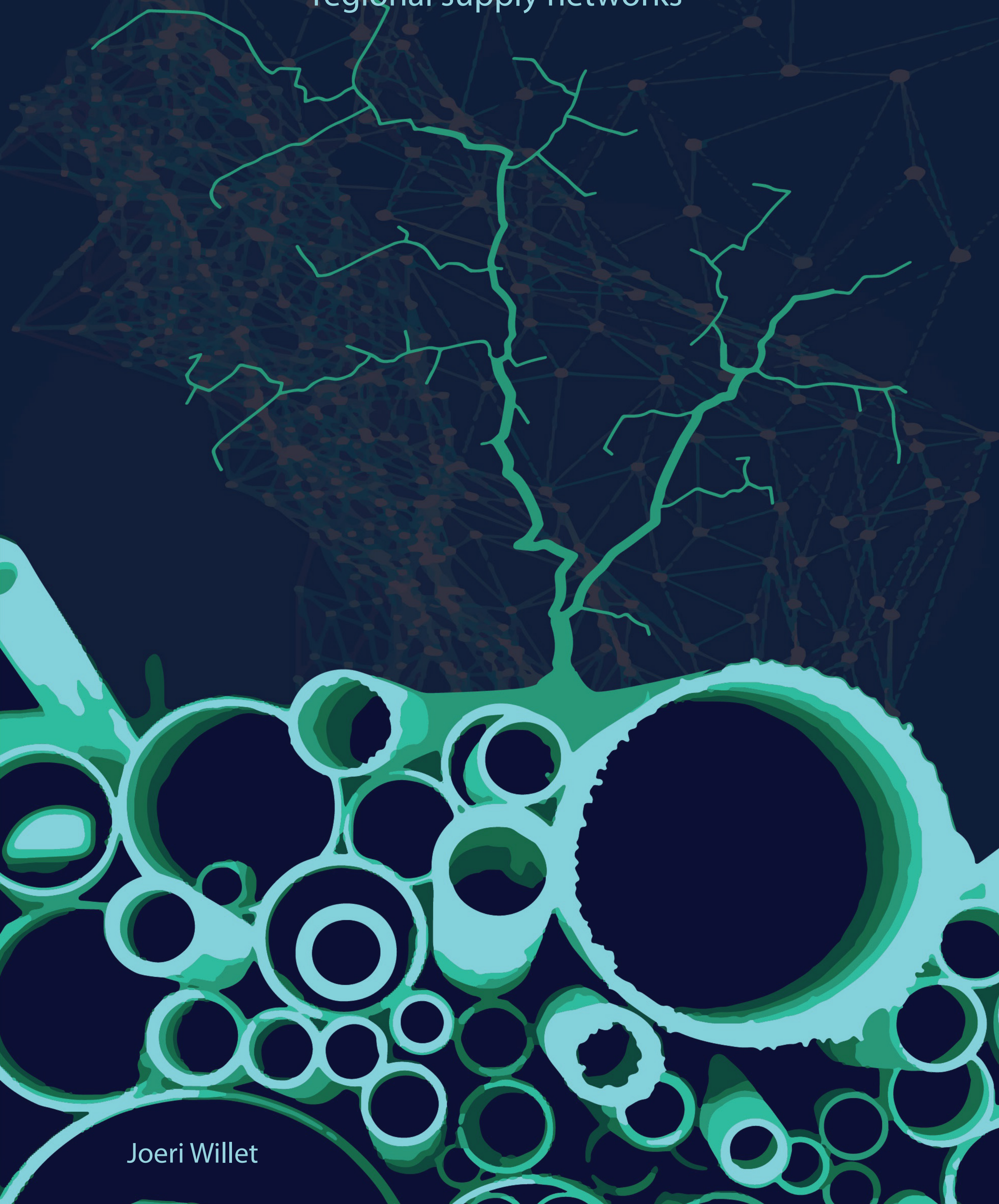
Alternative water resources for industry

Designing environmentally compatible regional supply networks



Joeri Willet

Propositions

1. The use of local alternative water resources will become a necessity for industry.
   (this thesis)

2. By evaluating sustainability with the wrong equipment, industry shows it is not willing to let go of current unsustainable practices.
   (this thesis)

3. Allowing science to be funded by businesses keeps humanity on track for the business-as-usual climate scenarios.

4. Acting on existing knowledge is delayed because of scientists that claim additional research is needed.

5. If free time is seen as a common good, then a tragedy of the commons is unfolding in science.

6. The current way society uses non-human animals confuses indulgence with necessity.

Propositions belonging to the thesis, entitled

Alternative water resources for industry: Designing environmentally compatible regional supply networks

Joeri Willet
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Alternative water resources for industry

Designing environmentally compatible regional supply networks

Joeri Willet

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Alternative water resources for industry

Designing environmentally compatible regional supply networks

Joeri Willet

Thesis

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Chapter 1
Introduction

1 Introduction

Human activities are reliant on the availability of water resources. Having access to water is needed for direct human consumption and sanitation and is a pre-requisite for human welfare (Folke, 1991; Kundzewicz, 1997; United Nations Development Programme, 2006; World Water Assessment Programme, 2009). Progress towards many, if not all, sustainable development goals are closely linked to the availability of clean water and sanitation (UN Water, 2018). As economies continue to develop and world population continues to grow the demand for water will increase (Boretti and Rosa, 2019). Paired with a finite availability of fresh water resources, a growing demand is expected to lead to increasing water scarcity (Hanasaki et al., 2013; Rijsberman, 2006).

Managing water resources in a way that alleviates water scarcity while allowing ecosystems to thrive is one of the main challenges in public policy and water management (Brown et al., 2015; M. Sophocleous, 2000; Poff et al., 2016; Postel and Richter, 2003). The current way humanity manages water resources is causing ecosystem degradation on a global scale (Millennium Ecosystem Assessment, 2005; Pittock and Lankford, 2010; Poff et al., 2016) ultimately leading to a reduction in water security for a large part of the global population (Liu et al., 2017; Mekonnen and Hoekstra, 2016; van Vliet et al., 2017; Vörösmarty et al., 2010). Maybe the clearest example of water resource (mis)management leading to ecological and human welfare reduction is the desiccation of wetlands, most notoriously the Aral Sea (Kingsford, 2000; Micklin, 1988; Micklin, 2007; Wang et al., 2020). Rethinking the way water is used and supplied for agriculture, domestic use, and industry (the focus of this thesis) is needed to ensure an adequate water availability in the future.

Industry contributes 20% to the total water use of humanity (Boretti and Rosa, 2019; United Nations World Water Assessment Programme (WWAP), 2014). Manufacturing accounts for 25% of the total industrial water use and energy production for 75% (United Nations World Water Assessment Programme (WWAP), 2014). The water demand of industry will continue to increase as countries become more industrialized and the need for manufactured goods continues to grow. The total water demand of the manufacturing industry alone is expected to increase by 400% globally in 2050 (Boretti and Rosa, 2019; Wada et al., 2016). Changing the way industry is supplied with water is needed to avoid overexploitation of the available renewable water resources.

This thesis explores alternative ways to supply industry with water through decentralized instead of the currently predominantly used centralized water supply systems. The use of decentralized systems can potentially reduce costs and environmental pressure while increasing supply security and flexibility (Leflaive, 2009). Most of the current research on decentralized water systems is focused on urban water services (Capodaglio, 2021). In this thesis the scope for decentralized water systems is expanded to include industrial areas. In addition to expanding the scope for decentralized water systems boundary conditions are set to ensure water resources are not overexploited. The boundary conditions for these new decentralized water supply systems are based on the concept of environmental compatibility, which is explained in the following section.

In the next section (Section 2) the concept of environmental compatibility is explained. In Section 3 the differences between centralized and decentralized water supply systems are discussed. The challenges that must be overcome to design decentralized water supply systems are explained in Section 4. In the fifth section the state of the art in modelling tools is presented, leading to the problem definition in Section 6 and objectives in Section 7. Background information on the mathematical tools used in this thesis are given in Section 8. Lastly, the outline of this thesis is presented in Section 9.

2 Environmental compatibility

In this thesis the concept of 'environmental compatibility' is used to define the boundary conditions for decentralized industrial water supply systems. Environmental compatibility is introduced to operationalize what is commonly referred to as sustainability or sustainable development. Environmental compatibility is used in this thesis because a clearer definition of sustainability is needed to guide policy and decision making (Holden et al., 2014).

Water use needs to be evaluated from the river basin scale down to specific watersheds to ensure local ecosystems, environments, economies, and human health are not overlooked (Cooper and Bottcher, 1993; Loucks, 2000). Environmental compatibility aims to include every scale in the evaluation of decentralized water supply systems because a consequence of decentralization is that environmental impacts are also decentralized. Environmental compatibility of a decentralized industrial water supply system means that environmental impacts are quantified and weighed at every location where water is used. 'Water use' refers to all the possible uses of a natural water system for industrial purposes. This means that environmentally compatible water use not only considers water extractions but also the discharge of wastewater which can affect aquatic ecosystems. The need for environmental compatibility is further explained through the historical developments around the exploitation of groundwater from aquifers.

