourly storms, a life cycle assessment that considers these quantities as monthly or annual aggregates might obscure the impacts of multiple short-duration peaks on both process efficiency and local environmental quality. Spatial heterogeneity is another important consequence of adapting LCA to fit local purposes. Characterization factors that convert impacts on specific local scales may not be appropriate for larger, heterogeneous land areas (Helmes et al., 2012). While scientists continue to work to improve the density and accuracy of local characterization factors and aggregation methods, clear communication is necessary to establish a policy standard for the scope and depth of LCA required to make process tradeoff decisions.

The objective of this work is to demonstrate how LCA can be used to evaluate tradeoffs in operational decision-making, with special focus on adapting the life cycle inventory and impact assessment process to the scope of the decision being made. This is especially critical when applying the global, long-term focused methods used in LCA to a decision with significant local impacts. Our process involves evaluating a multi-objective decision that involves a direct tradeoff between electricity use and effluent quality by increasing the spatiotemporal resolution and system modeling of environmental impacts at different tiers of evaluation. By comparing the results from a traditional aggregate LCA, locally calibrated environmental transport models, and a human and ecological health impact assessment, we hope to show the complexity of system impacts that can result from a process tradeoff decision. The overarching goal of this research is to use the questions raised by the Eindhoven case study example to further the discussion toward establishing a standard for systemic analysis of policy decisions for integrated urban water infrastructure.

# CHAPTER 2: BACKGROUND

As cities grow, sea waters rise, economies trade, populations urbanize, and climates change, it becomes increasingly imperative for modern cities to consider the urban water cycle in a holistic, integrated perspective. Initially, urban water problems were solved in a piecemeal fashion—stormwater drains were built to relieve flooding lots, drinking water treatment plants were placed near new urban centers, and wastewater treatment was improved in response to public health outbreaks. The growing complexity of urban water, energy, materials, and economic cycles, as well as our growing awareness of urban water impacts on the environment, mean that we must begin evaluating and optimizing these discrete subsystems in an integrated way. This review first explores the background of integrated urban water modelling (IUWM), including motivation and modeling structure. It then discusses the state-of-the-art in understanding the energy-water nexus in an urban context, with a particular focus on human and policy pressures. Then, the current standard of life cycle assessment (LCA) for environmental impact evaluation is discussed, with focus on the many modern applications of LCA and limitations and opportunities of the approach. The final section presents a detailed background of the Eindhoven case study explored later in this thesis.

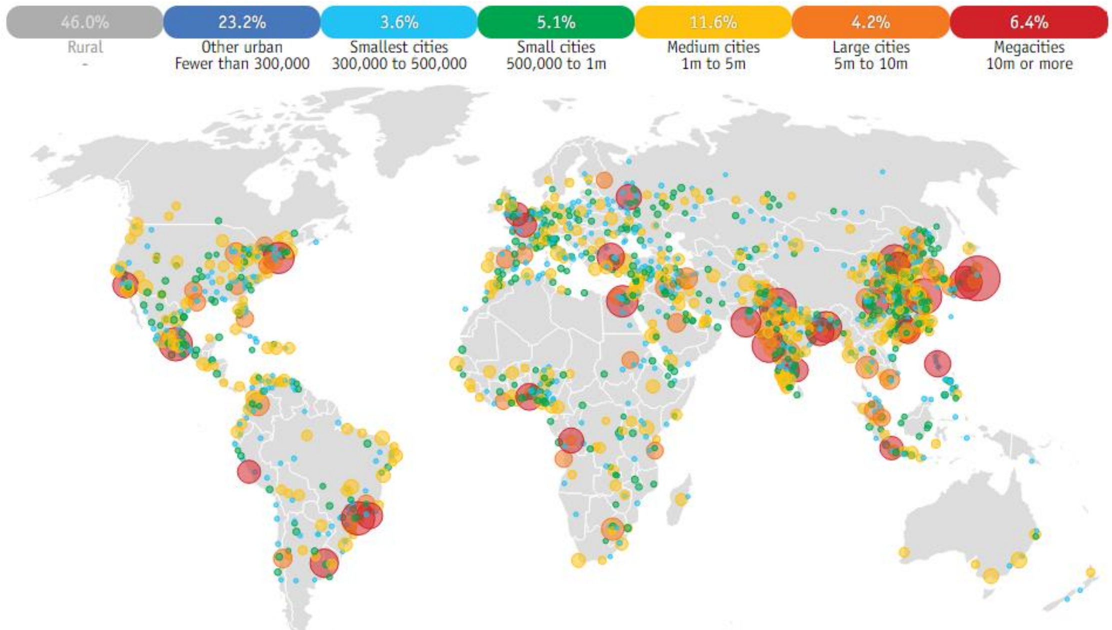
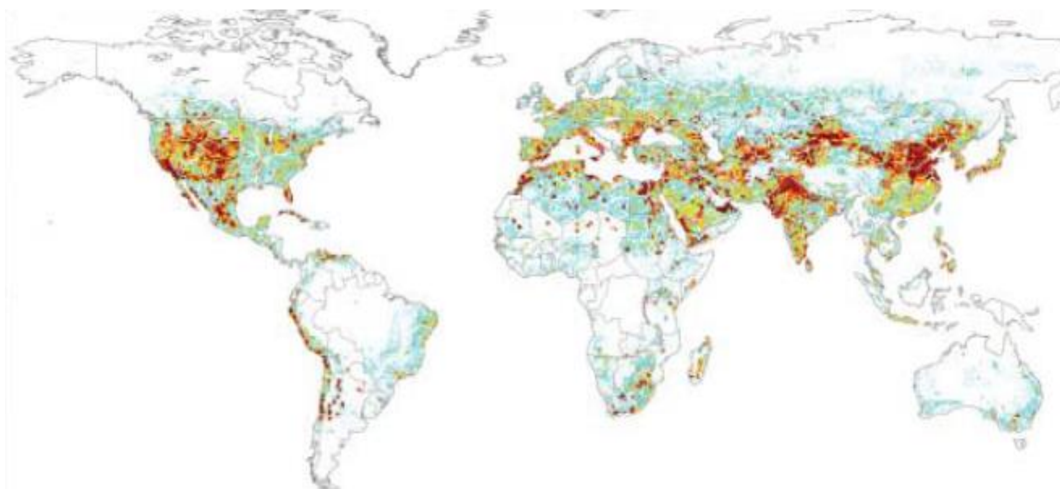



***Figure 1:*** *World population map of 2016 showing at least 30 megacities of at least 10 million people (red). Smallest cities shown are light blue, of at least 300,000 inhabitants (The Economist).*



## 2.1 Motivation for Integrated Urban Water Modelling (IUWM)

***Figure 2:*** *Global water scarcity index. Highest water scarcity (dark red) is felt in many highly urbanized, coastal areas.*

Earth is now home to 30 megacities with human populations over 10 million (Figure 1). Over half of the world's population lives in urban areas as of 2014 (The Economist, 2007). The largest wastewater treatment plant in the United States treats 700 million gallons of water a day—the demand placed by the 2 million people living in its service area (MWRD, n.d.). The size of urban water systems, like so many infrastructure systems created by humans (Bettencourt et al., 2007), has grown exponentially in the last half-century. Over one hundred years ago, engineers first recognized the problem that our knowledge of the impacts of our sanitary infrastructure extended no further than "the outfalls of our sewers" (Soper 1907). The local service area now covers tens of kilometers, while the downstream range of air- and water-shed impacts likely covers many hundreds of kilometers. Indeed, the rise of integrated urban water modeling (IUWM) first started as an attempt to develop more comprehensive urban drainage system models. Much of this research was driven by the objective to better understand urban water cycles and help conserve this scarce resource (Figure 2). The INTERURBA I conference (Lijklema et al., 1993) marks the start of a community committed to understanding the feedbacks and optimization of integrated urban water cycles.

In the wake of INTERURBA I, scientists almost immediately began looking to IUWM as an opportunity for real-time control of wastewater treatment systems (Bach et al., 2014). Water treatment subprocess models (i.e., for individual water bodies or sewer systems) had been under development for some time, coupling improved computation capacity for environmental fluid dynamics with the increased storage necessary for GIS datasets (Bach et al., 2014). However, as individual sectors began to commit to more sustainable infrastructure on a subsystem level (Marlow et al., 2013), engineers recognized the need to understand system interactions and possible feedbacks.

Brown et al. identified three institutions that shape our "patterns of practice": cognitive, normative, and regulative (Gessner et al., 2014). While the cognitive institutions—as engineers and research scientists—were shifting approaches from an experimental perspective, the regulatory institutions also provided pressure from an administrative perspective. The EU Water Framework Directive called for river-basin-wide management of surface water bodies to maintain their "good ecological and environmental quality" (European Council 2000), a novel call to manage environmental quality along biophysical boundaries rather than political ones. Finally, the normative institutions include social values and leadership. Scientific and political leadership has recognized that we have entered a geologic epoch called the Anthropocene, where human activity dominates environmental systems (Vidas et al., 2015). Thus, we should not study water cycles as solely physical systems—our models must incorporate human infrastructure, economic indicators, and ideally social impacts to provide a truly robust assessment of water resources (Oki 2006).

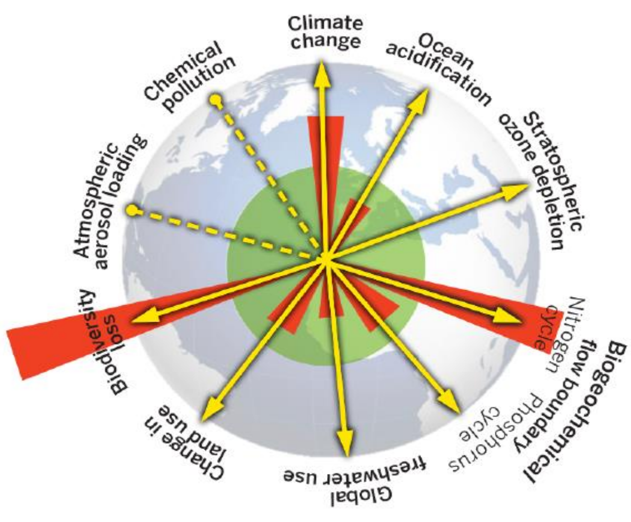



***Figure 3:*** *Planetary indicators showing highest anthropogenic impact on global ecosystem services. From Liu, et al.*

Anthropogenic influence doesn't only dominate water cycles—in the past several decades, scientists have begun identifying shifts in natural systems across scales due to direct or indirect human impacts. Rockstrom et al identified nine planetary indicators, ranging from freshwater use to aerosol loading, which represent global systems under great stress due to human activity. As shown in Figure 3, three of the sectors identified (nitrogen & phosphorus cycles, climate change, and biodiversity loss) have already crossed a threshold of sustainability which biophysical models suggest is irrecoverable (Liu et al., 2015; Rockström et al., 2009). Most human water use is for economic activities, including agriculture, power generation, domestic and industrial uses (Lund 2015). Meanwhile, economies are globalizing and interconnecting. Some economic decisions have faraway indirect impacts, such as fertilizer runoff from the American breadbasket in the Midwest flowing down the Mississippi and creating an anoxic zone at the New Orleans delta (Yaeger et al., 2013). Scientists are also beginning to understand the systems of virtual water, or water embodied in economic trade between distant communities (Dalin et al., 2012). Thus water systems may be critical for local economies, but their impacts extend across global scales.

On a local scale, water is the fluid connecting the urban metabolism—the way a city converts external resources to products and services, such as food and energy, to provide for the livelihood of its citizens (Gessner et al., 2014). This process produces various forms of waste (Beck and Walker, 2011), which have become a special interest of environmental engineers who seek to improve the balance between human society and its environmental impacts. Water as a resource plays a critical role in many sectors including agriculture, navigation and transportation, and public health, which have traditionally been viewed separately in sustainability assessments (Grant et al., 2012). However, emerging multilateral issues such as water scarcity and environmental quality will require communication among these different sectors to achieve effective solutions.

Energy is another critical, cross-sector resource which is limited in availability. Its provision often requires water, and in reverse the provision of useful water resources often requires an energy investment. This coupling is referred to in modern literature as the energy-water nexus. The intersection of these two systems is of special interest to scientists and policymakers because, just as increasing spatial and temporal scales might introduce tradeoffs between local and global optima, considering the energy and water systems working in unison presents a problem with multiple objectives and additional constraints. These objective functions may not even be based in the same units, such as investment decisions, water quality indicators, or resource scarcity (Bach et al., 2014).

To understand how the different systems within a city interact, we need to create models and designs on a local, rather than mechanistic or process-driven scale. This will be especially important to understand the long-range impacts of these technologies if they are implemented on a large scale. Collectively, wastewater treatment plants are feeling pressure to reduce their energy use and greenhouse gas emissions and become carbon neutral (Cabrera Marcet et al., 2014). If plants want to become carbon neutral, the electricity mix they consume becomes critical (Larsen 2015), underscoring the relevance of the energy-water nexus to this research. Indeed, reducing electricity use and by association, greenhouse gas emissions, have become a high policy priority for wastewater treatment plant operators (Caffoor 2008). One of the most promising areas of wastewater treatment research is resource recovery, or the development methods to capture energy and nutrients from wastewater (Guest et al., 2009). The advent of anaerobic and phototrophic technologies could even bring energy positive wastewater treatment to the mainstream (Shoener et al., 2014). Although several life cycle assessments and life cycle costing evaluations of different technologies have been completed (Iranpour, 1999; Ishii and Boyer, 2015; Shoener et al., 2014), these investigations have remained limited to the scope of an individual wastewater treatment plant. There remains a knowledge gap in how these new technologies can affect the urban-environment ecosystem, which is where integrated urban water modeling (IUWM) can play an important role. Some demonstrated benefits of IUWM include evaluating the economic and environmental impact of a phosphorus removal process (Clauson-Kaas et al., 2004), comparing centralized and decentralized treatment system scenarios (Tillman et al., 1998), and investigating the capital or production use carbon intensity of new technology (Caffoor, 2008; Rozenberg et al., 2015). Advances in computer modeling ability and big data availability in even the last five years have made it possible to develop models with high temporal resolution (Mitchell et al., 2007) and high reliability through local data calibration (van Loosdrecht and Brdjanovic, 2014).