2.1 Aquifers and sustainability

The overextraction of water from aquifers led to the awareness that surface water systems and groundwater systems are linked, and that alterations to one system will ultimately affect the other. The 'safe yield' concept was introduced in 1915 to establish the maximum amount of water extractable from aquifers (C. H. Lee, 1915). The safe yield concept is based on a balance between the extraction and the recharge of aquifers. Setting up a water balance for an aquifer shows that the safe yield ignores the natural discharge of aquifers (M. Sophocleous, 1997). When aquifer extractions are equal to the recharge of the aquifer this inevitably means a reduction in the natural discharge to downstream water systems and ecosystems (M. Sophocleous, 2000). Safe yield has therefore been labeled as a myth for long term sustainable water extractions from aquifers (Mays, 2013). Because of the shortcomings of the concept a transition towards 'sustainable yield' is needed (V.M. Ponce, 2007).

Sustainable yield incorporates the needs of water bodies and ecosystems dependent on aquifer discharge when determining the maximum water extraction from aquifers for human use. Since any form of extraction will alter the conditions of an unaltered natural system there is no single value representing sustainable yield (Maimone, 2004). Sustainable yield can therefore better be interpreted as a balance between the needs of different stakeholders, such as agriculture, industry, and nature. Figure 1 shows a simplified graphical representation of the water inflows and outflows from an aquifer under natural conditions, sustainable yield, and safe yield.

2.2 Environmentally compatible water supply systems

The interconnected nature of the hydrological cycle implies that the concept of sustainable yield is not only applicable to aquifers but to any water system. Environmentally compatible water use expands the concept of sustainable yield to include all the interactions between the water user and the (local) water system. Environmentally compatible water use not only considers the effects of water extractions but also considers the amount of (waste)water that can safely be

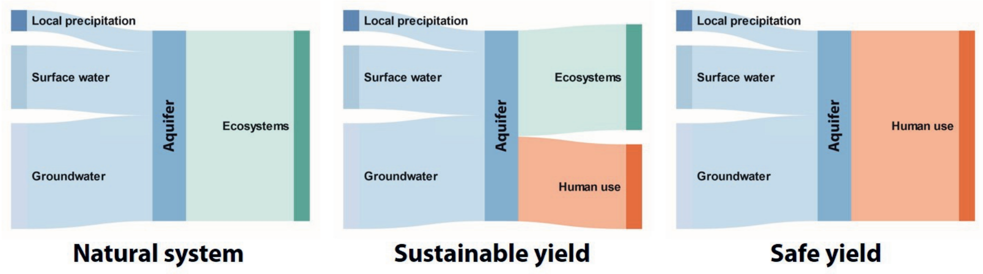


Figure 1 - Simplified representation of water flows in a natural aquifer system compared to the sustainable yield and safe yield concepts. In a natural system all the discharge from an aquifer is available for downstream ecosystems. In the safe yield scenario all the aquifer inflows can be appropriated for human use. In the sustainable yield scenario part of the inflows are used for human use and the remainder is available for ecosystems.

discharged back to a water system or the amount of water needed for other ecosystems. Such other functions could be the prevention of salinization or avoiding of land subsidence. The unique characteristics of each area imply that the limits on water use (indicated with question marks in Figure 2) must be (re)defined based on the local context. This means that environmentally compatible water use must be evaluated based on the unique conditions of every local water system (Figure 2).

Environmentally compatible water use can be expanded to any spatial or temporal scale. Applying the concept to every location where water is used is necessary to create a water supply system which is wholly environmentally compatible (Figure 3).

3 Centralized and decentralized water systems

For more than a century, water, wastewater, and stormwater services have been provided with centralized systems (Pahl-Wostl et al., 2011; Sapkota et al., 2015). Human communities have significantly benefited from the reliable supply, flood mitigation, and effective treatment that these centralized systems provide (Sharma et al., 2013). However, centralized systems may not be the most effective way to provide these functions than services considering the expected resource scarcity in the future. Centralized systems provide a single water quality for all users or mix all wastewater streams to be collectively treated (Cole et al., 2018; Sharma et al., 2013; van Roon, 2007). Having a single water quality in the complete system can lead to excessive environmental impacts and costs (Capodaglio, 2021).

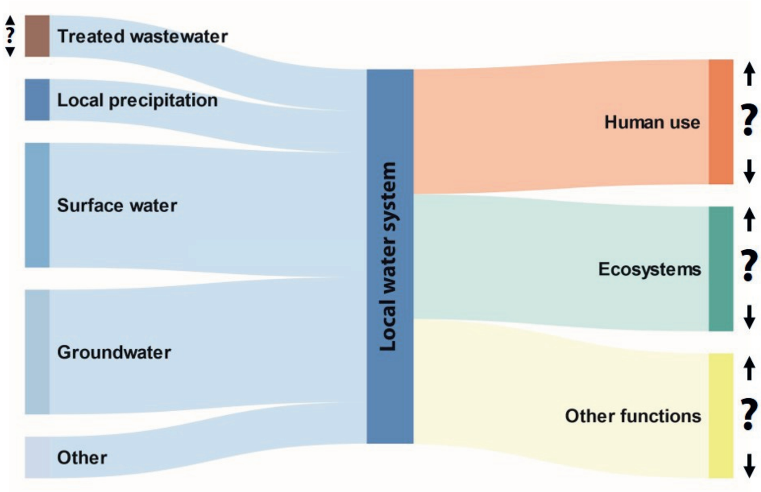


Figure 2 - Representation of water flows for environmentally compatible water use on a local scale. Besides extractions also return flows to the environment are considered. The question marks indicate that the amount of water required for these flows must be determined for each specific situation.

In several countries centralized infrastructures approach the end of their serviceable lifespan. Inevitably replacement of old infrastructure becomes necessary, which means there is the possibility to consider if decentralized systems are better suited in some cases. The availability of new water technologies can make a transition to decentralized, or a hybrid between centralized and decentralized, water management systems possible and economically attractive (Arora et al., 2015; Pahl-Wostl et al., 2011).

In this thesis decentralized water supply for industry is investigated. Decentralized water supply systems are defined as systems that use alternative water resources, including rainwater, wastewater, stormwater, treated wastewater, and brackish (ground)water to cover the demand of the user. Using a wide variety of alternative sources makes it possible to provide water based on the 'fit-for-purpose' concept (Sharma et al., 2013). Fit-for-purpose entails delivering water according to the required specifications of the user. The possibility to deliver water with a specific quality is especially relevant for industry since not all industrial processes require the same water quality (Leflaive, 2009). The benefit of delivering water at the desired quality is that unnecessary treatment costs can be avoided (Capodaglio, 2021). Besides the possibility to deliver 'fit-for-purpose' water, decentralized systems are more flexible and can be adapted to the local needs and opportunities more easily than centralized systems (Pahl-Wostl et al., 2011).

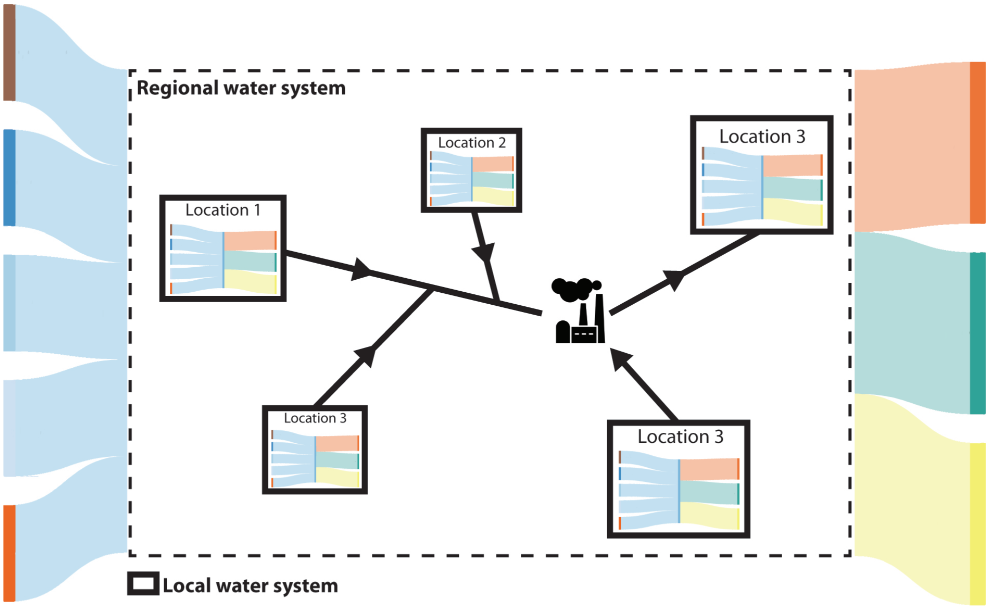


Figure 3 - Environmentally compatible water use applied to an entire decentralized water supply system.