In addition to evaluating local impacts of system changes, integrated urban water modeling provides the opportunity to see local impacts of global stressors such as climate change, population shifts, or policy pressures. Climate change can lead to different hydrologic impacts in various regions, such as changes in rainy or dry seasons, eutrophication, storm frequency and intensity, or temperature shifts. Integrated urban water modeling has been used to explore the local effects of increased eutrophication (Havens and Paerl, 2015), water availability (Paton et al., 2014), and storm impacts on water treatment (J. G. Langeveld et al., 2013). Such projects provide the additional challenge of coupling urban water models with non-technical scientific fields such as economics or sociology. It is certainly important to investigate these impacts, because water management serves a critical social need (Lund 2015). The additional complexity of these global phenomena increases the uncertainty of any such models.

## 2.2 Current State of IUWM

With INTERURBA I, the first conference to recognize the concept of integrated urban water modelling occurring over 20 years ago, the field has had its time to widen and deepen our understanding of local water systems. Many submodels are developed independently, or existing submodels have been adapted for use in IUWM (Bach et al., 2014). The basic system included in most integrated urban water models includes urban drainage, wastewater treatment plants, and the receiving waters.

Urban drainage models have been under development since the first designs of urban sanitary networks in the late 20$^{th}$ century (Rauch et al., 2002). In the current state of the art, urban drainage modeling is using advanced environmental flow models to evaluate the impacts of green infrastructure improvements on water quality and quantity (Casal-Campos et al., 2015). In this field, there is special emphasis on using a robust approach rather than optimization, because the uncertainty around flow parameters and water quality metrics is still quite high.

The Benchmark Simulation Model, originally developed for only activated sludge modeling by the IWA in 1999 (Jeppsson et al., 2013), has been extended to cover a range of pre- and post-treatment processes used in wastewater treatment plants. The uncertainty around the chemical kinetics of wastewater treatment is also still quite high, as found by the latest IWA task group on benchmarking control strategies of wastewater treatment plants. This group found that although the use of wastewater treatment process models, especially GPS-X (Hydromantis Environmental Software Solutions, Inc, 2016) and WEST (MIKE by DHI, 2016), is widespread among designers and operators alike, there remain several areas to improve. Namely, most wastewater treatment process simulators take inputs of constant model parameters, treating the process deterministically when due to the uncertainty around, for example, influent fractionation, sensor dependability, and chemical kinetics it would be more appropriate to use a stochastic approach (Jeppsson et al., 2013). Model runs using global sensitivity analysis have shown that it is not only the mechanistic models that require improvement, but uncertainty could be greatly reduced through more accurate sensing of influent fraction parameters (Sin et al., 2011). Both the model calibration and ultimate predictions depend on improved monitoring of water quality parameters throughout the water cycle (J. G. Langeveld et al., 2013).

The final, and possibly most critical for environmental impact assessment, component of many integrated urban water models is the receiving water. Receiving water often refers to a river, but may also include lakes and other surface waters or even groundwater. On the water quantity side, support from global climate modeling and GIS sensing and a drive to understand the impacts of flooding and storms has developed sophisticated systems for physical hydraulic analysis that can be directly linked to the effluent from wastewater treatment (Muschalla et al., 2014). Incorporating water quality in these models is more challenging for a series of factors, mostly due to a lack of monitoring data and uncertainty around biochemical parameters of reactions in receiving water. The most common used tanks-in-series models of receiving rivers are DuFlow (Rauch et al., 1998), originally developed by Wageningen University in 1996, and River Water Quality Model 1 (Shanahan et al., 2001) developed by an IWA task group in the early 2000s. DuFlow was originally focused on analyzing the environmental impacts covered by Dutch pollution permits, so it focused primarily on the dynamics of dissolved oxygen, organic matter, and ammonia. It is available in commercial software like WEST and SIMBA. It includes both biological processes like organic substrate degradation, nitrification, and photosynthesis, and physical processes like re-aeration, sedimentation, and diffusion. On the other hand, River Water Quality Model 1 (RWQM1) was developed in order to cover the missing gaps in industry models and is focused on a comprehensive, conservation of matter approach to track carbon, hydrogen, oxygen, phosphorus, and nitrogen (Saagi, n.d.).

The main challenges of integrating urban water models include the uncertainty of model parameters, setting system-wide objective functions, and connecting submodels. System models can suffer from both input uncertainty, where input values are either miscalculated or misrepresented as fixed values when they should be variable, or parameter uncertainty which is inherent to how the model mechanisms function (Schellart et al., 2010). A common source of uncertainty in large IUWMs is the simplified representation of spatial and temporal scales, done to reduce computing time (Blumensaat et al., 2012). Although it is important to match input and output scales when linking submodels, sometimes averaging or aggregating submodel output can lead to excluding important, acute results. This is because movement of water, solutes, and energy through a water system is characterized by steep gradients and high reaction rates (Gessner et al., 2014).

Another common problem is setting system-wide objective functions. The goals of sewer system designers, wastewater treatment operators, and environmental policy makers (to name a very few stakeholders) are very different and may depend on cost, environmental indicators, or process efficiency. Some scientists have even suggested that a true global optimum does not exist for integrated water systems (Bertrand-Krajewski, 2007; Khu and Madsen, 2005).

The final common challenge in integrated urban water modeling is developing a method to properly link submodels. Although it is possible to build a supermodel tailored to the specific plant and its parameters, this can be a very time- and capital-intensive process. It is often faster to adapt models used for other plants to new purposes. However, this approach, often called "interfaces", carries its own challenges because different submodels may handle certain parameters (COD fractionation, the description of organic nitrogen, the definition of pH, and the definition of inert materials, to name some of the most common ones) differently (Grau et al., 2009). It is very important to keep the big picture in mind when constructing an integrated model, focusing on keeping the system dynamics, spatial scale, and paradigms coherent (Voinov and Shugart, 2013). A particularly relevant quote states,

*"A complex model may be more realistic, yet more uncertain."* –(Oreskes, 2003)

Some of the more common approaches to successfully integrating these models include Petersen matrices (Vanrolleghem et al., 2005) and including data set modules (Voinov and Shugart, 2013). Still, scientists point out that much more monitoring is necessary both to calibrate and initialize models, and to validate the results of models across the entire urban water cycle (J. G. Langeveld et al., 2013).

Of course, integrated urban water models can be adapted and coupled to other models to facilitate different types of decisions making and planning purposes. Since the integrated urban water model allows for the propagation of effluent through the water cycle, scientists can connect wastewater process models to sustainability indicators like materials, energy, and costs for more comprehensive life cycle assessments (Fagan et al., 2010). Including submodels that have the ability to model micropollutants has helped explore the fate of these particles propagating downstream (Plósz et al., 2012; Vezzaro et al., 2014). On the water quantity side, nations like Australia which are highly concerned about water scarcity may include agent-based modeling and social metrics to evaluate water availability across a basin-wide water system, as well as the impacts of novel water-saving technologies (Welsh et al., 2013). And finally, studying system dynamics allows us to explore the life cycle impacts of individual material flows, rather than location-based processes. For example, a French group recently completed a LCA of urban water treatment from initial pumping station through to the wastewater treatment plant, essentially studying the life cycle of a kilogram of water through its lifespan in the city (Lassaux et al., 2007).

## 2.3 Using IUWM to evaluate the energy-water nexus

Although integrated urban water modeling may have its roots in the design and operation of urban water systems, it has since prompted scientists to take a closer look at the interactions of the water cycle with other flows in the urban metabolism such as energy, nutrients, and materials. The Water Environment Research Federation completed a quantitative analysis of the tradeoffs between eutrophication and electricity consumption for different wastewater treatment levels. Although wastewater treatment does produce some methane and greenhouse gas byproducts, the study found that the three largest contributors to greenhouse gas emissions were all energy related: aeration, pumping and mixing, and deep well injection. The study found that after a certain threshold of nutrient removal was achieved, electricity consumption increased exponentially to reduce additional eutrophication potential (Falk et al., 2013).

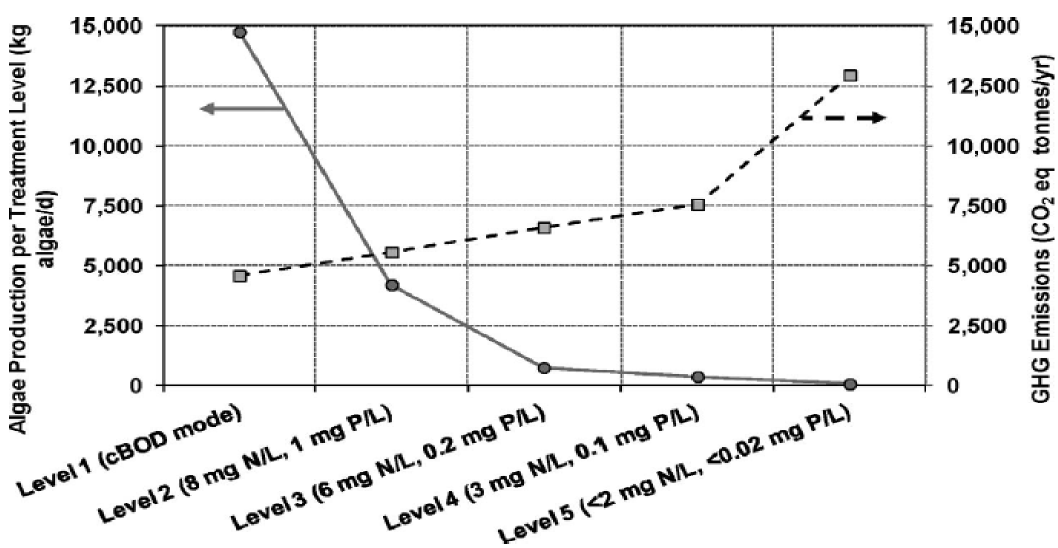



***Figure 4:*** *Results of a WERF study showing tradeoffs between effluent quality (levels 1-5) causing eutrophication (kg algae produced) vs. electricity used (GHG emissions). From Falk, et al.*

Another team at Wageningen University has recently developed the "urban harvest approach", which combines modeling of the integrated urban water cycle on short timesteps with an LCA-type assessment of water and energy fluxes through the city-wide system. They found that new water technologies benefit from a detailed analysis of their spatiotemporal impacts, because new technologies are often locally focused in contrast with traditional centralized treatment approaches (Leusbrock et al., 2015).

Finally, many separate scientific groups have combined these novel quantitative modeling approaches with LCA to develop "hybrid LCA" approaches. Traditional LCA establishes a method and characterization factors to facilitate the comparison of different processes for environmental impacts ranging from ecotoxicity to global warming potential. The goal of various hybrid LCA approaches is to layer on additional metrics of interest not covered by LCA libraries, which may include location-specific risk assessment or human health impacts. For example, scientists might evaluate pathogen risk using a quantitative microbial risk assessment with the output of disability-adjusted life years (DALYs), which provide a basis for indirect comparison with environmental impacts (Kobayashi et al., 2015). The biggest challenge of hybrid LCA lies in qualitatively assessing the tradeoffs from quantitative technical models when those models use environmental, economic, or social impact metrics (Harder et al., 2015). For example, it can be difficult to directly compare disability-adjusted life years against kilograms of greenhouse gases emitted, although both have human health implications. Some hybrid LCAs, therefore, try to integrate the economic or social models within the environmental system. For example, the THEMIS model couples LCA with regional electricity markets and climate change scenarios to constantly update the demand and impacts of different technological mitigation approaches (Gibon et al., 2015).

The challenge, from a wastewater treatment expert's perspective, is accurately capturing the impacts of the complex urban energy system. Most traditional wastewater treatment LCAs use a historical electricity mix to evaluate the electricity use impacts of a particular process, but researchers have established that this is not sufficient for capturing the impacts of local supplies or changing economic markets (Gibon et al., 2015; Lane et al., 2015). Mitigating water scarcity impacts by diversifying local supplies has been shown to increase the energy intensity of water provision by a factor of 2.3 (Lane et al., 2015). Properly accounting for electricity generation impacts is therefore critical to understanding urban water systems. However, most sources of electricity are highly location-dependent, which would require researchers to develop additional models of electricity generation to improve system understanding (Romero-Lankao et al., 2014; Stokes and Horvath, 2010). For example, the previously mentioned THEMIS model calculated the environmental impacts of 1 kwh of electricity using a linked environmental-economic market model, but the results showed significant variation due to regional differences in manufacturing (Gibon et al., 2015). Still, since policy directives such as the EU Water Framework Directive will require significant increases (60-100%) in energy consumption to meet more stringent effluent requirements (Caffoor 2008), incorporating accurate electricity generation models remains a high research priority.

## 2.4 Using IUWM for life cycle assessment (LCA)

Wastewater treatment plant designers and operators can choose from among many different technologies based on varying effluent quality requirements, biochemical processes, and hydraulic demand. LCA has been used to evaluate different parts of the urban water system since the late 1990s (Loubet et al., 2014). Although initial LCAs focused on evaluating individual processes, especially in wastewater and drinking water treatment, the early 2000s brought more critical, system-wide analyses of urban water treatment. As LCA has been applied to new fields and increasingly broad decision-making objectives, it is important to critically re-examine its potential and limitations. In the past two decades, LCA of urban water systems has been used to clarify economic implications of process decisions, evaluate new technology, and study interactions of different system subcomponents.

After water treatment processes meet their permitting standards, cost often becomes the most significant factor in making design decisions. Since most components of urban water treatment have lifespans on the order of decades, life cycle costing provides an opportunity to include the costs of operation, as well as the initial capital investment, in decision-making. It creates a life-cycle based approach to evaluate the economic viability of a product (Rebitzer and Seuring, 2003). Scientists have become more creative in incorporating economic principles in engineering design evaluations. For example, the principle of opportunity costs has also been incorporated as some IUWM evaluations use a “regret based approach” to determine the most robust system configuration that can weather a variety of environmental and economic scenarios (Casal-Campos et al., 2015). One of the most promising research fields in impact assessment of IUWM is in risk management of financial and infrastructural assets in various urban planning scenarios (Lund, 2015).

Of course, life cycle assessment can also be used in a comparative method to evaluate new technologies. The incorporation of integrated urban water models allows scientists to look at the impacts of decentralizing water provision and treatment systems (Tillman et al., 1998). One of the most common areas of research is in water recycling (Tangsubkul et al., 2005), which  may include such technologies as desalination (Ortiz et al., 2007) or struvite precipitation (Ishii and Boyer, 2015).

The IUWMs can be leveraged to compare the life cycle impacts of different control strategies and scenarios. For example, a robust analysis was performed of a single treatment subsystem, the activated sludge section, incorporating a multiobjective evaluation of the various life cycle impacts of subsystem controllers (Flores-Alsina et al., 2010). The WaLa model calculated the impact to service ratios of providing water treatment to different groups of end users in the Parisian metropolitan area (Loubet 2015). The life cycle assessment of an Australian catchment showed that life cycle impacts were dominated by the operations phase, and within that by energy consumption, across a variety of technology and control scenarios (Lane et al., 2015).

As scientists apply life cycle assessment methods to larger and more complex urban water system models, it becomes important check the scale and scope of the LCA method used. The data available from urban water models can improve the resolution and scope of LCA on both spatial and temporal scales. However, an overload of data provides its own problems (e.g., signal to noise ratios), so scientists must frame the model data in the context of the system they are working with. The main motivators for higher resolution

LCA of urban water systems include location-specific impact factors, assessing local versus global environmental impacts, and comprehensively evaluating risk.

Although life cycle assessment often focuses on global impacts such as greenhouse gas emissions, the processes studied in urban water systems are bound to the local environment with which they interact (Kobayashi et al., 2015). This means that the downstream impact models must be carefully tuned to local parameters, which can vary widely between cases. A recent study of freshwater eutrophication due to phosphorus in Europe showed that output uncertainty depended more on the variance of local characterization factors than on the model mechanics (Azevedo et al., 2013). This suggests that data verification of local impact factors is critical when constructing models of urban water systems, and when assessing the downstream life cycle impacts of local decision-making. Another study, of nitrogen loading to world rivers, showed that 75% of nutrient loading to rivers comes from diffuse sources and can vary widely between river sections (Mekonnen and Hoekstra, 2015). This means that monitoring must have not only high accuracy but high density to capture the spatial variability of water quality conditions. Some scientists are calculating “fate factors” for specific nutrients and pollutants which characterize, per spatial location, how long certain molecules remain in that environment (Helmes et al., 2012). This can help when assessing acute or chronic impacts per location, and also simplify the calculation of downstream impacts without incorporating complex environmental flow models. Since many life cycle assessments find that the operations phase of wastewater treatment, and specifically the electricity used by wastewater treatment plants, is the major contributor to environmental impacts, it is also important to verify the characterization factors for electricity use (Kobayashi et al., 2015). Integrated system models have been leveraged to connect the water system with an economically responsive energy system which provides more accurate feedback-based impact assessment (Gibon et al., 2015).

Life cycle assessment is traditionally based on aggregating sums of environmental impacts over the entire lifespan of the system in question, and comparing those volumes between different options (Gasparatos et al., 2009). Although this may make sense for binary decision-making on a global scale, it may not be optimal for local, multiobjective decisions. This is because local environmental systems do not respond linearly to external impacts, but rather change due to thresholds for concentrations and frequencies being exceeded (Mitchell et al., 2007). Indeed, some small amount of system variance may make the ecosystem more robust to external stressors. Bode's Law states that controlling the short-term variance of a system can increase variance on longer timescales (Carpenter et al., 2015). This system characteristic confronts a major shortcoming of LCA, which is based on accumulating and averaging impacts over the lifespan of a process as a basis for comparison (Blumensaat et al., 2012). Many life cycle assessments of wastewater effluent include errors such as summing the impacts of discrete discharges, or failing to consider high frequencies of moderate events, or ignore the effects of positive feedback or hysteresis in the downstream system. It is critical for modelers to understand the characteristics of their datasets and systems before applying life cycle methodology, which may over- or under-estimate impacts so drastically as to not provide any useful output (Gasparatos et al., 2009).

Finally, higher resolution life cycle assessment and modeling is necessary to evaluate the risks associated with emerging pollutants in the urban water system. As water is a conveyor of many processes used in our daily lives, we continue to find new components and interactions with environmental systems downstream. Most modern treatment systems focus on eliminating pathogens, heavy metals, and nutrient pollution which contribute to eutrophication and ecotoxicity. However, an analysis of a Spanish wastewater treatment plant found that personal care products and pharmaceuticals were the main contributors to ecotoxicity of wastewater effluent (Muñoz et al., 2008). Improved environmental flow models and geospatial data are also allowing for better data collection and modeling of micropollutants on regional scales (Vezzaro et al., 2014).

## 2.5 Eindhoven Case Study Background

The International Water Association organizes communities of scholars called "working groups" whenever it sees a particularly significant new area of research on the horizon. In this way the Modeling of Integrated Urban Water Systems (MIUWS) working group was established in 2012 with the goal of gathering information on the current state of the art of IUWM and necessary areas of research. Through participation in this working group we found an opportunity to work with a calibrated integrated urban water model of the wastewater treatment process of the city of Eindhoven in the Netherlands.

The model was originally developed by Waterschap de Dommel as part of the KALLISTO project (Weijers, 2012) for real time control of this highly sensitive local water system. The Waterschap de Dommel is one of 24 regional water boards in the Netherlands responsible for the water supply, sanitation, flood mitigation, and water quality health of all waters in its service boundary. The service area covers roughly 1,500 square kilometers and one million people and can be seen in the orange section of Figure 5. Although the Waterschap de Dommel was founded in the 19$^{th}$ century with the goal of flood mitigation, the region did not commit to water quality efforts until over a century later. Up until the 1950s, the large city of Eindhoven discharged all its wastewater effluent directly to the Dommel, the largest river in the service region. Built in 1963, the Eindhoven wastewater treatment plant (Dutch: rioolwaterzuiveringsinstallatie, RWZI), serves an equivalent population of about 750,000 individuals.

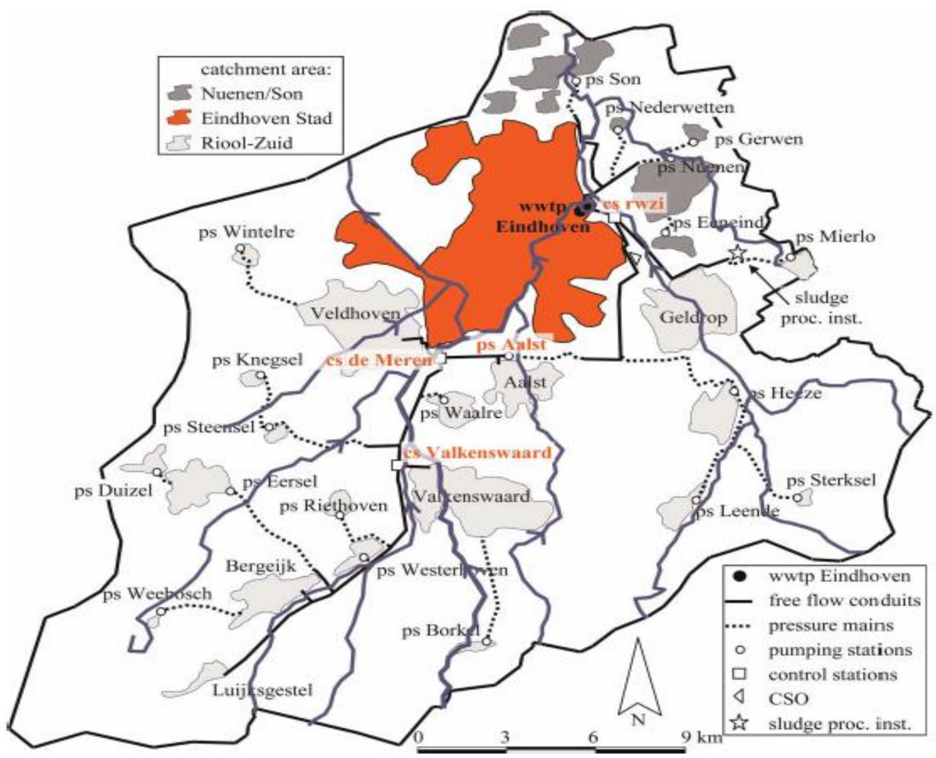



***Figure 5:*** *The complex urban drainage system of the Dommel River around the urban area of Eindhoven (orange). From Weijers, et al 2012.*

The Dommel River faces water quality challenges from many different fronts, including the large urban drainage area, domestic population, local zinc industry, and intensifying agriculture. The Dommel itself discharges about 1.5 $m^3/s$ and runs about 85 km from the Netherlands-Belgium border to the larger Meuse river (Benedetti et al., 2013b). Urban runoff presents both a hydraulic problem as it intensifies and shortens the runoff peaks from particular rainfall patterns, relative to the natural norm, and a water quality problem as it can flush metals, particulate matter, and other toxins off paved roads and to the receiving waters. Stormwater from the Eindhoven and surrounding urban areas discharges to the Dommel through some 200 combined sewer outflows (Benedetti et al., 2013b; J. Langeveld et al., 2013). The local metal industry, especially focused on zinc smelting has contributed to significantly elevated levels of zinc and cadmium in regional soils and sulfur dioxide emissions to the atmosphere (Petelet-Giraud et al., 2009). About 62% of the catchment is covered by agricultural lands (Rozemeijer and Broers, 2007). In the past two decades, agriculture in this region has shifted from dairy farming to intensive livestock farming, which results in the spreading of manure with high nitrogen, phosphorus, and metal contents (Petelet-Giraud et al., 2009). Since the groundwater table is generally within 1-3 meters of the surface, fertilizer use can greatly contribute to escalated levels of nutrients in river discharge (Rozemeijer and Broers, 2007). Although the impact is expected to be significant, the quantified impact of these nonpoint sources of nutrient pollution has not yet been compared to the known impact of the effluent from the Eindhoven wastewater treatment plant and linked CSOs.

The impact of the Eindhoven wastewater treatment plant and linked CSO effluent has become a matter of great concern for the municipality especially in the face of rising quality standards through the EU Water Framework Directive and Dutch national surface water goals(Benedetti et al., 2013a). In 2006 the city budgeted and began installing a large monitoring network comprising of rain gauges and radar, sewer system flow and water depth sensors, UV-VIS and ammonium sensors at the WWTP influent, WWTP reactor sensors testing ammonium, phosphate, nitrate, and dissolved oxygen levels, and ammonium and dissolved oxygen sensors along several kilometers of the Dommel River both up- and down-stream of the treatment plant discharge (J. Langeveld et al., 2013). This extensive monitoring campaign has yielded unprecedented amounts of data that allowed the calibration of a full integrated urban water system model (IUWM) used in this project. This integrated urban water model was one of the first efforts to bridge two EU water quality directives on opposite ends of the spatiotemporal spectrum: the EU Urban Waste Water Treatment Directive, which regulates point source emissions from wastewater treatment plants, and the EU Water Framework Directive, which specifies water quality standards and management of river basins (European Council, 2000). The KALLISTO project identified the need for both higher-quality resolution water system models to understand how to design wastewater treatment plants to comply with both objectives, and the critical importance of monitoring campaigns to develop these models (Benedetti, Langeveld, Comeau, et al.).

The Eindhoven wastewater treatment plant, as mentioned, treats an average of 200,000 $m^3$ of domestic effluent per day from about 750,000 individuals. This is approximately 5% of the population of the Netherlands, which makes the Eindhoven system a significantly sized case study to explore policy-compliant design options for the rest of the nation. The Eindhoven wastewater treatment plant (Eindhoven RWZI) uses a modified UCT process to biologically treat influent in three parallel lines. The maximum hydraulic load for treatment is 26,000 $m^3$/hr. A separate stormwater settling tank bumps up the maximum hydraulic load to 35,000 $m^3$/hr. After passing through a primary settling tank, the effluent enters one of the three biological reactors which are shaped like rings, as shown in Figure 6. The concentric rings function like plug-flow reactors, with the initial inner ring functioning for the anaerobic treatment, the central ring switching between anoxic and aerobic treatment depending on the weather and seasonal conditions. The outer ring functions fully as an aerobic plug-flow reactor and is the last stage before the effluent moves on to the secondary settling tank.

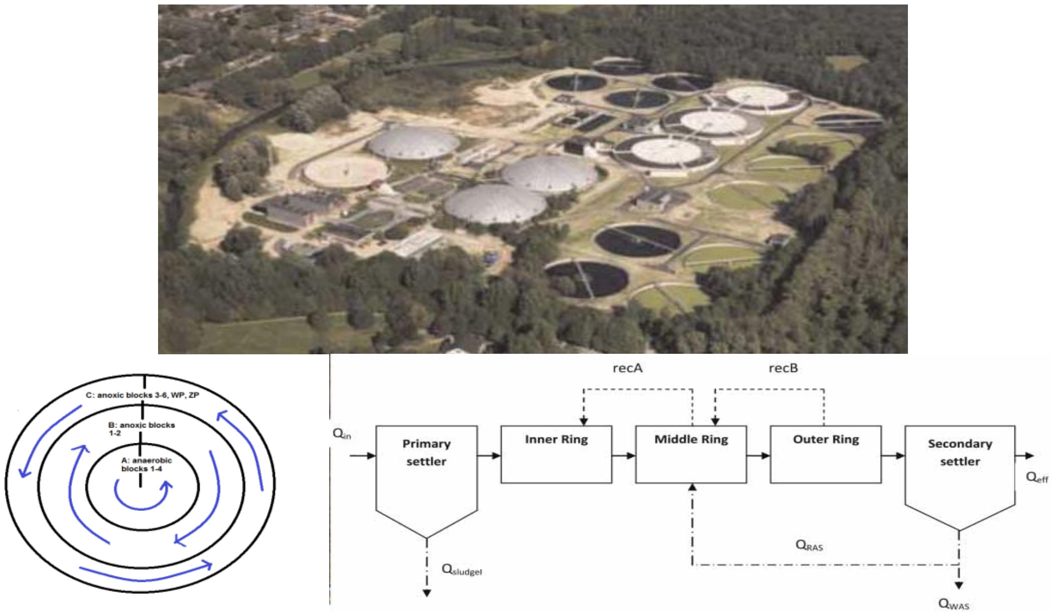



***Figure 6:*** *Above, a Google Maps overview of the Eindhoven WWTP showing 3 parallel treatment lines leading to a cluster of secondary settlers. Below left, a sketch of a circular primary settler treatment system. Below right, the process model of the modified UCT process used by the wastewater treatment plant (Weijers et al 2012).*

The software WEST (MIKE by DHI, 2016) was used by the KALLISTO project to model the Eindhoven wastewater treatment plant. Although the river model was initially built using DuFlow and a detailed sewer model was developed in InfoWorks, these subsystems were simplified and integrated into the WEST-based model of the wastewater treatment plant. This required simplifying some of the geometry and most significant physical processes of these subsystems, but ultimately yielded a fast-functioning, highly accurate integrated model for the analysis of the impacts of process design decisions on receiving water quality (Benedetti et al., 2013b). This is an example of a "standard supermodel", which uses a general software package to model the entire integrated water system (Grau et al., 2009). The sewer and receiving river models were likely simplified to preserve the general spatial scale of the model, which is critical when developing a useful integrated model (Voinov and Shugart, 2013). The WEST model uses blocks in series to model both the plug-flow reactors of the wastewater treatment plant and the separate river sections of the receiving river, as can be seen in Figure 7.