Currently decentralization of water supply in industry mainly takes place in the form of (waste)water exchange between industries. This form of decentralization, called industrial symbiosis, can increase resource use efficiency (Chertow, 2007; Jacobsen, 2006) and can increase the resilience of the system by diversification, multifunctionality, and redundancy (Chopra and Khanna, 2014). At present, the spatial scale of water exchange between industries is limited and mainly occurs between co-located companies (Jacobsen, 2006). This thesis takes a broader view and expands the spatial scale for decentralized industrial water systems and explores alternative water resources on a regional scale.

Examples of regionally available alternative water resources are brackish (ground)water, treated wastewater, or harvested rainwater. Brackish water is available in large quantities around the world and is increasingly seen as an alternative to freshwater. Brackish water can either be used directly for some industrial processes such as cooling or can be desalinated to obtain freshwater. In response to increasing water scarcity the installed desalination capacity around the world is steadily increasing (Eke et al., 2020). Treated wastewater is seen as a potential alternative water source depending on the purpose for which it is used (Capodaglio, 2021). Rainwater harvesting has a long history as an adaptation strategy to changes in water availability (D.N. Pandey et al., 2003). Appropriate sizing and planning of rainwater harvesting systems can yield significant water savings in urban areas (Campisano et al., 2017; Zhang et al., 2019) but is not yet widely applied in industry.

Using a wide range of alternative water resources in decentralized water supply systems means that the supply and demand of water needs to be connected spatially and temporally. The challenges that this can bring are explained in the next section.

4 Spatial and temporal challenges of water supply systems

Water supply systems make it possible to overcome the disconnect between the demand and supply of water resources in space and time. In addition, water quantity and water quality must be considered simultaneously when connecting supply with demand with decentralized water supply systems. For decentralized water supply systems to be effective the selection of an appropriate scale – spatially and temporally – is important (Arora et al., 2015). In this section the spatial and temporal challenges for water supply systems are highlighted.

4.1 Spatial challenges

The supply of and demand for water is unevenly distributed around the world (Biswas, 2008; Oki and Kanae, 2006). The annual precipitation in an area can be considered as the renewable amount of water available when upstream water is unusable due to pollution or consumptive use (Oki et al., 2001). Yearly precipitation ranges from an annual average of 18 mm per year in Egypt to 3240 mm in Colombia (World Bank, 2021), a difference of more than two orders of magnitude. Within countries water availability is also highly variable and can vary significantly between catchment basins.

The spatial challenge that needs to be overcome by water supply systems is to physically connect the demand for water with suitable supply locations. Overcoming this challenge makes it possible for communities to exist in places where water would normally be insufficiently available. The many water transfer projects around the world and their large scale reflects the need for water transport to make human activities possible in areas where water is scarce (Shumilova et al., 2018).

The possibility to overcome the challenges associated with water transport depend on the locations of the demand sites and the supply sites in relation to the local characteristics of a region. Depending on the local characteristics of a region water transport can be prohibitively expensive or technically infeasible. For example, transporting water in a mountainous region poses different challenges compared to transporting water through a desert, a densely populated area, or a protected nature area.

An alternative way to deal with the uneven distribution of water resources is to treat water with a lower quality. In some areas water transport is economically or politically infeasible and treating water of a lower quality is considered as a better alternative. An example where treatment is preferred of transport is the desalination of seawater in some places. Desalination, due to its high (energy) costs, is generally only preferred when other water supply options are unavailable or infeasible (Voutchkov, 2018). The possibility to combine transport with treatment also exists. However, water treatment, or the combination of treatment and transport, is not considered in this thesis.

4.2 Temporal challenges

The availability and demand of water resources is not static in time. Seasonal differences in precipitation and temperature around the globe can result in significant variations in the monthly water balance of each region (C.J. Willmott and K. Matsuura, 2018). Besides seasonal variations there are long term changes to precipitation patterns which alter water availability. Between 1900 and 2014 the average monthly precipitation in some countries increased up to 67% while in other countries it decreased up to 76% (Kenji Matsuura and Cort J. Willmott, 2018). As the global climate changes the period of the year that glaciers melt also changes, which in turn affects the discharge patterns of rivers. The demand for water resources is not static either. Water demand can vary within a single day on a small spatial scale (Blokker et al., 2017), and over a longer time period for complete regions or sectors (Amarasinghe and Smakhtin, 2014).

The quality of water resources also varies in time. Variability in quality is caused by a combination of natural and anthropogenic factors. The (unintentional) discharge of contaminants into water bodies can lead to short- and long-term changes in water quality. High intensity rainfall events can temporarily increase turbidity. Salinization of fresh groundwater can affect surface water quality through different forms of exfiltration (Aydin, 2020). Sea level rise (natural and climate change induced) and land subsidence further accelerate the process of salinization.

The temporal challenge for water supply systems is to ensure that sufficient water – with an adequate quality – is supplied despite the variations in water availability and demand. A short-term mismatch in the supply and demand of water can be solved with storage facilities or by (temporarily) altering the demand for water. Here, 'short-term' refers to the inter-annual variability of water demand and supply and to periods of drought of a few years. A structural water deficit cannot be solved with water storage and can only be overcome with transport, treatment, or by reducing demand. The Cape Town drought between 2015 and 2017 is an example of how demand reductions were able to avoid a complete stop of water supply services (Sousa et al., 2018).

When water storage is used to overcome the temporal challenges of water supply this can happen at large and at small scales. The capacity of water storage facilities can range from less than one cubic meter (domestic rainwater tanks) to millions of cubic meters (dammed rivers). When designing water storage infrastructure the challenge is to a balance between water supply security, costs, and environmental impacts (McCartney, 2009).

4.3 From challenges to water supply network design

The design of water supply networks must address the spatial and temporal variability of water demand and supply while remaining economically feasible. In Figure 4 a graphical representation of water supply network design is given when transitioning from a single water supply location to multiple alternative water resources. When a single water supply location is considered, the main challenge is to determine the best pipeline route to the demand location. When multiple alternative water supply sources are considered the design complexity of the water supply network increases (Figure 4).

Using locally available alternative water resources, such as brackish groundwater, rainwater, or treated wastewater, increases the number of potential water supply locations in decentralized water supply networks. Each additional water source increases the complexity of the water supply problem to the point where modelling approaches are needed to find a solution which is both feasible and desirable.

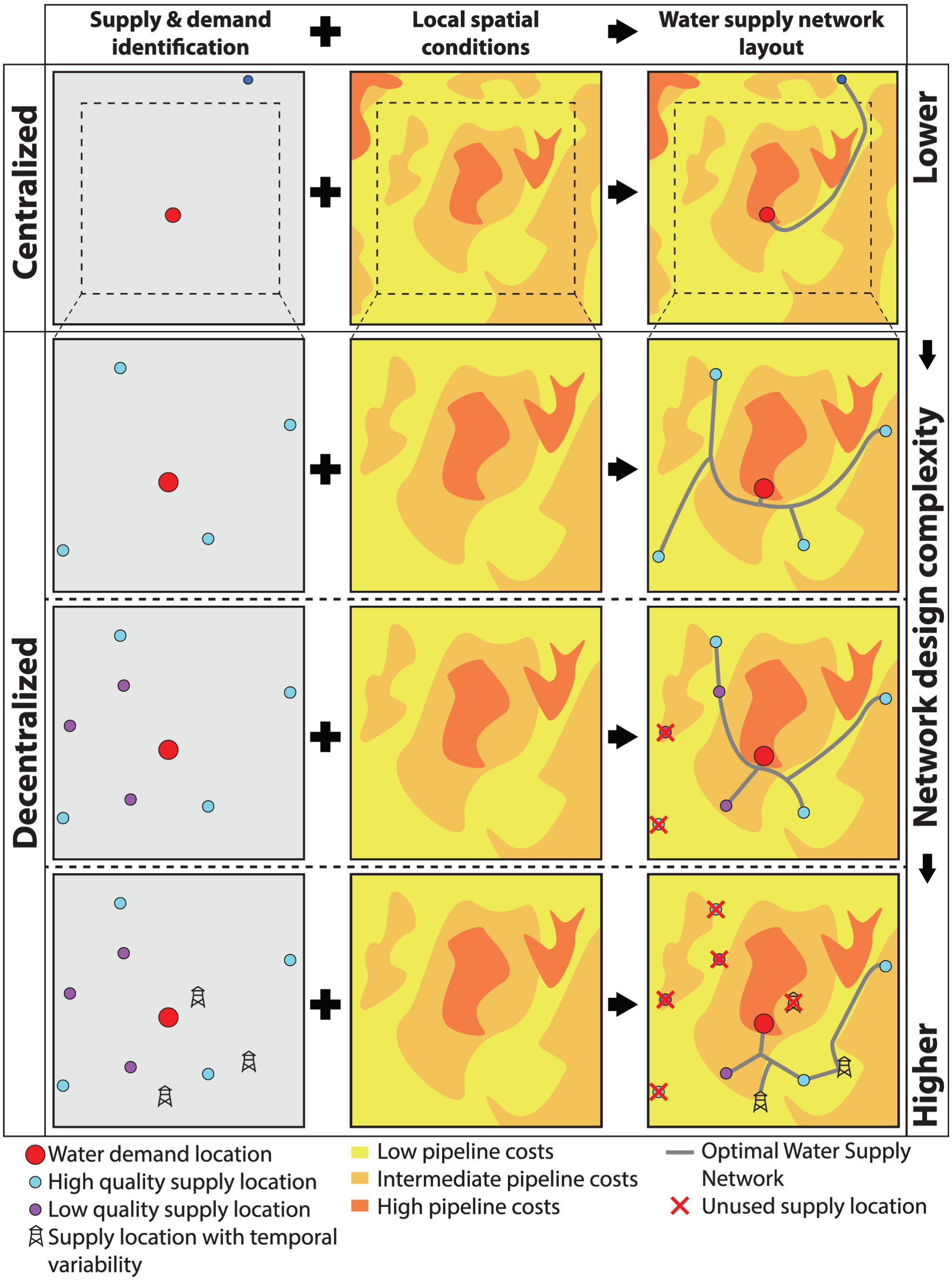


Figure 4 - Water supply network design complexity in relation to spatial and temporal challenges.

5 Water resources management modelling tools – state of the art

Modelling tools are often used in water resources management to aid decision making. In the following section an overview of existing modelling tools which can partly address decentralized water supply network design using alternative water resources is given.

5.1 Simulation or optimization

In the area of water resources management a distinction can be made between two main types of models: simulation models and optimization models. Simulation models tend to address 'what if' questions, while optimization models attempt to answer 'what should be' questions (Loucks and van Beek, 2017). Determining the amount of water which can be extracted from a specific aquifer for industrial activities without excessive negative impacts (environmental compatibility) is typically a problem approached through simulation models. Planning and design of water supply networks on the other hand requires some type of optimization model.

Because of limitations in the underlying assumptions of optimization models the results of these models should not be considered as the best overall solution. Optimization models should rather be considered as a preliminary screening of feasible alternatives which can be used as inputs for the scenarios in simulation models (Loucks and van Beek, 2017).

5.2 Regional scale models

There are many modelling tools for water resources management that function on a regional scale. Several of these tools combine simulation and optimization in a single tool. These models are suitable to evaluate regional strategies and to model water flows in a region. However, these models are not suitable to design detailed new water supply network configurations. Combining regional scale simulation with the optimization of water supply network configurations is done in this thesis. The following models are examples of regional scale models useful for regional planning but that lack the possibility to design water supply networks based on location specific infrastructure costs:

MODSIM is a decision support system for river basin management. It assists decision makers in developing regional strategies for short-term water management, operational planning over longer time periods, contingency planning for droughts, and the analysis of water rights (John W. Labadie, 2010). MODSIM represents the water system as a capacitated flow network and features a dedicated solver for network flow optimization problems.

Water Evaluation and Planning System (WEAP) is an integrated water system simulation model which assists in developing and examining alternative water management strategies (Sieber and Purkey, 2015). WEAP can be used to simulate different water management strategies but also includes optimization capabilities.

WaterCRESS tracks the flow of water through natural and constructed water systems over a continuous time series. WaterCRESS is useful to evaluate current system performance or to evaluate the performance of alternative water supply system configurations (Clark and Cresswell, 2011). These configurations must be determined by the user and are not generated by the model.

RIBASIM is a model to simulate the hydrological behavior of river basins as a result of changes in climate, hydrology, and human activities (W.N.M. van der Krogt and A. Boccalon, 2013). RIBASIM can take a large number of input scenarios and link them to water-using activities within a basin (W.N.M. van der Krogt and A. Boccalon, 2013).

5.3 Water distribution network models

Water distribution network models focus on the detailed design and operation of distribution networks. In general these models are not linked to simulation models which evaluate the environmental compatibility of water use in an area and do not connect water infrastructure costs to the local conditions. Examples of water distribution network models include:

EPANET simulates pressurized pipe networks in terms of hydraulics and water quality (Lewis A. Rossman et al., 2000) and can be used to assess alternative management strategies. EPANET is mainly focused on the operation of networks rather than design of new ones.

BRANCH is a model to design branched water supply networks based on elevation, pipeline length, and friction in pipelines (Awe et al., 2019). This model can only handle a limited number of pipeline connections.

WaterModels is a modelling platform for computational evaluation of optimization and design algorithms in the area of network design and optimal water flow (B. Tasseff, 2021).

A more extensive overview of water distribution system modelling can be found in Awe et al., 2019 and Sonaje and Joshi, 2015.

6 Problem definition

Over the years model accuracy, functionality, and complexity have increased in regional scale models as well as in water distribution network models. However, tools which specifically address the design of decentralized water supply networks using alternative water resources are missing.

The quantification of water demand and supply is taking place with an increasing level of detail in space and time (Alcamo et al., 2003). These higher levels of detail reveal when and where a certain demand for resources can be covered with local renewable (alternative) resources (Agudelo Vera, 2012; Li and Kwan, 2018; Metson et al., 2018; Wielemaker, 2019). However, quantifying the demand and supply of water resources is not enough to design decentralized water supply networks.

To go from quantification to actually connecting an existing water demand with new alternative water resources requires new infrastructure. The possibility to implement new water infrastructure depends on the local context of a study area. For example, the placement of new pipeline infrastructure which crosses existing roads is very costly or completely impossible in protected nature areas.

Modelling and design tools which connect the demand and supply of alternative water resources in space and time within the boundaries of environmental compatibility are missing. Such tools must also consider the local characteristics of an area which influence the costs of water infrastructure to be of value for decision makers.

7 Objective and research questions

The objective of this thesis is to offer modelling tools to design environmentally compatible water supply networks which can deliver fit-for-purpose water for industry. Environmentally compatible water supply networks consider the sustainable availability of water on a local scale as a boundary condition in the design stage. Fit-for-purpose entails delivering water with the quality required for the intended use. Delivering fit-for-purpose water can be achieved by using decentralized water supply networks using local alternative water resources.

In this thesis the design of decentralized water supply networks is determined by minimizing costs from an economic perspective. The local conditions which affect water infrastructure costs are included in the modelling tools to optimize the water supply network configuration. The modelling tools developed in this thesis can be used by knowledge institutes, researchers, and decision makers to design and optimize industrial water supply networks which effectively use alternative water resources.

Two main research questions were formulated to reach the objective of this thesis. The first research question aims to create a better understanding of the way water use is currently evaluated in industry, and is formulated as follows:

> *Which methods are available to effectively evaluate the sustainability of industrial water use and to what extent are these methods currently used?*

The outcomes from the first research question are used to understand and define the boundary conditions for environmentally compatible water supply networks. Based on these boundary conditions the development of modelling tools for water supply network design can take place. Effective water supply network design is guided by the second research question of this thesis:

> *What is an effective modelling framework to optimize environmentally compatible water supply networks based on the spatial and temporal variability of water supply and demand in terms of both water quantity and water quality?*

8 Mathematical background

Simulation and optimization are both used to reach the objective of this thesis. Simulation techniques are used to understand the local hydrological conditions of an area. By understanding the local hydrological conditions potential alternative water supply locations can be identified and the amount of water available can be determined. The amounts of water available at each location become the constraints for the optimization models. Optimization models are used to determine the configuration of decentralized water supply networks.

Determining the configuration of water supply networks is based on a water balance in the network. This means that water that enters the network must be accounted for throughout the network and must also leave the network at the demand location. By ensuring that the water balance is obeyed it is possible to formulate the decentralized network design problem as a mathematical optimization problem.

In this section the mathematical optimization principles used in this thesis are explained. Mathematical optimization is used to determine which supply locations and which pipelines should be used in decentralized water supply networks (the third column in Figure 4). Three examples are given to connect the formulas with a concrete situation.

Example 1: There is an industrial facility with a water demand of 1000 m^3 day^{-1} and two potential water supply sources (Figure 5). The water supply sources – groundwater and surface water – both have more than 1000 m^3 day^{-1} available.

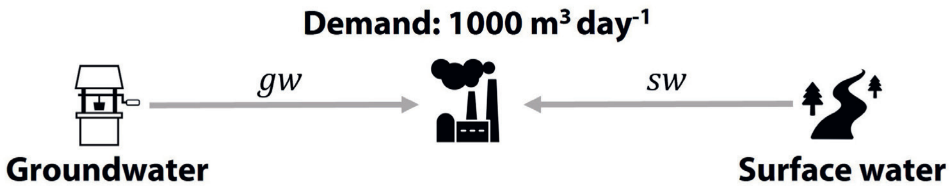


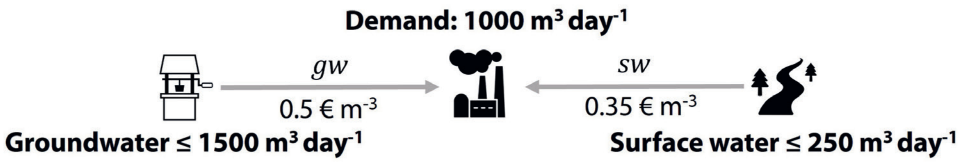
Figure 5 - Graphical representation of Example 1.