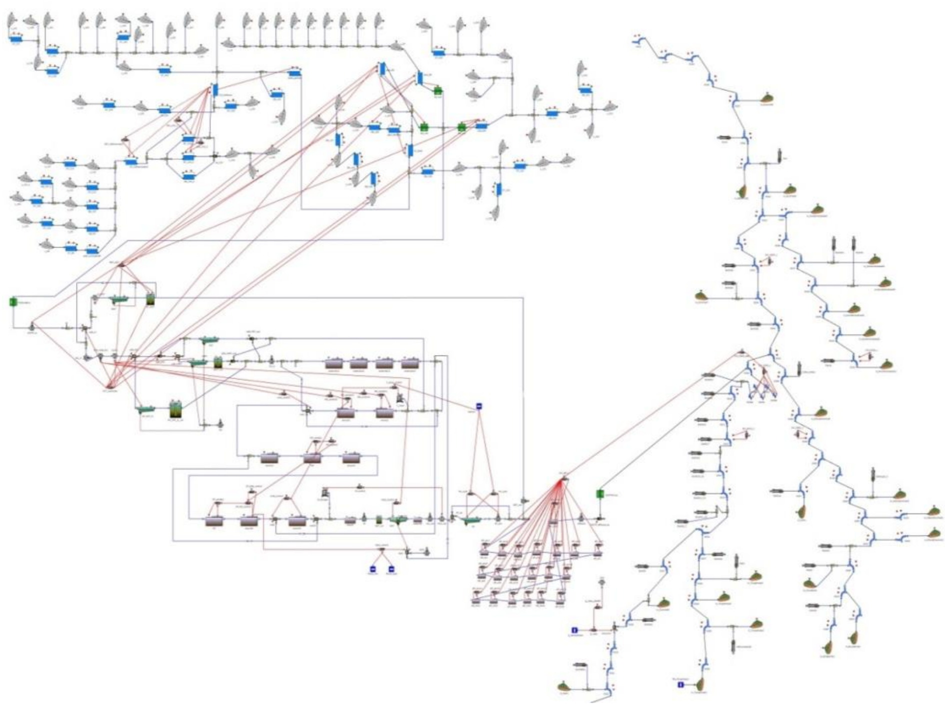


***Figure 7:*** *Integrated model of the Eindhoven urban water system in WEST (Mike by DHI). The urban drainage blocks and sewer system are on the upper left, the wastewater treatment plant process blocks in the lower left, and the river submodel is on the right.*

To critically examine the design decisions of investing additional energy into the wastewater treatment process, a spatiotemporally discrete model of the emissions associated with electricity generation was necessary. This model was built in-house, and the data collection for the calculations of the electricity emissions are described in greater detail in the methods section. The open-source HYSPLIT model (NOAA, 2016) was selected for the calculation of the dispersion of air-borne emissions for its efficiency, simple interface, and meteorological data integration. HYSPLIT is typically used for general meteorology studies or air pollution studies using back-trajectory calculation to determine the source of some pollution. Based on NOAA's guidelines and the European Environmental Agency data on significant emissions factors of particulate matter from fossil fuel and biomass-based power plants, a regional model of particulate matter concentration was developed to assess the environmental impacts of electricity investment design decisions. Figure 8 below shows the ability of HYSPLIT to utilize open-source meteorology data and user inputs of geospatial locations of particle emissions to calculate the trajectories of individual particles moving across a region and also through the atmosphere (Cohen, 2011; Heinzerling et al., 2005).

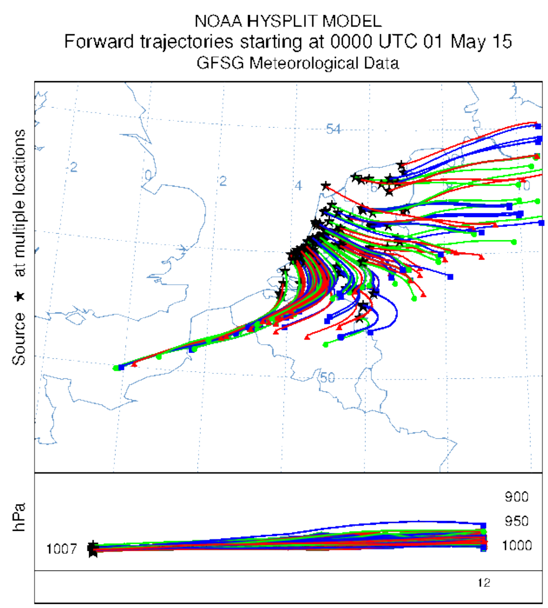



***Figure 8:*** *Example of HYSPLIT trajectory calculations for single particles emitted from Dutch power plants (original content).*

# CHAPTER 3: METHODS AND RESULTS

## 3.1 METHODS

### *3.1.1 POLICY CONTEXT*

With the 2008 Water Framework Directive, the European Union has committed to improving the ecological and chemical quality of its surface water bodies using an intergovernmental, river-basin-wide management approach. According to a 2011 European Environment Agency report (EEA 2012), 50% of Dutch rivers are classified as "poor "ecological quality unfit to support wildlife habitats. In this research, we analyze the way a local water authority in Eindhoven, the Netherlands responds to these national policies and trajectories when tasked with mitigating electricity consumption while protecting the quality of the water in its highly sensitive receiving Dommel River. The Waterschap de Dommel, the public company responsible for storm- and waste-water management in the city of Eindhoven and surrounding areas (Overzichtskaart Waterschap de Dommel, 2015), made its mission to provide "clean, sufficient, and safe" water for its regulatory region (Waterschap de Dommel 2010). To support this objective, the KALLISTO project was established to develop a sophisticated integrated model of the urban water system in Eindhoven (STOWA 2012), including a 20-kilometer stretch of the downstream receiving river. On the energy use side, the water utilities in Eindhoven share a commitment made by the European Environment Agency and World Water Forum to reduce electricity use by 20% by 2020 (European Environment Agency, World Water Forum).

### 3.1.2 Operational decision-making

The multiple policy objectives of reducing utility electricity demand while improving surface water quality present a dilemma for wastewater treatment plant operators. In the Eindhoven case, wet weather events temporarily intensify the load of ammonium through the treatment system and can cause high ammonium loadings to the receiving river. To mitigate this effect, additional fine bubble aerators were installed in the anoxic tanks of the biological treatment system to reduce ammonium in the effluent. The additional aeration capacity can be activated at different setpoints measured by an ammonium sensor in the plant effluent. In this project, we characterize the impacts of increasing the setpoint of this sensor, varying it in four levels through 7.5, 8.5, 9.5, and 10.5 mg/L. This incrementally reduces aeration demand and thereby the electricity demand of the plant over extended timeseries. The evaluation of this tradeoff can be viewed as a microcosm of large-scale policy decisions that must be made to satisfy the dual objectives of local water quality and regional electricity demand.

### 3.1.3 Estimation of aggregate environmental impacts

To understand the long-term impacts of the tradeoff between additional electricity use and releasing additional ammonium to the local environment, a life cycle assessment was performed on these specific cross-boundary flows. Because this is purely an operational decision (infrastructure construction, equipment needs, etc., do not change as a result of this decision), the system boundary excludes construction and demolition of the treatment plant. The functional unit evaluated was one day’s worth of water treatment by the Eindhoven plant based on the average treatment flow of 200,000 $m^3$/day. This allowed us to test the kilowatt hours of electricity consumed, versus kilograms of ammonium released at each of the four treatment levels. The inventory data for medium-voltage electricity in the Dutch market comes from the Ecoinvent database, while the ammonium and biochemical oxygen demand (BOD) characterization factors come from the ReCiPe database in SimaPro software. ReCiPe midpoint (H) is used as the impact assessment method because it was developed by Dutch consultants and the midpoint indicators can be best compared to later physical model results.

### 3.1.4 *Integrated urban water system modeling*

The KALLISTO project created an integrated urban water system model simulating the entire storm- and waste-water collection and treatment system of the Eindhoven municipality, including an ASM2d-based wastewater treatment system process model and a DuFlow-based receiving river model (Weijers 2012).

This model was run with one-year dynamic hydrologic input based on precipitation data measured for the KALLISTO project (J. Langeveld et al., 2013). To examine the spatiotemporal variation of water quality impacts in the downstream river solely due to wastewater treatment plant operation, the influence of CSO inflows from Eindhoven to the river was removed.

### 3.1.5 *Water quality and ecological implications*

The integrated urban water system model calculates the water quality conditions based on concentrations of ammonium, dissolved oxygen, and BOD in 20 kilometers of the Dommel River downstream of the wastewater treatment plant. Certain thresholds of ammonium and dissolved oxygen concentration, when exceeded for particular lengths of time within a certain recurrence interval, can highly stress the local ecosystem. The Urban Pollution Management Manual (Urban Pollution Management Manual (3rd Edition) 2012) provides fundamental intermittent standards matrices specifying these thresholds, durations, and recurrence intervals. These matrices were used by the KALLISTO project to calculate the total number of ecological exceedances in the Dommel River due to the wastewater plant effluent. In this project, the number of exceedances are calculated for the four ammonium setpoints with a high degree of spatial resolution.

### 3.1.6 *AIRBORNE EMISSIONS AND HUMAN HEALTH IMPLICATIONS*

To further investigate the spatiotemporal dimension of electricity consumption impacts, a model of air emissions combining open-source energy grid data and the HYSPLIT atmospheric transmission model was created. The Eindhoven wastewater treatment plant purchases electricity from Essent utility (Lako, 2015), but the grid is maintained by TenneT B.V., a government-owned distributor. Individual power plant locations, generating capacity, type, and efficiency were sourced from Enipedia (Netherlands/Power Plants 2010), an open-source energy industry wiki published by T.U. Delft. The air pollution effects of Dutch domestic biomass, natural gas, and coal plants were modeled, as they contribute 49.9% of the local utility's electricity mix (Stroometiket 2014 Essent, 2014). Particulate matter exposure based on local concentrations was selected as a proxy for long-term health effects. Emissions factors for particulate matter were sourced from the European Environmental Agency, separated by fuel type

(EMEP/EEA air pollutant emission inventory guidebook, 2013). The Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model was used for modeling the particulate matter emissions from individual plants over a one-month period in May 2015 (Draxler, 2000). The model was run as a concentration calculation (*hycs_std.exe*) with Gaussian-plume horizontal, particle vertical motion as suggested by the NOAA emissions modeling guidelines (NOAA Air Resources Laboratory, 2009a). Meteorological data for May 2015 was sourced from the NOAA Global Data Assimilation System archive on a 3-hourly, 0.5 degree global grid (NOAA Air Resources Laboratory, 2015). From the Enipedia archives, 215 coal, natural gas, or biomass burning plants were identified to be included in the calculations. Each plant's particulate matter emissions rate was calculated based on plant type and its proportional contribution to the national electricity generation. Concentration data were then calculated at 10, 100, and 500 meters above ground in 6-hour time intervals over the course of the month. According to the NOAA guidelines, this yielded a good representation of the particle spread in space and time without requiring excessive computing capacity (NOAA Air Resources Laboratory, 2009b). Finally, the human health impacts of the local particulate matter concentrations were calculated using population density data (CIESIN and CIAT, 2005) and literature-based concentration-response curves (Krewski et al., 2010).

### *3.1.7 UNCERTAINTY AND SENSIVITY ANALYSES*

The largest source of uncertainty in the electricity generation life cycle assessment has been identified as variability in the national electricity production mix (Gibon et al., 2015; Lund 2015). In the Netherlands, the amount of fossil fuels in the mix have fluctuated by about 5% over the past 10 years (The World Bank 2016). The transport mechanism of ammonium in the local environment also varies greatly on spatial timescales, with recent literature on fate factors of phosphorus worldwide (Helmes et al., 2012) showing that the retention time of nutrients in Dutch watersheds varies by as much as 75%. In the aggregate life cycle assessment, these impacts are implicit in the impact assessment methodologies because most include generalized environmental transport models. In the physical modelling approach, the WEST model allows for greater discretization of spatiotemporal scales. However, the WEST model was run deterministically in this project because varying the inputs and model parameters was deemed too computationally burdensome for the scope of this study, without contributing meaningful details to the tradeoff decision being made.. Published uncertainties about the HYSPLIT trajectory model (Draxler 2000) and the GDAS meteorological dataset (NOAA Air Resources Laboratory 2015) are significantly smaller than the uncertainties associated with our electricity mix assumptions. Finally, in converting the physical model data to quantifiable human health and ecological system impacts, it is critical to consider the appropriateness of local characterization factors. The ecological indicators used here were also previously used to characterize Eindhoven effluent impact in the KALLISTO project (STOWA 2012). The concentration-response curves carry a human health impact uncertainty explained in detail in various review literature (Krewski et al., 2010).

## 3.2 RESULTS

### *3.2.1 AGGREGATE ENVIRONMENTAL IMPACTS*

The plant used for this review uses additional aeration energy to compensate for increased ammonium levels during wet weather flows. When analyzing the tradeoff using a traditional life cycle analysis approach, the electricity consumption and effluent quality are quantified as flows within the system boundary. The flow of electricity used by the plant is measured in kilowatt hours, which is then converted using LCA characterization factors to specific impact categories of interest: eutrophication and global warming. The impacts of ammonium in the wastewater effluent are calculated based on the total quantity of ammonia in kilograms released per day at different setpoint treatment levels. The models used to calculate the environmental flows and transformations of the electricity production process outputs to soil, water, and air are included in the LCA inventory which means they are standardized across all cases in which the LCA characterization factors are applied.

Figure 9 shows the output of the traditional LCA metrics for the Eindhoven wastewater treatment plant, considering the endpoint indicators of global warming and eutrophication. Although other impact categories are affected, especially by electricity production, the global warming impacts were selected to show a representative trend across varying treatment levels. The impacts are normalized to the highest impact treatment level to better show trends. There is a clear tradeoff showing that as the treatment standard increases, the aggregate level of eutrophication impact decreases while the total global warming impact increases.