In **Example 1** the only constraint for the water supply network is to ensure that the water balance imposed by the demand location is obeyed. The sum of groundwater (gw) and surface water (sw) entering and leaving the water supply network must be 1000 m^3 day^{-1}. This means that $gw + sw = demand$ = 1000 m^3 day^{-1}.

Additional criteria are needed to decide on the optimal configuration of a water supply network in a situation where water availability is limited. One of such criteria can be the costs to pump water from the water supply locations to the demand location.

Example 2: The industrial facility of the previous example still has a demand of 1000 m^3 day^{-1} but limits on water extractions are now in place. The groundwater location has a maximum of 1500 m^3 day^{-1} available and the pumping costs towards the demand location are 0.50 € m^{-3}. The surface water has a maximum of 250 m^3 day^{-1} available and pumping costs towards the demand location are 0.35 € m^{-3}.

Based on the maximum allowed extraction from each supply location and the pumping costs per cubic meter the lowest cost water supply network can be determined (Figure 6). The lowest cost water supply network can cover the demand of 1000 m^3 day^{-1} at a cost of 462.5 € day^{-1}. The lowest costs are achieved by using 750 m^3 day^{-1} from groundwater and 250 m^3 day^{-1} from surface water. If more surface water were available costs could be further reduced. However, a water supply system which uses more than 250 m^3 day^{-1} from surface water is not compatible with the local water availability and is considered an infeasible solution to the design problem.



Groundwater (gw) (m^3 day^{-1})	Surface water (sw) (m^3 day^{-1})	Costs (€ day^{-1})
1000	-	500
900	100	485
750	250	**462.5**
650	**350** ✖	**Infeasible**

Figure 6 - Graphical representation of Example 2.

The situation in **Example 2** can be written as a mathematical optimization problem:

$$\text{minimize } Costs = 0.5 \cdot gw + 0.35 \cdot sw \qquad (1.a)$$

subject to

$$gw + sw = demand = 1000 \qquad (1.b)$$

$$gw \leq 1500 \qquad (1.c)$$

$$sw \leq 250 \qquad (1.d)$$

$$gw \geq 0, sw \geq 0 \qquad (1.e)$$

where Equation (1.a) is the objective function that measures the desirability of a specific combination of values of the decision variables. In this case the objective is to minimize the total costs based on the decision variables gw and sw. The constraints of the optimization problem are given by Equation (1.b), (1.c), (1.d), and (1.e). The water balance is achieved with the equality constraint in Equation (1.b), which ensures that the demand is met. The equations (1.c) and (1.d) ensure that the maximum amount of water available at each supply location is respected. The Equation (1.e) ensures that a (physically impossible) negative flow is not allowed.

Besides the costs to pump water from each supply location the configuration of a water supply network can be important to minimize costs. The cost to place and maintain a new pipeline are significant and therefore excessively long water supply networks should be avoided.

Example 3: There is an industrial facility which is considering switching to alternative local groundwater and surface water resources. The configuration of the new water supply network still needs to be decided depending on the water demand of the industrial facility. The spatial configuration and water availability for this example are shown in Figure 7. The grey lines in Figure 7 represent the possible pipeline connections and their length (l_i) in km. In total there are five – i = 1,2,…,5 – pipeline connections to choose from. In this example the pumping costs depend on the distance the water needs to be transported and are 0.0005 € m^{-3} km^{-1}. The costs to place and maintain a pipeline are 8 € km^{-1} day^{-1}.

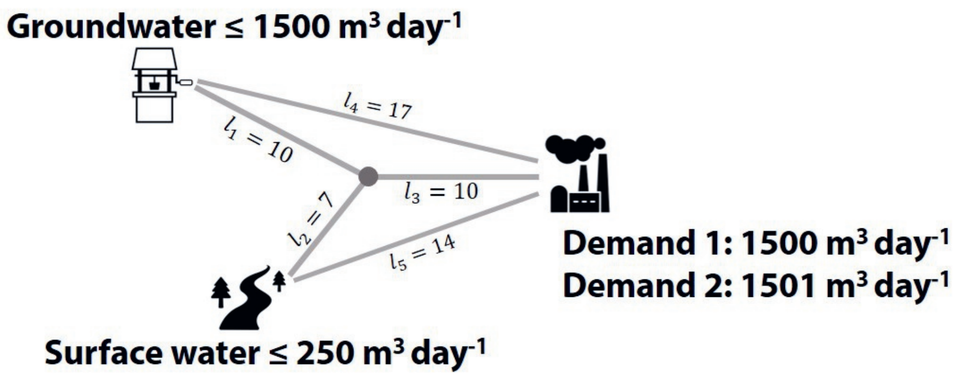


Figure 7 - Graphical representation of Example 3.

The lowest cost water supply network in this example depends on the water demand of the industrial facility. To illustrate the potential effect of slightly increasing the water demand two situations are examined in this example. One situation where the demand is 1500 m^3 day^{-1} and another where it is 1501 m^3 day^{-1}.

The objective of the design problem in this example is to determine which pipeline sections should be used and how much water should be transported through them. The situation in **Example 3** can be written as a mathematical optimization problem by assigning two variables – x_i and y_i – to each of the possible pipelines (Figure 8). The variable x_i represents the amount of water flowing over a pipeline in m^3 day^{-1}. The binary variable y_i is used to represent if a pipeline is used (y_i=1) or not used (y_i=0). The binary variable is used to include the pipeline placement and maintenance costs in the objective function.

The mathematical optimization problem representing **Example 3** is written as:

$$\text{minimize } Costs = \sum_{i=1}^{n}(0.0005 \cdot x_i \cdot l_i + 8 \cdot y_i \cdot l_i) \tag{2.a}$$

subject to

$$x_3 + x_4 + x_5 = demand \tag{2.b}$$

$$x_1 + x_2 = x_3 \tag{2.c}$$

$$x_1 + x_4 \leq 1500 \tag{2.d}$$

$$x_2 + x_5 \leq 250 \tag{2.e}$$

$$x_i \leq y_i \cdot M \qquad \forall i \tag{2.f}$$

$$y_i \in \{0,1\} \qquad \forall i \tag{2.g}$$

$$x_i \geq 0 \qquad \forall i \tag{2.h}$$

where x_i are the decision variables representing the flow of water over each possible pipeline section. The objective function is given by Equation (2.a). The first term ($0.0005 \cdot x_i \cdot l_i$) of Equation (2.a) represents the pumping costs depending on the amount of water transported over each pipeline. The second term ($8 \cdot y_i \cdot l_i$) of Equation (2.a) represents the pipeline placement and maintenance costs which are not dependent on the amount of water transported. The objective is to minimize the sum of the costs of the individual pipeline sections. The mass balance at the demand location is ensured by Equation (2.b). The mass balance at the intersection between x_1 and x_2 is ensured by Equation (2.c). The mass balance at

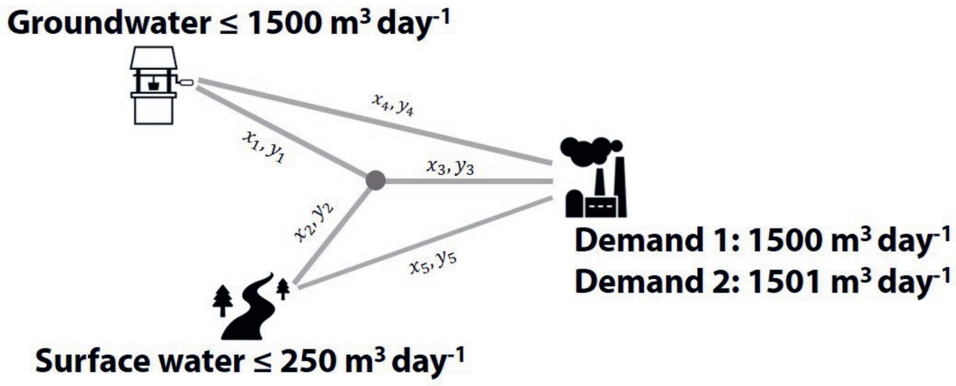


Figure 8 – Graphical representation of Example 3 including the variable x_i and y_i.

the supply locations is ensured by Equation (2.d) and Equation (2.e). The function (2.f) ensures that if there is a flow over a pipeline the binary variable y_i must be equal to 1. In Equation (2.f) the value for M must be chosen manually. In this example there should never be a flow larger than the demand over any pipeline, so M can be set equal to the demand ($M = demand$). When y_i is equal to 1 the pipeline placement and maintenance costs are incurred in the objective function. The function (2.g) ensures that y_i can only take a value of 0 or 1. The function (2.h) ensures that flows cannot be negative.

If the demand is 1500 m^3 day^{-1} the optimal solution has a cost of 148.75 € day^{-1} and surface water is not used at all (Figure 9-A). The costs of 148.75 € day^{-1} are composed of 12.75 € day^{-1} for pumping (1500 m^3 day^{-1} × 0.0005 € m^{-3} km^{-1} × 17 km) and 136 € day^{-1} (8 € km^{-1} day^{-1} × 17 km) for the pipeline placement and maintenance. If the demand slightly increases to 1501 m^3 day^{-1} then both groundwater and surface water need to be used (Figure 9-B). For this demand value the groundwater location is operated at 1251 m^3 day^{-1} and the surface water at 250 m^3 day^{-1}. The costs for a demand of 1501 m^3 day^{-1} are 213.13 € day^{-1}.

Example 3 shows how the water demand and the water availability at each supply location can have significant effects on costs and network configuration. By increasing water demand with 1 m^3 day^{-1} the network configuration must include an additional supply location and the costs increase by 64.38 € day^{-1}.

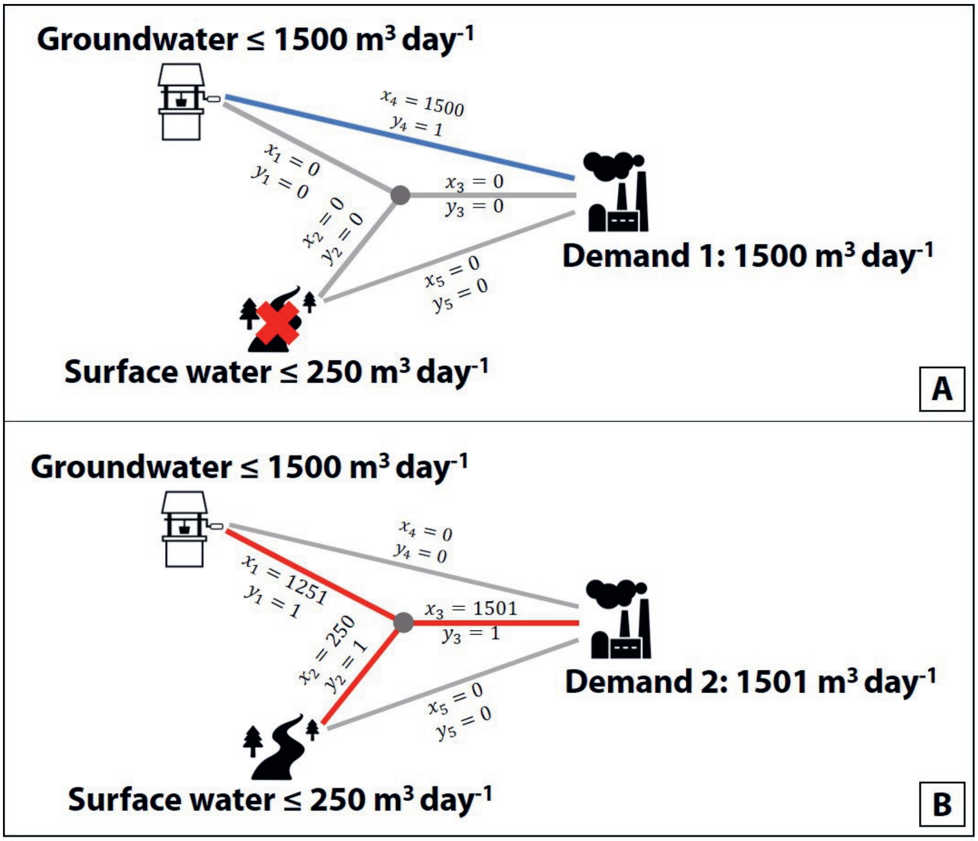


Figure 9 - Optimal solutions for the water supply network problem of Example 3.

The examples in this section can be solved with logic and intuition. As water supply networks grow computer models are needed to handle all the potential network configurations and water flows. In this thesis more complex and extensive water supply network design is investigated based on the basic principles explained in this section. The mathematical formulation of the network design problem elaborated in this section is used to design networks with many more potential pipelines and water supply locations.

9 Thesis outline

In **Chapter 2** a systematic literature review is performed to better understand the field of industrial water use and the way industrial water use is currently evaluated. An existing assessment framework is used to compare and categorize the evaluation methods used in the scientific literature on industrial water use. The assessment framework distinguishes evaluation methods which effectively assess water supply system sustainability from evaluation methods which only do so to a limited extent. **Chapter 2** aims to answer the first research question of this thesis and is used to identify the boundary conditions for environmentally compatible industrial water supply systems.

The complex interplay between spatial and temporal aspects when matching water supply with demand requires a stepwise approach. **Chapters 3, 4, and 5** are all dedicated to the development of the modelling framework to answer the second research question.

The focus of **Chapter 3** is the development of optimization methods for decentralized water supply network design based on the local land use in a region. Land use affects the costs for water infrastructures (pipelines, storage basis, etc.) and therefore needs to be included in the design of decentralized water supply networks. The integration of land use data and optimization is achieved by using geographic information systems (GIS) in combination with mathematical programming. The methods developed in this chapter consider a single water quality in the water supply system.

In **Chapter 4** the focus shifts towards including water quality and delivering fit-for-purpose water with decentralized water supply networks. In this chapter the quality of water, in terms of salt content, is added to the optimization procedure. The effects of salinization of groundwater resources in combination with different salinity requirements at the demand location are investigated in relation to network design. Hydrological modelling on long-term changes to groundwater salinity are used to define the maximum environmentally compatible extraction rates of groundwater wells. Again, mathematical programming is used to optimize the network layout.

Chapter 5 is dedicated to including the temporal variability of water resource availability in the design of water supply networks. This temporal variability is addressed by including storage capacity in the design of water supply networks. In this chapter a steady flow of water from groundwater resources is combined with the variable water availability of rainwater harvested from urban areas.

Chapter 6 is a synthesis and discussion of the findings of this thesis. The contributions of the work are examined in relation to different research fields, the modelling tools developed are discussed, and a reflection on the requirements for a transition towards sustainable industrial water systems is given.

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Chapter 2

Review of methods to assess sustainability of industrial water use

Abstract

The projected increase of industrial water demands raises the need to assess the environmental sustainability of industrial water use. Assessment methods need to use Sustainable Systems Indicators (SSIs) which relate resource use to the carrying capacity of the local environment. SSIs for water use evaluate whether water use exceeds the natural water renewal (quantity) and whether emissions remain within the assimilation capacity of ecosystems (quality). We systematically reviewed the scientific literature to show which methods are used to assess industrial water use, and of these, which methods incorporate SSIs. In total, 82 assessment methods were identified in 340 papers. The methods were assigned to five categories: Key Performance Indicators, Composite Indices, Environmental Accounting, Material and Energy Flow Analysis, and Life Cycle Analysis. In 26% of the reviewed papers, the assessment methods used SSIs. The number of papers incorporating SSIs is growing at a slower rate than the overall number of papers in the area of sustainability assessments of industrial water use. Considering the expected growth in industrial water use this poses a risk to sustainable water use. The best performing category in terms of incorporating SSIs is Material and Energy Flow Analysis (42% of papers). Papers assessing several industrial sectors in the same study incorporate SSIs more frequently (68%) than research focused on a single industry or process (20%). We discuss examples from the reviewed papers which successfully incorporate SSIs, in order to: (1) identify the elements needed to create SSIs for industrial water use, (2) aid researchers and practitioners in selecting methods which incorporate SSIs, and (3) provide a starting point for future methodological development incorporating SSIs.

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1 Introduction

Both human societies and natural ecosystems depend on the availability of adequate water resources. Water is not only needed to satisfy basic human needs but is also crucial for sustainable economic development (Kundzewicz, 1997). On a global scale, the rate at which water resources are naturally replenished is more than enough to meet the demand of humanity (Oki and Kanae, 2006). However, water resources and water demand are heterogeneously distributed around the globe. This results in some areas having a water surplus while other areas have a water deficit. On a local scale, anthropogenic water use often exceeds the watersheds natural recharge rate, resulting in water scarcity (Gleick and Palaniappan, 2010).

Global water demand is projected to increase from 3500 km^3 year^{-1} in 2000 to around 5500 km^3 year^{-1} in 2050 (OECD, 2012). In many places around the world the response to the increasing water demand is to increase the extraction of non-renewable water (i.e. water not replenished through the hydrological cycle). This leads to the overdraft of aquifers (Wada et al., 2010), depletion of surface reservoirs, and ecosystem water shortages. Overdrafting the water resources that are needed to maintain the local ecosystems leads to the degradation of those ecosystems, and ecosystem services, on which societies depend (Hoekstra, 2011a; Poff et al., 2010). The 'Aral Sea Disaster' is one example of how local over extraction leads to ecosystem degradation. The impact of this over extraction was the disappearance of fish populations, desertification and decreased air quality which led to severe ecological and human welfare damage (Micklin, 2007). The negative effects of water extraction can be avoided by balancing human water demand with renewable water availability, for both the global and the local scale.