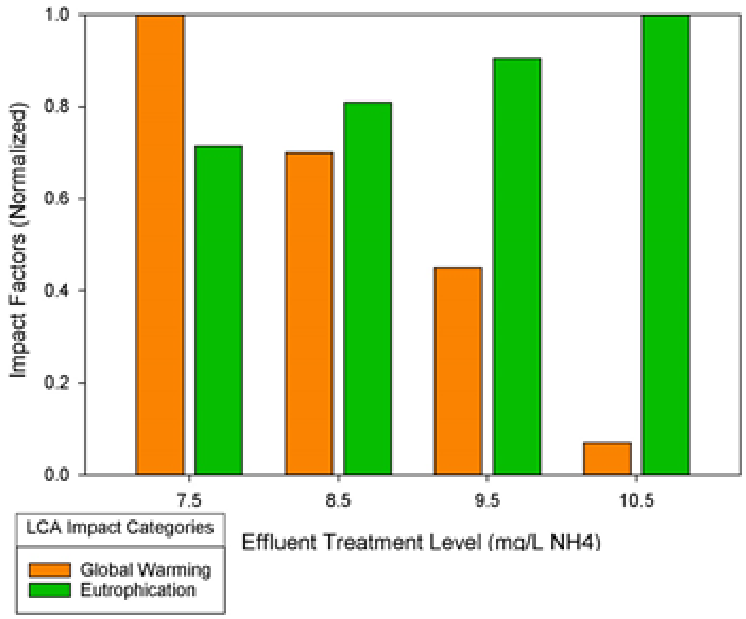



***Figure 9:*** *Normalized LCA output of ammonium and electricity generation processes, showing clear tradeoff at different effluent treatment standards.*

However, this LCA output gives no information about the spatial or temporal spread of these impact factors. The processes, which in an environmental flow model would be considered as concentrations and fluxes, are now measured in absolute and volumetric terms. Such reductionist quantities make it difficult to determine if critical environmental thresholds have been crossed, or if impacts are localized to a specific area or time period. This means that the actual enduring influence of the processes on human wellbeing and the environment cannot be assessed, so the approach does not meet Water Framework Directive requirements.

### *3.2.2 Spatial Environmental Quality Impacts*

To better assess the spatial and temporal distribution of electricity and water quality impacts, two models were used to separately study the flows of electricity- and wastewater effluent- associated pollutants away from the wastewater treatment plant. The electricity production model calculated particulate matter concentrations caused by the electricity generation necessary to operate the wastewater treatment plant. The top half of Figure 10 shows the distribution of particulate matter concentration at the measurable level of at least 1 picogram per cubic meter for the daily electricity generation emissions associated with powering the aeration of the wastewater treatment process. For most scenarios, the impact of particulate matter concentration extends far beyond the local utility boundaries of Eindhoven, across Holland and into Germany and Belgium. However, because of the large spatial distribution of emissions, the concentration of particulate matter is quite low in most locations. Scenario A, with the strictest treatment standard, affects the largest spatial region with its air-emissions impacts. On the other hand, the air emission impacts of Scenario D, the most lax treatment standard, are localized to a much smaller area.

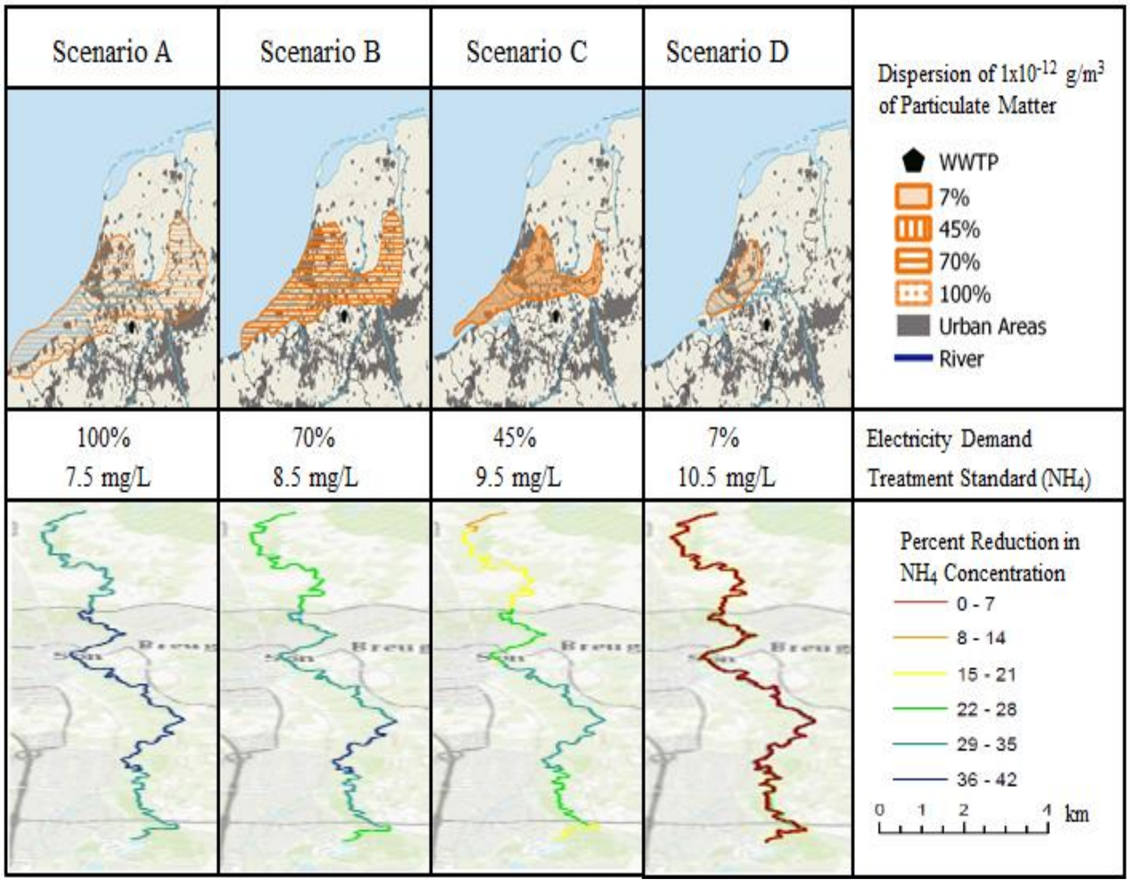



***Figure 10:*** *Biophysical model outputs showing particulate matter concentrations (top) and worst-case ammonium concentrations (bottom) at four different treatment standards.*

The spatial distribution of water quality impacts was assessed using an integrated urban water system model developed by the Waterschap de Dommel for the city of Eindhoven and surrounding areas, implemented in the WEST simulator (MIKE by DHI, 2016). The model output calculates the water quality in the receiving river, the Dommel, as "tanks in series", essentially dividing the river into separate blocks in space. The bottom half of Figure 10 shows the worst case impacts for all river sections over the 10-year time period studied, for different levels of water quality treatment. Improving the spatial distribution by using physical modelling allows policymakers to see explicit downstream impacts, possibly allowing regulators to demarcate how far downstream engineers must consider when designing water quality improvements. Figure 10 shows the percent reduction in $NH_4$ concentration from a "do-nothing" control scenario. Scenario D, when the treatment standard is at 10.5 mg/L $NH_4$, shows almost no difference in the worst-case ammonium concentrations. On the other hand, there is significant improvement in Scenario A, where the worst case has been reduced in most river sections by about 40%.

### 3.2.3 HUMAN AND ECOLOGICAL HEALTH IMPACTS

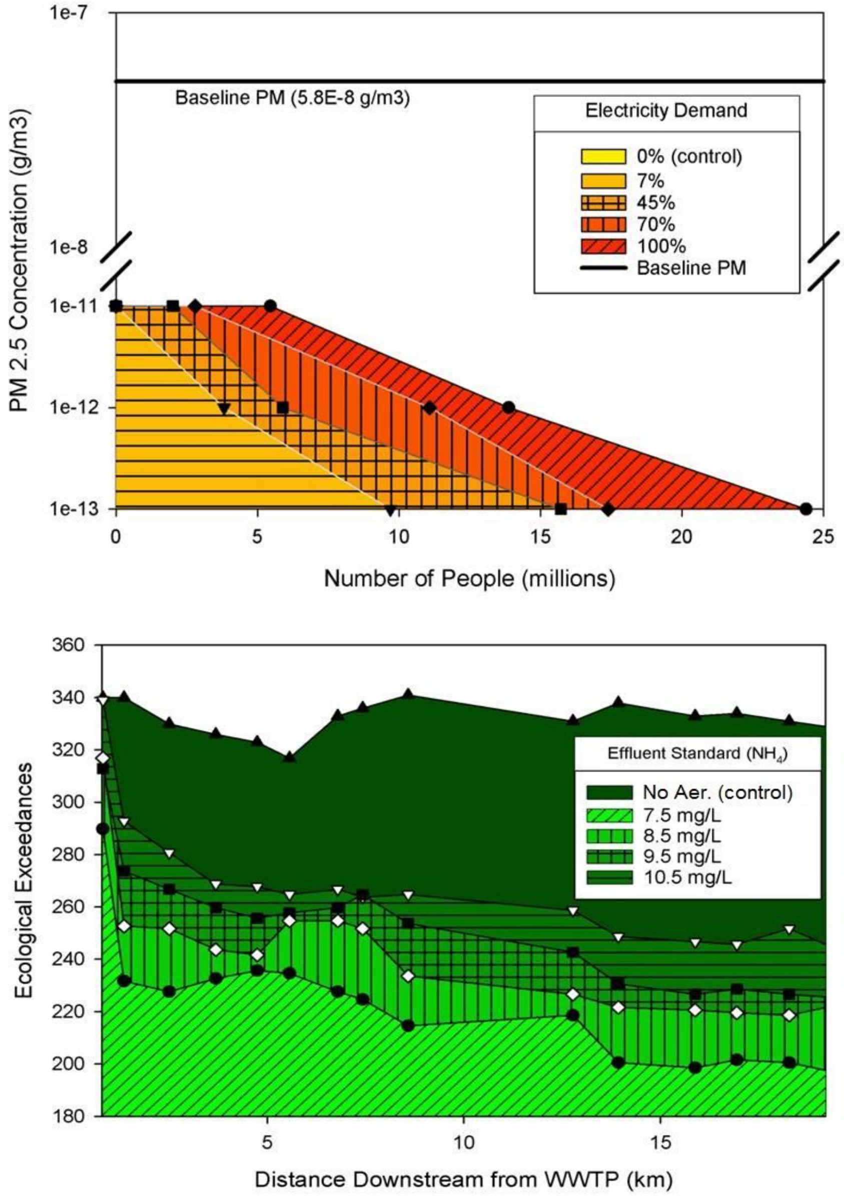



***Figure 11:*** *The human (top) and ecosystem (bottom) impacts of different treatment levels. The number of individuals exposed to different levels of PM2.5 concentration are shown, compared with the environmental baseline of 5.8 micrograms per cubic meter. At right, the ecological exceedances calculated using FIS matrices are shown for different sections of the river. The control scenario is based on no additional aeration treatment being provided in the anoxic zone of the treatment system, although other biological processes continue to run. In this way, the quantitiative spatial impacts of varying ammonium standards on human and ecological systems can be compared.*

While the Tier 2 physical model outputs can be useful for defining the system boundary more specifically, the objective of LCA is to connect design decisions with their environmental and human impacts. To achieve this goal, we use separate methods for the air and water emissions that account for local system characteristics. Our goal is to determine the spatial scales and intensities of human and ecological system effects, and compares those with the results of the aggregate LCA performed in Tier 1. In the case of the water emissions, we used literature-based FIS matrices to determine the exposure of local ecosystem fauna to significant levels of ammonium or oxygen deprivation. For air emissions, we considered important thresholds for human health exposure to particulate matter and overlaid our physical model data onto a population density map.

In the air pollution case, the average particulate matter concentration due to each treatment tier is calculated as well as the number of people exposed to concentrations above certain thresholds of particulate matter. This presents an opportunity to decision makers to choose to "flatten the curve", by decreasing the number of individuals exposed to the highest concentration thresholds. Scenarios which use less electricity or different combinations of power plants can be tested through Tier 2 and Tier 3 methods to provide alternatives to decision makers. Figure 11 shows the millions of individuals exposed to particular concentrations of particulate matter, as well as the average background concentration of 58 $\mu g/m^3$ (Van Dingenen et al., 2004).

In the water pollution case, fundamental intermittent standards (FIS) matrices describing the critical threshold intensities of specific pollutants sorted by event duration and recurrence interval, allow us to determine how many acute events that could cause significant ecosystem damage occur at each treatment level. These factors are taken from the industry standard Urban Pollution Manual, which considers system resilience and hysteresis in order to account for the impacts of both acute and chronic poor water quality. The spatial resolution offered by the model in Tier 2 analysis remains, as it is possible to see in which geospatial sections of the river ecosystems might be especially vulnerable to high-frequency intense emissions. However, the FIS matrices allow us to convert the water quality metrics directly to quantified ecological impacts. Here, again, there is an opportunity to select a lower-impact curve across the spatial region of interest, or to compare tradeoffs with the air emissions impacts curves. Figure 11 shows the summation of all exceedance events with a 1-year return period. The results are displayed per river block starting at the point of the WWTP outlet and ending approximately 20 km downstream. It is evident that the worst treatment threshold would have a worse impact at the point of the wastewater effluent. However, the impact continues far downstream, where with each additional 1 $g/m^3$ ammonium allowed in the effluent, the chance of exceedance events increases by about 15%.

# CHAPTER 4: DISCUSSION

New policy goals are calling for water treatment authorities to plan on a river-basin level scale. As decision makers are confronted with the task of evaluating these larger and more complex systems, they will look to use geospatial data to develop more comprehensive life cycle evaluations of their options. This can yield high-resolution valorization of environmental flows resulting from specific processes. While our understanding of the linkages between economic, environmental, and social systems continues to grow, we must be careful to develop a standard for decision-making based on multilevel environmental impact assessment. Traditional LCA impact methods are rooted in a global, long-term perspective, but impacts on human health and ecosystems may need to be evaluated on a range of spatiotemporal scales. It is important for decision makers and researchers to coordinate the goals and scope of a LCA with the information available for environmental impact assessment.

In some highly localized or self-contained systems, LCA analysis using the traditional, "first-tier" methods presented in this paper may suffice for the decisions being made. For example, determining whether hydraulic piping should be made from PVC or cast iron would only involve looking at the sourcing and construction processes of these pipes. Since there is no difference in energy usage or efficiency between these two options, full physical modeling of the energy use or water quality impacts would not yield any meaningful results. The Tier 1 metrics presented in this paper are sufficient for design decisions that do not affect process performance or effluent quality.

However, if engineers find that there is some sort of reaction between the cast iron material and the water influent, which perhaps creates pollutants whose dispersion and impact cannot be measured using traditional LCA metrics, the second-tier approach used in this paper might be helpful. Bilateral communication among stakeholders, especially between policymakers and those conducting the LCIA, is crucial to defining which pollutants are critical to examine and clarifying the limitations of transport models. Engineers can then determine if the amount of pollutants produced by the cast iron choice provides a considerable threat to local environmental function, and compare the results with LCA analysis to create a more robust environmental analysis. These Tier 2 metrics are useful for assessing spatiotemporal scale impacts beyond the boundaries of wastewater treatment operation.