Industry is one of the main users of water and their water use is expected to increase (OECD, 2012). Water demand is expected to increase with 400% by 2050 (OECD, 2012) for the manufacturing industry. This increased industrial demand can have severe consequences on the local environment and ecosystems. This paper focuses specifically on the environmental sustainability of industrial water use, in terms of quantity and quality.

Industrial water use needs to be based on sustainable water extraction rates that are adequately determined and evaluated. Several assessment methods have been developed to evaluate the sustainability of industrial (water) resource use (Angelakoglou and Gaidajis, 2015). Most of these assessment methods have been effective at increasing resource use efficiency (Bakshi, 2011). However, increasing resource use efficiency alone is not enough to reach a sustainable system (Bakshi, 2011). To create a sustainable water system, industries need assessment methods which can quantify their water use in relation to renewable water availability, and the ability of ecosystems to purify pollutants, across all relevant spatiotemporal scales. The relationship between sustainability, industrial (or any other) resource use, and assessment methods is captured by the concept of 'Sustainable Systems Indicators' (SSIs) introduced by Veleva et al. (2001). Assessment methods using SSIs link resource use to the carrying capacity of ecosystems providing the resources. An evaluation of assessment methods based on the use of SSIs has not yet been performed within the area of industrial water use. With this in mind, a review of the assessment methods themselves, instead of their results is needed. Establishing which assessment methods effectively incorporate SSIs for water use is needed to move past efficiency gains and towards sustainable industrial water use. The interrelations between water use and energy use, in the water-energy nexus, are not addressed directly in this paper.

Research Objective. The objective of this research is to gain insight into the effectiveness of commonly used assessment methods to evaluate the environmental sustainability of industrial water use. This paper categorizes and qualitatively assesses the methods used to evaluate industrial water use based on data gathered through a systematic literature review. The results of the review allow for more thorough selection of assessment methods and for better interpretation of assessment results. Additionally, this review serves as a starting point for future assessment methodology development. Such a review is needed to adequately assess water resource use considering the natural variability in supply and the expected increases in (industrial) water demand. The remainder of this paper is organized as follows: Section 2 presents the methodology used for the review; Section 3 presents the background theory on assessment methodologies; Section 4 presents and discusses the extent to which SSIs are incorporated in assessment methods and within industrial sectors; and Section 5 summarizes and concludes our findings.

2 Methodology

2.1 Systematic review

Previous review papers on sustainability assessments of industrial systems (e.g. Angelakoglou and Gaidajis (2015), Bakshi (2011), and Singh et al. (2009)) were used for a meta-review to define the search strategy for this research (Table 1) and to guide the development of the evaluation framework.

Papers found through the search strategy were screened according to four criteria:

Industry: Only articles focusing on industrial processes were included. The industrial sectors included were: energy production, manufacturing, mining, (petro)chemical, and waste processing. The (petro)chemical industry is often considered part of the manufacturing industry (European Commission, 2020). We make a distinction between the (petro)chemical and other manufacturing industry due to large quantities of water used in the petrochemical industry (Eurostat, 2017). By making this distinction the difference in assessment practices for these sectors can become apparent. A 'mixed' sector was created for papers that evaluated water use in multiple sectors. Industrial processes that focused on the refinement of agricultural products (e.g. cheese and wine production) fall under manufacturing category since raw materials are converted into a final product. The production of agricultural products, livestock, or aquaculture were considered out of scope.

Environmental sustainability: Papers incorporating the environmental aspect of sustainability, and more specifically the sustainability of water use (quantity/quality) were included. Assessments solely addressing social or economic sustainability of industrial activities were excluded.

Assessment methodology: The definition of a sustainability assessment method used by Angelakoglou and Gaidajis (2015) is "a method which can provide quantitative information that can potentially help industries to assess their environmental sustainability". This definition was used to include papers. Articles elaborating on a product, technology, or industrial system, that did not elaborate on the assessment method used to evaluate the product, technology or industrial system were excluded.

Table 1 - Overview of the systematic literature review process.

Source	***Number of papers***	***Cumulative number of papers***
Scopus[a]	3373	3373
Web of knowledge[b]	1717	5090
Duplicate removal	-1212	3878
Not retrievable papers	-137	3741
Screening according to inclusion criteria	-3401	340
Papers included in the review		340

[A] TITLE-ABS-KEY (water) AND TITLE-ABS-KEY (industry OR industrial OR factory) AND TITLE-ABS-KEY (sustainable OR sustainability) AND TITLE-ABS-KEY (assessment* OR indicator* OR evaluation* OR index OR indices)

[B] TOPIC: (water) AND TOPIC: (industry OR industrial OR factory) AND TOPIC: (sustainable OR sustainability) AND TOPIC: (assessment* OR indicator* OR evaluation* OR index OR indices)

[A,B] Both searches were performed on 15-1-2019 and cover the time period from 1995-2018

Case studies: The aim of this research is to identify the methods used to evaluate industrial water use in real cases. Papers elaborating on a specific industry, or method to evaluate an industrial sector were included. Papers evaluating water resource use of a country or region excluded.

2.2 Assessment framework

The purpose of the assessment framework used in this research is to determine which assessment methods are suitable to evaluate the environmental sustainability of industrial water use. The evaluation framework for this research is based on the Lowell Center for Sustainable Production (LCSP) indicator framework as developed by Veleva et al. (2001). The LCSP framework is used because it provides a structured way to evaluate assessment methods which focus specifically on environmental sustainability. In this research, the LCSP framework is used to determine the extent to which the indicators used in different assessment methods include threshold values based on the renewable availability of water resources. The LCSP framework ranks indicators on 5 levels where indicators that reach level 5 can be considered ‘Sustainable Systems Indicators’ (Veleva et al., 2001). The different levels are intended to be evolutionary, meaning indicators that reach levels 1 through 4 are the building blocks to create level 5 indicators. Level 1 and 2 indicators limit assessment to processes and (water) resource use within the company/facility boundaries. Level 3 and 4

Table 2 - LCSP levels and associated indicator criteria, adapted from Veleva et al. (2001).

Level	***Criteria***	***Example***
1: Facility Compliance/conformance indicators	Show the degree to which industrial operations comply with regulations	Number of spills/fines
2: Facility Material Use and Performance indicators	Show overall resource efficiency at the facility level	Water use per kilogram of product
3: Facility Effects indicators	Show potential effects of a facility on the environment	Kilograms of eutrophic substances released in PO_4^{-3} equivalents (Eutrophication potential)
4: Supply Chain and Product Life-Cycle indicators	Show environmental impacts through the life-cycle of a product	Embodied/virtual water use (Chen et al., 2012)
5: Sustainable Systems Indicators (SSIs)	Show the performance of a single company in relation to sustainable resource use as a whole. SSIs show the extent to which resource use fits within the carrying capacity of ecosystems by setting resource use by the company in relation to the availability, renewal rate or assimilation capacity of the ecosystem on a local and global scale	Percentage of water sourced from renewable vs non-renewable sources Water abstraction rate vs natural renewal rate Local emissions in relation to local assimilation capacity

indicators expand the boundary of the assessment to the effects of the company/facility on the outside environment. Level 5 indicators place company/facility resource use and emissions in relation with sustainable renewal rates of (water)resources and the assimilation capacity of the environment.

The LCSP framework has previously been used to evaluate sustainability indicators used in the petrochemical (Samuel et al., 2013) and pharmaceutical industries (Veleva et al., 2003). The framework has not yet been used to compare assessment methods specifically for industrial water use. In this research, the original criteria of the LCSP framework are used and operationalized to assess how SSIs are incorporated in the assessment methods for water use in industry. The different levels and associated operationalization of the LCSP framework for this research are shown in Table 2.

In the systematic review, indicators were evaluated according to the criteria presented in Table 2 irrespective of the aspect they assess, such as water quality or quantity. Papers using several water related indicators were ranked based on the highest scoring indicator.

3 Theory

After the Brundtland report in 1987 the importance of sustainable development gained increased attention. Consequently, methods were then needed to evaluate progress towards sustainable development (Mitchell, 2006). To date there is a multitude of assessment methods to evaluate the environmental sustainability of industrial systems (Angelakoglou and Gaidajis, 2015; Fowler and Hope, 2007; Gasparatos et al., 2008; Singh et al., 2009). Because of the plethora of methods, categorization is required for further analysis. Angelakoglou et al. (2015) argue that the classification used by the OECD (Organization for Economic Co-operation and Development, 2009) is the most suitable since it is the closest to practice within industry, and is used in this research. The OECD classification consists of six categories: (1) Key Performance Indicators, (2) Socially Responsible Investment Indices, (3) Composite Indices, (4) Material and Energy Flow Analysis, (5) Environmental Accounting, (6) Life Cycle Analysis. The interconnections between the proposed categories (e.g. Material and Energy Flow Analysis and Life Cycle Analysis) (Angelakoglou and Gaidajis, 2015) are relevant when determining if the combination of methodology categories results in better performance in terms of SSIs. The OECD categories used to group papers in this research are described in Sections 3.1–3.6.