Finally, if engineers find that the micropollutants do present a quantifiable environmental impact and want to determine how broadly they affect human or ecological systems, they can supplement the Tier 3 approach presented in this paper. This approach requires additional data about characterization factors, those LCA parameters which convert system outputs to standardized environmental impacts. For the approach to provide additional insight, the characterization factors must be locally specific and validated. This connects the environmental process studied to its larger social and ecological system impacts, the core goal of LCA. This approach has been implemented using other modeling tools as well, such as quantitative microbial risk assessment (Kobayashi et al., 2015), water footprinting for water quantity analysis (Mekonnen and Hoekstra, 2015), and social life cycle impact assessment (Lund, 2015).

Reviewing the environmental impact assessment across the three tiers of analysis used in this paper, we found that the traditional LCA analysis showed a clear tradeoff between global warming and eutrophication impacts in the four scenarios with no discernable optimal choice. In the biophysical modeling completed for the Tier 2 analysis, it seemed that on the eutrophication side, each incremental improvement in effluent standard had a drastic effect on the worst-case ammonium levels in the receiving river, with a 50% increase in effluent treatment standard leading to river ammonium levels comparable with no wastewater treatment at all. However, the air emissions impacts also seemed to be significant, with particulate matter emissions associated with the treatment process's typical electricity use crossing international borders. In the Tier 3 analysis, these environmental quality impacts were put in a human and ecosystem frame of reference. The electricity demand was found to contribute a negligible amount, far below the human health impact threshold, to regional particulate matter concentrations. Alternatively, the eutrophication due to effluent produced a large number of local "ecological exceedance" events that could be dramatically reduced with marginal improvements in treatment levels.

Wastewater treatment operators target a hierarchy of objectives in accordance with our historical understanding of the impact of effluent on local ecosystems. The top priority is to protect public health through wastewater treatment. Thereafter, policy objectives on long-term human health or climate change mitigation are now encouraging plants to choose processes that reduce chemical use (like disinfection byproducts) and electricity use (and greenhouse gas emissions). There is little operational or political priority for the local ecosystem at the point of effluent discharge, which absorbs the brunt of acute process impacts. A conservative sustainability perspective would flatten this hierarchy, considering that all aspects of the environmental system are interconnected. However, our understanding of ecosystem-human-system links remains too limited to make decisions in that manner with confidence. As we develop our decision-making standard based on comprehensive environmental impact assessment methods, this may be a goal to work toward.

The operational decision considered in this paper may seem to have relatively low system impacts, when considering the particulate matter concentration relative to the baseline or the ecological exceedances for one small, highly sensitive river. However, this approach is not only intended to be used for evaluating local operational decisions but also high-level policy structures. The Eindhoven WWTP treats water for approximately 4% of the Dutch population, so the tradeoff decisions made here would have compound effects if all wastewater treatment operators were to align themselves along the same policy rationale. Therefore, with a growing abundance of geospatial data and understanding of human-environmental-system interactions, we need to establish a standard for making these tradeoff decisions based on comprehensive environmental impact assessment.

# CHAPTER 5: ENGINEERING AND POLICY SIGNIFICANCE

This thesis studied the various levels of environmental impact modeling that could be employed by scientists and engineers tasked with evaluating the sustainability of certain operational and policy decisions made in the wastewater treatment sector. The significance of this work must be seen bilaterally in how it helps to build the bridge of communication between engineers and policy decision makers. In this chapter, the most insightful portions of the research are discussed as well as potential avenues for future investigation.

## 5.1 MAJOR INSIGHTS

The major themes explored in this thesis include the complementary use of biophysical models and life cycle assessment methods, the importance of local characterization factors to understand human and ecological impacts of environmental transport models, and the role that wastewater utilities play in urban environmental impacts.

- *Traditional LCA approaches can be augmented with biophysical modeling.* Traditional LCA approaches—using standardized inventories and characterization factors—are inherently long-term and global in scope. This is led by the core value that rigid sustainability flattens the hierarchy of spatial and temporal impacts, so that ecological or human impacts felt far away in time or space carry the same weight as those close by. On the other end of the spectrum, biophysical modeling is based on concretely characterizing the environmental transport of pollutants in a specific local region. Those impacts are quantified and often, the most critical areas are identified for further research. This is often valuable to local regulators and businesses who respond to the demands of current, local stakeholders. As mentioned in the background literature review, many other researchers are trying to bridge this gap by making LCA more inclusive of local human and ecological health priorities. This thesis attempts to contribute to the discussion by simultaneously evaluating a case study using traditional LCA and extensive modeling approaches.

- *Even in simple case studies, spatial models and local characterization factors can be used to understand interactions with human-ecological systems.*

  The growth of integrated urban water models has allowed research, including that presented in this thesis, to become more creative in linking process decisions to external systems including energy demand, resource use, and economic impacts. Datasets in sectors important to sustainability research are also increasingly open-source. This permits increased innovation and collaboration on case studies with local information and characterization factors. For human and ecological systems impacts, which are nonlinear and highly uncertain, analyzing a large set of these simple case studies would go a long way to developing our understanding of system mechanics and feedbacks.

- *Wastewater treatment plant operations strongly influence the environmental impacts of urban water systems.*

  Through its link with energy and food systems, wastewater treatment is a complex inflection point in the analysis and management of the urban water cycle. The evaluation in this thesis showed that the electricity demand of modern biological wastewater treatment is significant and, when coming from an electricity production sector focused on fossil-fuel based sources, can have direct human health and environmental impacts in regions far beyond the water treatment plant's service area.

## 5.2 Mitigation Strategies

As discussed previously, it is vital for both scientists and policymakers to contribute to the bilateral discussion that allows us to incorporate environmental impact assessment to make informed choices toward a sustainable future. This communication requires effort on both sides to understand the other's values, uncertainty, and consequences driving data-informed decision-making. The roadmap established in Chapter 4 for evaluating the use of piping material at different tiers shows one path that lets policymakers make strategic investments in researching the environmental impacts of a specific policy based on interpreting the results presented by scientists at lower tiers of evaluation.

However, this project was very limited in scope in that it only analyzed the human health impacts of particulate matter emissions and the ecological impacts of nutrient pollution, based on a single tradeoff decision between energy investment and nutrients in the effluent. In values-driven policymaking, a more comprehensive Tier 1 study would have to be completed to enumerate all the potential consequences of a process decision. Further analysis using modeling and characterization factors might then show the sensitivity of certain consequences to the process decision being made. Then the engineering task becomes limiting the most sensitive constraint of the multiobjective problem. This is simply a multi-variable or multi-constraint extension of the two-constraint tradeoff presented in this thesis.

## 5.3 Potential future work

As our ability to model the long-term impacts of decision-making and our data resolution continues to improve, it is important to guide future research in a direction that will support our understanding and application of these model outputs. With that aim in mind, the following research areas seem interesting to pursue in continuation of the work presented here:

- *Improved local spatial and temporal resolution of standardized LCA-type characterization and impact factors.* Even though this work focused on a tradeoff among different processes happening in a singular location, other projects may look to tradeoffs among different locations or timepoints. This work highlighted the relevance of local characteristics (for example, the highly sensitive receiving river) in impact evaluation. Research should continue to improve the spatial and temporal discretization of impact factors.

- *Understanding wastewater effluent pollution in context of local diffuse pollutions sources like agriculture.* The dramatic increase in agricultural intensity in this watershed likely overpowers any effluent mitigation attempts made by the local water management authority. At the same time, the research here showed that the existing background concentration of particulate matter was far beyond the production associated with generating electricity for this plant's wastewater treatment. If the water management authority is responsible for the water quality in the entire region, it should focus on placing individual subsystem (i.e. the wastewater treatment plant, or the agricultural sector) in appropriate context relative to the state of the full system. This way, it can prioritize policies and resources to projects that have the most significant sustainability impact (low hanging fruit).

- *Explore interactions of wastewater operation with food and energy systems, potentially through energy and resource positive wastewater treatment.* Wastewater treatment plants are a critical link between the urban water cycle and energy and food systems. Rather than having the wastewater treatment operation sink resources from these other systems, recent research has made significant advances in energy- and resource-positive wastewater treatment. This could potentially make wastewater treatment a source for energy and food systems. The application of these new technologies will have to be evaluated within human and environmental system contexts, potentially using some of the approaches outlined in this thesis.

# REFERENCES


Azevedo, L.B., Henderson, A.D., van Zelm, R., Jolliet, O., Huijbregts, M.A.J., 2013. Assessing the Importance of Spatial Variability versus Model Choices in Life Cycle Impact Assessment: The Case of Freshwater Eutrophication in Europe. Environ. Sci. Technol. 47, 13565–13570. doi:10.1021/es403422a

Bach, P.M., Rauch, W., Mikkelsen, P.S., McCarthy, D.T., Deletic, A., 2014. A critical review of integrated urban water modelling – Urban drainage and beyond. Environ. Model. Softw. 54, 88–107. doi:10.1016/j.envsoft.2013.12.018

Baresel, C., Destouni, G., 2007. Uncertainty-accounting environmental policy and management of water systems. Environ. Sci. Technol. 41, 3653–3659.

Beck, B., Walker, R.V., 2011. Global Water Crisis: A Joined-Up View From The City. SAPIENS Surv. Perspect. Integrating Environ. Soc.

Benedetti, L., Langeveld, J., Comeau, A., Corominas, L., Daigger, G., Martin, C., Mikkelsen, P.S., Vezzaro, L., Weijers, S., Vanrolleghem, P.A., 2013a. Modelling and monitoring of integrated urban wastewater systems: review on status and perspectives. Water Sci. Technol. 68, 1203. doi:10.2166/wst.2013.397

Benedetti, L., Langeveld, J., van Nieuwenhuijzen, A.F., de Jonge, J., de Klein, J., Flameling, T., Nopens, I., van Zanten, O., Weijers, S., 2013b. Cost-effective solutions for water quality improvement in the Dommel River supported by sewer–WWTP–river integrated modelling. Water Sci. Technol. 68, 965. doi:10.2166/wst.2013.312

Bertrand-Krajewski, J.-L., 2007. Stormwater pollutant loads modelling: epistemological aspects and case studies on the influence of field data sets on calibration and verification. Water Sci. Technol. 55.

Bettencourt, L., Lobo, J., Helbing, D., Kühnert, C., West, G., 2007. Growth, innovation, scaling, and the pace of life in cities. Proc. Natl. Acad. Sci. 104, 7301–7306.

Blumensaat, F., Staufer, P., Heusch, S., Reußner, F., Schütze, M., Seiffert, S., Gruber, G., Zawilski, M., Rieckermann, J., 2012. Water quality-based assessment of urban drainage impacts in Europe – where do we stand today? Water Sci. Technol. 66, 304. doi:10.2166/wst.2012.178

Borken-Kleefeld, J., Fuglestvedt, J., Berntsen, T., 2013. Mode, Load, And Specific Climate Impact from Passenger Trips. Environ. Sci. Technol. 47, 7608–7614. doi:10.1021/es4003718

Bradford-Hartke, Z., Lane, J., Lant, P., Leslie, G., 2015. Environmental Benefits and Burdens of Phosphorus Recovery from Municipal Wastewater. Environ. Sci. Technol. 49, 8611–8622. doi:10.1021/es505102v

Brown, R.R., Keath, N., Wong, T.H.F., 2009. Urban water management in cities: historical, current and future regimes. Water Sci. Technol. 59, 847. doi:10.2166/wst.2009.029

Cabrera Marcet, E., Jeffrey, P., Parsons, D., 2014. Carbon sensitive urban water futures.

Caffoor, I., 2008. Business Case: Energy Efficient Water and Wastewater Treatment.

Carpenter, S.R., Brock, W.A., Folke, C., van Nes, E.H., Scheffer, M., 2015. Allowing variance may enlarge the safe operating space for exploited ecosystems. Proc. Natl. Acad. Sci. 112, 14384–14389. doi:10.1073/pnas.1511804112

Casal-Campos, A., Fu, G., Butler, D., Moore, A., 2015. An Integrated Environmental Assessment of Green and Gray Infrastructure Strategies for Robust Decision Making. Environ. Sci. Technol. 49, 8307–8314. doi:10.1021/es506144f

CIESIN, CIAT, 2005. Gridded Population of the World, Version 3 (GPWv3): Population Density Grid.

Clauson-Kaas, J., Poulsen, T.S., Neergaard-Jacobsen, B., Guildal, T., Thirsing, C., 2004. Economic and environmental optimization of phosphorus removal. Water Sci. Technol. 50, 243–248.

Cohen, M., 2011. An integrated example of using command line functionality of HYSPLIT and DOS batch scripts to carry out various kinds of trajectory frequency analyses.

Collet, P., Lardon, L., Steyer, J.-P., Hélias, A., 2014. How to take time into account in the inventory step: a selective introduction based on sensitivity analysis. Int. J. Life Cycle Assess. 19, 320–330. doi:10.1007/s11367-013-0636-7

Dalin, C., Konar, M., Hanasaki, N., Rinaldo, A., Rodriguez-Iturbe, I., 2012. Evolution of the global virtual water trade network. Proc. Natl. Acad. Sci. 109, 5989–5994. doi:10.1073/pnas.1203176109

De Lange, W.J., Prinsen, G.F., Hoogewoud, J.C., Veldhuizen, A.A., Verkaik, J., Oude Essink, G.H.P., van Walsum, P.E.V., Delsman, J.R., Hunink, J.C., Massop, H.T.L., Kroon, T., 2014. An operational, multi-scale, multi-model system for consensus-based, integrated water management and policy analysis: The Netherlands Hydrological Instrument. Environ. Model. Softw. 59, 98–108. doi:10.1016/j.envsoft.2014.05.009

Dolan, T., Howsam, P., Parsons, D.J., Whelan, M.J., 2013. Is the EU Drinking Water Directive Standard for Pesticides in Drinking Water Consistent with the Precautionary Principle? Environ. Sci. Technol. 47, 4999–5006. doi:10.1021/es304955g

Draxler, R., 2000. HYSPLIT 4 User’s Guide.

EEA, 2012. European waters-- assessment of status and pressures (No. 8). European Environment Agency.

EMEP/EEA air pollutant emission inventory guidebook 2013 (Technical report No. 12), 2013. . European Environment Agency.

EPA, 1972. Federal Water Pollution Control Act.

Erbe, V., Frehmann, T., Geiger, W.F., Krebs, P., Londong, J., Rosenwinkel, K.H., Seggelke, K., 2002. Integrated modelling as an analytical and optimisation tool for urban watershed management. Water Sci. Technol. 46, 141–150.

European Council, 2000. Directive 2000/60/EC of the European Parliament and of the Council establishing a framework for community action in the field of water policy.

Fagan, J.E., Reuter, M.A., Langford, K.J., 2010. Dynamic performance metrics to assess sustainability and cost effectiveness of integrated urban water systems. Resour. Conserv. Recycl. 54, 719–736. doi:10.1016/j.resconrec.2009.12.002

Falk, M.W., Reardon, D.J., Neethling, J.B., Clark, D.L., Pramanik, A., 2013. Striking the Balance between Nutrient Removal, Greenhouse Gas Emissions, Receiving Water Quality, and Costs. Water Environ. Res. 85, 2307–2316. doi:10.2175/106143013X13807328848379

Flores-Alsina, X., Gallego, A., Feijoo, G., Rodriguez-Roda, I., 2010. Multiple-objective evaluation of wastewater treatment plant control alternatives. J. Environ. Manage. 91, 1193–1201.

Freni, G., Mannina, G., 2010. Uncertainty in water quality modelling: The applicability of Variance Decomposition Approach. J. Hydrol. 394, 324–333. doi:10.1016/j.jhydrol.2010.09.006

Fu, G., Butler, D., 2012. Frequency analysis of river water quality using integrated urban wastewater models. Water Sci. Technol. 65, 2112. doi:10.2166/wst.2012.127

Fu, G., Butler, D., Khu, S.-T., 2008. Multiple objective optimal control of integrated urban wastewater systems. Environ. Model. Softw. 23, 225–234. doi:10.1016/j.envsoft.2007.06.003

Gallego, A., Hospido, A., Moreira, M.T., Feijoo, G., 2008. Environmental performance of wastewater treatment plants for small populations. Resour. Conserv. Recycl. 52, 931–940. doi:10.1016/j.resconrec.2008.02.001

Gasparatos, A., El-Haram, M., Horner, M., 2009. The argument against a reductionist approach for measuring sustainable development performance and the need for methodological pluralism. Account. Forum 33, 245–256. doi:10.1016/j.accfor.2008.07.006

Gessner, M.O., Hinkelmann, R., Nützmann, G., Jekel, M., Singer, G., Lewandowski, J., Nehls, T., Barjenbruch, M., 2014. Urban water interfaces. J. Hydrol. 514, 226–232. doi:10.1016/j.jhydrol.2014.04.021

Gibon, T., Wood, R., Arvesen, A., Bergesen, J.D., Suh, S., Hertwich, E.G., 2015. A Methodology for Integrated, Multiregional Life Cycle Assessment Scenarios under Large-Scale Technological Change. Environ. Sci. Technol. 49, 11218–11226. doi:10.1021/acs.est.5b01558

Grant, S.B., Saphores, J.-D., Feldman, D.L., Hamilton, A.J., Fletcher, T.D., Cook, P.L.M., Stewardson, M., Sanders, B.F., Levin, L.A., Ambrose, R.F., Deletic, A., Brown, R., Jiang, S.C., Rosso, D., Cooper, W.J., Marusic, I., 2012. Taking the “Waste” Out of “Wastewater” for Human Water Security and Ecosystem Sustainability. Science 337, 681–686. doi:10.1126/science.1216852

Grau, P., Copp, J., Vanrolleghem, P.A., Takács, I., Ayesa, E., 2009. A comparative analysis of different approaches for integrated WWTP modelling. Water Sci. Technol. 59, 141. doi:10.2166/wst.2009.589

Guest, J.S., 2012. Sustainable Design of Wastewater Treatment Systems: Evaluations of Operational Flexibility and Phototrophs for Resource Recovery. University of Michigan.

Guest, J.S., Skerlos, S.J., Barnard, J.L., Beck, M.B., Daigger, G.T., Hilger, H., Jackson, S.J., Karvazy, K., Kelly, L., Macpherson, L., Mihelcic, J.R., Pramanik, A., Raskin, L., Van Loosdrecht, M.C.M., Yeh, D., Love*, N.G., 2009. A New Planning and Design Paradigm to Achieve Sustainable Resource Recovery from Wastewater [1]. Environ. Sci. Technol. 43, 6126–6130. doi:10.1021/es9010515

Harder, R., Holmquist, H., Molander, S., Svanström, M., Peters, G.M., 2015. Review of Environmental Assessment Case Studies Blending Elements of Risk Assessment and Life Cycle Assessment. Environ. Sci. Technol. 49, 13083–13093. doi:10.1021/acs.est.5b03302

Havens, K.E., Paerl, H.W., 2015. Climate Change at a Crossroad for Control of Harmful Algal Blooms. Environ. Sci. Technol. 49, 12605–12606. doi:10.1021/acs.est.5b03990

Heinzerling, D., Turner, J.R., Corsi, R.L., 2005. HYSPLIT TRAJECTORY MODELING AND CLUSTERING TECHNIQUES: COMPUTATION, ERROR ANALYSIS, AND APPLICATIONS.

Helmes, R.J.K., Huijbregts, M.A.J., Henderson, A.D., Jolliet, O., 2012. Spatially explicit fate factors of phosphorous emissions to freshwater at the global scale. Int. J. Life Cycle Assess. 17, 646–654. doi:10.1007/s11367-012-0382-2

Huhne, C., 2011. The Carbon Plan: Delivering Our Low Carbon Future.

Hydromantis Environmental Software Solutions, Inc, 2016. GPS-X: Wastewater Process Simulation.

Iranpour, R., 1999. Environmental Engineering: Energy Value of Replacing Waste Disposal with Resource Recovery. Science 285, 706–711. doi:10.1126/science.285.5428.706

Ishii, S.K.L., Boyer, T.H., 2015. Life cycle comparison of centralized wastewater treatment and urine source separation with struvite precipitation: Focus on urine nutrient management. Water Res. 79, 88–103. doi:10.1016/j.watres.2015.04.010

Jeppsson, U., Alex, J., Batstone, D.J., Benedetti, L., Comas, J., Copp, J.B., Corominas, L., Flores-Alsina, X., Gernaey, K.V., Nopens, I., Pons, M.-N., Rodríguez-Roda, I., Rosen, C., Steyer, J.-P., Vanrolleghem, P.A., Volcke, E.I.P., Vrecko, D., 2013. Benchmark simulation models, *quo vadis* ? Water Sci. Technol. 68, 1. doi:10.2166/wst.2013.246

Kates, R., Clark, W., 2001. Sustainability Science. Science 292, 641–642.

Khu, S.T., Madsen, H., 2005. Multiobjective calibration with Pareto preference ordering: An application to rainfall-runoff model calibration. Water Resour. Res. 41.

Kobayashi, Y., Peters, G.M., Ashbolt, N.J., Heimersson, S., Svanström, M., Khan, S.J., 2015. Global and local health burden trade-off through the hybridisation of quantitative microbial risk assessment and life cycle assessment to aid water management. Water Res. 79, 26–38. doi:10.1016/j.watres.2015.03.015

Krewski, D., Jerrett, M., Burnett, R., Ma, R., Hughes, E., Shi, Y., Turner, M., Pope, A.I., Thurston, G., Calle, E., Thun, M., 2010. Extended Follow-Up and Spatial Analysis of the American Cancer Society Study Linking Particulate Air Pollution and Mortality.

Kuczera, G., Kavetski, D., Franks, S., Thyer, M., 2006. Towards a Bayesian total error analysis of conceptual rainfall-runoff models: Characterising model error using storm-dependent parameters. J. Hydrol. 331, 161–177. doi:10.1016/j.jhydrol.2006.05.010

Lai, E., Lundie, S., Ashbolt, N.J., 2008. Review of multi-criteria decision aid for integrated sustainability assessment of urban water systems. Urban Water J. 5, 315–327. doi:10.1080/15730620802041038

Lako, P., 2015. Utility or energy company supplying electricity to waste water treatment plant (RWZI) Eindhoven.

Lane, J.L., de Haas, D.W., Lant, P.A., 2015. The diverse environmental burden of city-scale urban water systems. Water Res. 81, 398–415. doi:10.1016/j.watres.2015.03.005

Langeveld, J.G., Schilperoort, R.P.S., Weijers, S.R., 2013. Climate change and urban wastewater infrastructure: There is more to explore. J. Hydrol. 476, 112–119. doi:10.1016/j.jhydrol.2012.10.021

Langeveld, J., Nopens, I., Schilperoort, R., Benedetti, L., de Klein, J., Amerlinck, Y., Weijers, S., 2013. On data requirements for calibration of integrated models for urban water systems. Water Sci. Technol. 68, 728. doi:10.2166/wst.2013.301

Larsen, T.A., 2015. CO2-neutral wastewater treatment plants or robust, climate-friendly wastewater management? A systems perspective. Water Res. 87, 513–521. doi:10.1016/j.watres.2015.06.006

Lassaux, S., Renzoni, R., Germain, A., 2007. Life Cycle Assessment of Water from the Pumping Station to the Wastewater Treatment Plant. LCA Case Stud. 12, 118–126.

Leusbrock, I., Nanninga, T.A., Lieberg, K., Agudelo-Vera, C.M., Keesman, K.J., Zeeman, G., Rijnaarts, H.H.M., 2015. The urban harvest approach as framework and planning tool for improved water and resource cycles. Water Sci. Technol. 72, 998. doi:10.2166/wst.2015.299

Lijklema, L., Tyson, J.M., Lesouef, A., 1993. Interactions Between Sewers, Treatment Plants and Receiving Waters in Urban Areas: A Summary of the Interurba '92 Workshop Conclusions. Water Sci. Technol. 27, 1–29.

Lim, S.-R., Suh, S., Kim, J.-H., Park, H.S., 2010. Urban water infrastructure optimization to reduce environmental impacts and costs. J. Environ. Manage. 91, 630–637. doi:10.1016/j.jenvman.2009.09.026

Liu, J., Mooney, H., Hull, V., Davis, S.J., Gaskell, J., Hertel, T., Lubchenco, J., Seto, K.C., Gleick, P., Kremen, C., Li, S., 2015. Systems integration for global sustainability. Science 347, 1258832–1258832. doi:10.1126/science.1258832

Logan, B., 2015. Urgency at the Nexus of Food, Energy, and Water Systems. Environ. Sci. Technol. Lett. 2, 149–150. doi:10.1021/acs.estlett.5b00122

Loubet, P., Roux, P., Loiseau, E., Bellon-Maurel, V., 2014. Life cycle assessments of urban water systems: A comparative analysis of selected peer-reviewed literature. Water Res. 67, 187–202. doi:10.1016/j.watres.2014.08.048

Lund, J.R., 2015. Integrating social and physical sciences in water management: INTEGRATING SOCIAL AND PHYSICAL SCIENCES IN WATER MANAGEMENT. Water Resour. Res. 51, 5905–5918. doi:10.1002/2015WR017125

Makropoulos, C.K., Natsis, K., Liu, S., Mittas, K., Butler, D., 2008. Decision support for sustainable option selection in integrated urban water management. Environ. Model. Softw. 23, 1448–1460. doi:10.1016/j.envsoft.2008.04.010

Marlow, D.R., Moglia, M., Cook, S., Beale, D.J., 2013. Towards sustainable urban water management: A critical reassessment. Water Res. 47, 7150–7161. doi:10.1016/j.watres.2013.07.046

Mekonnen, M.M., Hoekstra, A.Y., 2015. Global Gray Water Footprint and Water Pollution Levels Related to Anthropogenic Nitrogen Loads to Fresh Water. Environ. Sci. Technol. 49, 12860–12868. doi:10.1021/acs.est.5b03191

MIKE by DHI, 2016. WEST: Modelling and simulation of wastewater treatment plants.

Mitchell, Vg., Duncan, H., Inman, M., Rahilly, M., Stewart, J., Vieritz, A., Holt, P., Grant, A., Fletcher, T., Coleman, J., Maheepala, S., Sharma, A., Deletic, A., Breen, P., 2007. Integrated urban water modelling - past, present, and future [WWW Document]. URL http://search.informit.com.au/documentSummary;dn=889043199381845;res=IELENG (accessed 7.31.14).

Muga, H.E., Mihelcic, J.R., 2008. Sustainability of wastewater treatment technologies. J. Environ. Manage. 88, 437–447. doi:10.1016/j.jenvman.2007.03.008

Muñoz, I., José Gómez, M., Molina-Diaz, A., Huijbregts, M., Fernandez-Alba, A.R., Garcia-Calvo, E., 2008. Ranking potential impacts of priority and emerging pollutants in urban wastewater through life cycle impact assessment. Chemosphere 74, 37–44. doi:doi:10.1016/j.chemosphere.2008.09.029

Muschalla, D., Vallet, B., Anctil, F., Lessard, P., Pelletier, G., Vanrolleghem, P.A., 2014. Ecohydraulic-driven real-time control of stormwater basins. J. Hydrol. 511, 82–91. doi:10.1016/j.jhydrol.2014.01.002

Mutel, C.L., Pfister, S., Hellweg, S., 2012. GIS-Based Regionalized Life Cycle Assessment: How Big Is Small Enough? Methodology and Case Study of Electricity Generation. Environ. Sci. Technol. 46, 1096–1103. doi:10.1021/es203117z

MWRD, n.d. Stickney Water Reclamation Plant.

Nair, S., George, B., Malano, H.M., Arora, M., Nawarathna, B., 2014. Water–energy–greenhouse gas nexus of urban water systems: Review of concepts, state-of-art and methods. Resour. Conserv. Recycl. 89, 1–10. doi:10.1016/j.resconrec.2014.05.007

Netherlands/Power Plants, 2010. . Enipedia.

NOAA, 2016. HYSPLIT.

NOAA Air Resources Laboratory, 2015. Global Data Assimilation System (GDAS1) Archive Information.

NOAA Air Resources Laboratory, 2009a. Presentation from the NOAA workshop on using HYSPLIT for Mercury Emissions Calculations.

NOAA Air Resources Laboratory, 2009b. Presentation from the NOAA workshop on using HYSPLIT for Concentration/Deposition Calculations.

Oki, T., 2006. Global Hydrological Cycles and World Water Resources. Science 313, 1068–1072. doi:10.1126/science.1128845

Oreskes, N., 2003. The Role of Quantitative Models in Science Naomi Oreskes. Models Ecosyst. Sci. 13.

Ortiz, M., Raluy, R.G., Serra, L., 2007. Life cycle assessment of water treatment technologies: wastewater and water-reuse in a small town. Desalination 204, 121–131.

Overzichtskaart Waterschap de Dommel, 2015.

Paton, F.L., Maier, H.R., Dandy, G.C., 2014. Including adaptation and mitigation responses to climate change in a multiobjective evolutionary algorithm framework for urban water supply systems incorporating GHG emissions. Water Resour. Res. 50, 6285–6304. doi:10.1002/2013WR015195

Petelet-Giraud, E., Klaver, G., Negrel, P., 2009. Natural versus anthropogenic sources in the surface- and groundwater dissolved load of the Dommel river (Meuse basin): Constraints by boron and strontium isotopes and gadolinium anomaly. J. Hydrol. 369, 336–349. doi:10.1016/j.jhydrol.2009.02.029

Pizzigallo, A.C.I., Granai, C., Borsa, S., 2008. The joint use of LCA and emergy evaluation for the analysis of two Italian wine farms. SPIn-Eco Sustain. Siena Prov. Ecodynamic Indic. 86, 396–406. doi:10.1016/j.jenvman.2006.04.020

Plósz, B.G., Benedetti, L., Daigger, G.T., Langford, K.H., Larsen, H.F., Monteith, H., Ort, C., Seth, R., Steyer, J.-P., Vanrolleghem, P.A., 2012. Modelling micro-pollutant fate in wastewater collection and treatment systems: status and challenges. Water Sci. Technol. 67, 1. doi:10.2166/wst.2012.562

Rauch, W., Bertrand-Krajewski, J.-L., Krebs, P., Mark, O., Schilling, W., Schütze, M., Vanrolleghem, P.A., 2002. Mathematical modelling of integrated urban drainage systems. Water Sci. Technol. 45, 81–94.

Rauch, W., Henze, M., Koncsos, L., Reichert, P., Shanahan, P., SomlyóDy, L., Vanrolleghem, P., 1998. River water quality modelling: I. state of the art. Water Qual. Int. 98 Part 9 Water Qual. Manag. Proc. 19th Bienn. Conf. Int. Assoc. Water Qual. 38, 237–244. doi:10.1016/S0273-1223(98)00660-X

Rebitzer, G., Seuring, S., 2003. Methodology and application of life cycle costing. Int. J. Life Cycle Assess. 8, 110–111.

Renou, S., Thomas, J.S., Aoustin, E., Pons, M.N., 2008. Influence of impact assessment methods in wastewater treatment LCA. J. Clean. Prod. 16, 1098–1105. doi:10.1016/j.jclepro.2007.06.003

Rice, J., Westerhoff, P., 2015. Spatial and Temporal Variation in De Facto Wastewater Reuse in Drinking Water Systems across the U.S.A. Environ. Sci. Technol. 49, 982–989. doi:10.1021/es5048057

Risch, E., Gutierrez, O., Roux, P., Boutin, C., Corominas, L., 2015. Life cycle assessment of urban wastewater systems: Quantifying the relative contribution of sewer systems. Water Res. 77, 35–48. doi:10.1016/j.watres.2015.03.006

Rockström, J., Steffen, W., Noone, K., Persson, \AAsa, Chapin, F.S., Lambin, E.F., Lenton, T.M., Scheffer, M., Folke, C., Schellnhuber, H.J., others, 2009. A safe operating space for humanity. Nature 461, 472–475.

Romero-Lankao, P., Gurney, K.R., Seto, K.C., Chester, M., Duren, R.M., Hughes, S., Hutyra, L.R., Marcotullio, P., Baker, L., Grimm, N.B., 2014. A critical knowledge pathway to low-carbon, sustainable futures: Integrated understanding of urbanization, urban areas, and carbon. Earths Future 2, 515–532.

Rozemeijer, J.C., Broers, H.P., 2007. The groundwater contribution to surface water contamination in a region with intensive agricultural land use (Noord-Brabant, The Netherlands). Environ. Pollut. 148, 695–706. doi:10.1016/j.envpol.2007.01.028

Rozenberg, J., Davis, S.J., Narloch, U., Hallegatte, S., 2015. Climate constraints on the carbon intensity of economic growth. Environ. Res. Lett. 10, 095006. doi:10.1088/1748-9326/10/9/095006

Saagi, R., n.d. Modelling River Water Quality for System-Wide Benchmark Simulation Models.

Schellart, A.N.A., Tait, S.J., Ashley, R.M., 2010. Towards quantification of uncertainty in predicting water quality failures in integrated catchment model studies. Water Res. 44, 3893–3904. doi:10.1016/j.watres.2010.05.001

Shanahan, P., Borchardt, D., Henze, M., Rauch, W., Reichert, P., Somlyódy, L., Vanrolleghem, P., 2001. River Water Quality Model no. 1 (RWQM1): I. Modelling approach. Water Sci. Technol. 43, 1–9.

Shoener, B.D., Bradley, I.M., Cusick, R.D., Guest, J.S., 2014. Energy positive domestic wastewater treatment: the roles of anaerobic and phototrophic technologies. Environ. Sci. Process. Impacts 16, 1204. doi:10.1039/c3em00711a

Sills, D.L., Paramita, V., Franke, M.J., Johnson, M.C., Akabas, T.M., Greene, C.H., Tester, J.W., 2013. Quantitative Uncertainty Analysis of Life Cycle Assessment for Algal Biofuel Production. Environ. Sci. Technol. 47, 687–694. doi:10.1021/es3029236

Sin, G., Gernaey, K.V., Neumann, M.B., van Loosdrecht, M.C.M., Gujer, W., 2011. Global sensitivity analysis in wastewater treatment plant model applications: Prioritizing sources of uncertainty. Water Res. 45, 639–651. doi:10.1016/j.watres.2010.08.025

Smith, A.L., Stadler, L.B., Cao, L., Love, N.G., Raskin, L., Skerlos, S.J., 2014. Navigating Wastewater Energy Recovery Strategies: A Life Cycle Comparison of Anaerobic Membrane Bioreactor and Conventional Treatment Systems with Anaerobic Digestion. Environ. Sci. Technol. 48, 5972–5981. doi:10.1021/es5006169

Soper, G.A., 1907. The Sanitary Engineering Problems of Water Supply and Sewage Disposal in New York City. Science 601–605.

Stokes, J., Horvath, A., 2010. Life-cycle assessment of urban water provision: tool and case study in California. J. Infrastruct. Syst. 17, 15–24.

STOWA, 2012. KALLISTO, samen slim schoon.

Stroometiket 2014 Essent, 2014.

Tangsubkul, N., Beavis, P., Moore, S.J., Lundie, S., Waite, T.D., 2005. Life Cycle Assessment of Water Recycling Technology. Water Resour. Manag. 19, 521–537.

The Economist, 2007. Bright lights, big cities: Urbanization and the rise of the megacity. The Economist.

The World Bank, 2016. Electricity production from coal sources (% of total)-- from International Energy Agency statistics.

Tillman, A.M., Svingby, M., Lundström, H., 1998. Life cycle assessment of municipal waste water systems. Int. J. Life Cycle Assess. 3, 145–147.

Urban Pollution Management Manual (3rd Edition), 2012.

Urich, C., Bach, P.M., Sitzenfrei, R., Kleidorfer, M., McCarthy, D.T., Deletic, A., Rauch, W., 2013. Modelling cities and water infrastructure dynamics. Proc. Inst. Civ. Eng. - Eng. Sustain. 166, 301–308. doi:10.1680/ensu.12.00037

Van Dingenen, R., Raes, F., Putaud, J.-P., Baltensperger, U., Charron, A., Facchini, M.-C., Decesari, S., Fuzzi, S., Gehrig, R., Hansson, H.-C., Harrison, R.M., Hüglin, C., Jones, A.M., Laj, P., Lorbeer, G., Maenhaut, W., Palmgren, F., Querol, X., Rodriguez, S., Schneider, J., Brink, H. ten, Tunved, P., Tørseth, K., Wehner, B., Weingartner, E., Wiedensohler, A., Wåhlin, P., 2004. A European aerosol phenomenology—1: physical characteristics of particulate matter at kerbside, urban, rural and background sites in Europe. Atmos. Environ. 38, 2561–2577. doi:10.1016/j.atmosenv.2004.01.040

van Loosdrecht, M.C.M., Brdjanovic, D., 2014. Anticipating the next century of wastewater treatment. Science 344, 1452–1453. doi:10.1126/science.1255183

Vanrolleghem, P.A., Rosén, C., Zaher, U., Copp, J., Benedetti, L., Ayesa, E., Jeppsson, U., 2005. Continuity-based interfacing of models for wastewater systems described by Petersen matrices. Water Sci. Technol. 52, 493–500.

Vezzaro, L., Benedetti, L., Gevaert, V., De Keyser, W., Verdonck, F., De Baets, B., Nopens, I., Cloutier, F., Vanrolleghem, P.A., Mikkelsen, P.S., 2014. A model library for dynamic transport and fate of micropollutants in integrated urban wastewater and stormwater systems. Environ. Model. Softw. 53, 98–111. doi:10.1016/j.envsoft.2013.11.010

Vidas, D., Fauchald, O.K., Jensen, Ø., Tvedt, M.W., 2015. International law for the Anthropocene? Shifting perspectives in regulation of the oceans, environment and genetic resources. Anthropocene 9, 1–13. doi:10.1016/j.ancene.2015.06.003

Villarroel Walker, R., 2012. Innovation, multi-utility service businesses and sustainable cities: where might be the next breakthrough? Water Pract. Technol. 7, 1–8. doi:10.2166/wpt.2012.084

Voinov, A., Shugart, H.H., 2013. “Integronsters”, Integral and Integrated Modeling. Env. Model Softw 39, 149–158. doi:10.1016/j.envsoft.2012.05.014

Vorosmarty, C.J., Hoekstra, A.Y., Bunn, S.E., Conway, D., Gupta, J., 2015. Fresh water goes global. Science 349, 478–479. doi:10.1126/science.aac6009

Wackernagel, M., 2002. Tracking the ecological overshoot of the human economy. Proc. Natl. Acad. Sci. 99, 9266–9271.

Wackernagel, M., Silverstein, J., 2000. Big things first: focusing on the scale imperative with the ecological footprint. Ecol. Econ. 32, 391–394.

Waterschap de Dommel, 2010. Waterbeheerplan 2010-2015.

Weijers, S.R., 2012. KALLISTO: cost effective and integrated optimization of the urban wastewater system Eindhoven. Water Pract. Technol. 7, 1–9. doi:10.2166/wpt.2012.036

Welsh, W.D., Vaze, J., Dutta, D., Rassam, D., Rahman, J.M., Jolly, I.D., Wallbrink, P., Podger, G.M., Bethune, M., Hardy, M.J., Teng, J., Lerat, J., 2013. An integrated modelling framework for regulated river systems. Environ. Model. Softw. 39, 81–102. doi:10.1016/j.envsoft.2012.02.022

Xue, X., Schoen, M.E., Ma, X. (Cissy), Hawkins, T.R., Ashbolt, N.J., Cashdollar, J., Garland, J., 2015. Critical insights for a sustainability framework to address integrated community water services: Technical metrics and approaches. Water Res. 77, 155–169. doi:10.1016/j.watres.2015.03.017

Yaeger, M.A., Sivapalan, M., McIsaac, G.F., Cai, X., 2013. Comparative analysis of hydrologic signatures in two agricultural watersheds in east-central Illinois: legacies of the past to inform the future. Hydrol. Earth Syst. Sci. 17, 4607–4623. doi:10.5194/hess-17-4607-2013

Zachary, D.S., 2014. On the sustainability of an activity. Sci. Rep. 4. doi:10.1038/srep05215

APPENDIX A: Sample HYSPLIT control file

The MATLAB code used to generate these files is available at https://github.com/smashkia/MSThesis2016.git.

HYSPLIT control files are very sensitive to spacing and newline characters. Best practice is to copy the files from sample tutorials and insert your own parameters as necessary.

```
00 00 00 00        %starting time in {yy mm dd hh} format
1                  %number of starting locations
53.5 5.7 150       %latitude, longitude, and height (m) of starting
location
24                 %total run time (hours)
0                  %vertical motion option (0: data, 1:isob, etc)
10000              %top of model domain (MAGL)
1                  %number of input meteorological data grids
C:/hysplit4/working/meteofile %meteo data file location

1                  %number of pollutants being emitted
HgII               %4-character pollutant ID name (mercury in this case)
1.0                %emissions rate (mass/hr)
24.0               %hours of emission
00 00 00 00 00     %starting time in {yy mm dd hh mm} format

1                  %number of concentration grids
52.0  5.0          %grid center {lat lon}
0.3  0.3           %grid spacing {lat lon} [degrees]
20.0  20.0         %grid extent {lat lon} [degrees]
./test1            %directory for grid output file
Cdump              %name of grid output file
4                  %number of vertical levels
0 100 500 1000     %elevations of these output levels (MAGL)
00 00 00 00 00     %sampling start time {yy mm dd hh mm}
00 00 01 00 00     %sampling end time {yy mm dd hh mm}
00 06 00           %sampling interval {rate hh mm} (rate: avg=0, now=1,
max=2)

1                  %number of deposition parameters defined (same as
# of pollutants)
0.0 2.0 1.0        %particle diameter (microns), density (g/cc),
shape
0.0 271.5 1.0 2.0 1400000  %deposition velocity (m/s), pollutant
molecular weight (g/mole), surface reactivity ratio, diffusivity
ratio, effective Henry’s constant
140000 40000 0.00005  %wet removal: actual Henry’s constant, in-
cloud (L/L), below-cloud (l/s)
0.0                %radioactive decay half-life [days]
0.0                %pollutant resuspension factor [1/m]
```

Appendix B: FIS Matrices for ecosystem responses

DO concentration limits for salmonid ecosystem (when $NH_4$ also below 0.02 mg/L)

| | Dissolved Oxygen Concentrations (mg/L) | | |
|---|---|---|---|
| Return Period | 1 hour | 6 hours | 24 hours |
| 1 month | 5.0 | 5.5 | 6.0 |
| 3 months | 4.5 | 5.0 | 5.5 |
| 1 year | 4.0 | 4.5 | 5.0 |

DO concentration limits for cyprinid ecosystem (when $NH_4$ also below 0.02 mg/L)

| | Dissolved Oxygen Concentrations (mg/L) | | |
|---|---|---|---|
| Return Period | 1 hour | 6 hours | 24 hours |
| 1 month | 4.0 | 4.5 | 5.0 |
| 3 months | 5.5 | 6.0 | 6.5 |
| 1 year | 5.0 | 5.5 | 6.0 |