3.1 Key Performance Indicators (KPIs)

The selection and development of KPIs aims to reduce the amount of data which needs to be collected and tracked to evaluate system performance. Key Performance Indicators (KPIs) were originally used to evaluate the economic performance of organizations (Angelakoglou and Gaidajis, 2015). More recently, sets of KPIs have been developed to evaluate the environmental sustainability of human activities.

Careful selection of KPIs is needed to make sure the complete system is evaluated (Bai and Sarkis, 2014). KPIs do not always reveal the underlying reasons for system performance or show which changes are needed to improve performance (Parmenter, 2007). These shortcomings are reinforced by the fact that development and disclosure of environmental KPIs is predominantly voluntary (Perrini and Tencati, 2006), while the selection of indicators is largely based on the "realities, values, and culture" of the organization using them (Keeble et al., 2003). Even so, the implementation and monitoring of KPIs is useful for tracking developments within an organization (Chae, 2009).

3.2 Composite Indices (CI)

Composite Indices (CI) are built by aggregating separate indicators (KPIs) into a single metric according to a specified method (Ciegis et al., 2009; Gasparatos et al., 2009). The apparent simplicity of CI outputs makes them appealing for policy and decision makers since large amounts of information can be condensed into more manageable and comparable values (Gasparatos et al., 2009). The benefits of CI include: ease of interpretation, ability to rank alternatives, facilitating communication, and making performance and progress central within the policy arena (Nardo et al., 2008).

The main critique within CI research is the subjective nature of the weighing scales (Böhringer and Jochem, 2007; Singh et al., 2009). Determination of weights is generally done through participative (expert inputs) or non-participatory methods (Gasparatos et al., 2009). Procedures such as the analytic hierarchy process (Saaty, 2008) can be used to standardize the process of deriving priority weights but the input for such procedures still has a subjective nature. The participatory method can be valuable in relation to SSIs due to the possibility for local experts to give added emphasis to locally relevant issues.

After weight determination the individual KPIs are aggregated to generate the final index. The aggregating procedure can also have significant influence on the final outcome of the assessment (Munda and Nardo, 2005). Due to internal assumptions (weighting and aggregating), the outcome of a CI can yield different results when analyzing the same system. The effects of this internal bias was shown when evaluating the overall sustainability of different countries (Mayer, 2008) and where results were dependent on methodological choices.

The economic and social sustainability aspects included in many CI were not taken into account when evaluating CI papers based on the LCSP framework. To evaluate CI methods according to the LCSP framework the underlying indicators specifically related to the environmental sustainability of water use were considered. The weighting and aggregation steps of CI were not considered because these only affect the extent to which environmental, economic and social sustainability are represented in the final index score.

3.3 Socially Responsible Investment Indices (SRI)

SRI are used by stakeholders and investors to benchmark the sustainability performance of organizations and corporations (Organization for Economic Co-operation and Development, 2009). In most cases this takes the form of a ranking list (Angelakoglou and Gaidajis, 2015). Over the last decades, the number of corporate social responsibility indices and metrics for the assessment of corporate performance has steadily grown (Sadowski et al., 2010). While the underlying motives for companies to engage in corporate social responsibility can be debated (Searcy, 2012), the development of SRI does foster competition among companies to enhance their environmental performance (Sadowski et al., 2010). The environmental performance of companies, measured through SRI, is frequently highlighted in sustainability reports (Searcy and Elkhawas, 2012). The extent to which SRI reflects whether a company contributes to a sustainable future is still lacking. In part because many SRI do not yet relate company resource use to the carrying capacity of ecosystems (Sadowski et al., 2010).

3.4 Material and Energy Flow Analysis (MEFA)

The underlying principle of MEFA is the law of conservation of mass and energy (Huang et al., 2012) to assess the flows of materials or energy in a given system (Bringezu et al., 1997; Brunner and Rechberger, 2004). The use of MEFA to evaluate the environmental performance of human activities began in the 1970s (Brunner and Rechberger, 2004) and has become an important tool for decision making in many fields (Huang et al., 2012). Combination of MEFA with other methodologies (such as Life Cycle Analysis) is expected to increase accuracy and relevance and has been on the research agenda for years (Huang et al., 2012).

MEFA methods systematically quantify stocks and flows within the system and connect these to their respective sources and sinks. MEFA methods are frequently used in the Life Cycle Inventory phase within Life Cycle Analysis. This approach makes it possible to relate resource utilization to the carrying capacity of the ecosystem (Huang et al., 2012; Naohiro et al., 2015). The above process is generally performed with either materials/substances or energy as units of measurement.

There is a range of methodologies within MEFA which can lead to differing outcomes for the same case based on the boundary conditions chosen (Brown and Herendeen, 1996). Even so, MEFA make it possible to determine the direction of change in terms of resource utilization and material/energy flows (Haberl, 2007).

3.5 Environmental Accounting (EA)

Environmental accounting methods convert environmental value (ecosystem services) to economic value in order to evaluate the costs or benefits of resource exploitation (Angelakoglou and Gaidajis, 2015). Conversion of environmental to economic value allows organizations to assess their environmental performance and report their progress to external stakeholders (Yakhou and Dorweiler, 2004). The monetization of ecosystem services can make them subject to market mechanisms of exchange and sale (Gómez-Baggethun et al., 2010). The exchange and sale of ecosystem services can be problematic when not all ecosystem services can be captured in a monetary value or there is missing knowledge on the interdependence of ecosystem services. It is recognized that EA could theoretically contribute towards more sustainable practices, but the current voluntary nature (in contrast to economic accounting) can also undermine this purpose. In a world where decision maker acceptance of personal accountability is severely lacking (Owen, 2014), and organizations actively work to avoid accountability (Gray et al., 2014), it is hard to reconcile transparent disclosure with voluntary accountability. Without obligatory independent assessments, the quality of EA is considered very low in comparison to traditional/monetary accounting practices (Gray and Milne, 2015). Additionally, improvements tend to be overruled by business interests (Deegan, 2016).

Despite the shortcomings of EA, there are also arguments for the added value of this type of assessment. Sunstein (2005) concludes that Cost-Benefit Analysis, a sub-methodology within EA, "does not tell regulators all they need to know; but without it, they will know far too little". EA can be a powerful tool to inform decision makers about environmental sustainability, and can be even more effective when used alongside other methods (Gómez-Baggethun and Ruiz-Pérez, 2011).

3.6 Life Cycle Analysis (LCA)

LCA calculates the environmental impact of a product or service over its lifetime. In the 1970s, LCA mostly focused on the analysis of energy (McManus and Taylor, 2015). Since then LCA methods have grown to cover a wide variety of environmental impacts (McManus and Taylor, 2015). The most relevant impact categories in relation to water use are: water use, freshwater ecotoxicity, marine ecotoxicity, and freshwater eutrophication (Huijbregts et al., 2017). Between 1990 and 2000, LCA entered policy and legislation as a tool for decision makers. From 2000 to 2010, LCA methods started to diverge in order to address some of the drawbacks of the method such as system boundaries and allocation (Guinée et al., 2011). Currently, LCA methods are expanding from attributional LCA (aLCA) to consequential LCA (cLCA) (McManus and Taylor, 2015). The aLCA focuses on the environmental impacts of specific products or services per functional unit of the product. In cLCA the systems boundaries are increased to evaluate impacts over larger spatiotemporal scales and to investigate how resource flows and their associated environmental impacts will change as a consequence of changes in demand for the functional unit (Weidema et al., 2018). The transition towards cLCA increases the complexity of analysis but also makes it possible to holistically assess environmental impacts (McManus and Taylor, 2015).

The strengths of LCA include that it provides a comprehensive and structured investigation and assessment, highlights potential environmental tradeoffs, can challenge conventional wisdom, advances the knowledge base, and fosters communication and discourse (Curran, 2014). LCA can also incorporate an increasing number of relevant impact categories and can be applied to a wide range of systems such as products, industrial sectors, or countries. Despite these strengths, LCA has limitations which hinder assessing system sustainability. Arguably the most prominent drawback is the difficulty for integration of results across different temporal and spatial scales (Reap et al., 2008). For some environmental impacts the location of emissions and associated effects are almost independent, as is the case for ozone depletion and climate change (Reap et al., 2008). Other environmental impacts can vary by orders of magnitude due to variations in local sensitivities (Reap et al., 2008). In addition to the above limitations, LCA is unable to account for changes of conditions outside the geographic system boundaries which can affect the system being studied (Finnveden et al., 2009). These issues are on the LCA research agenda and have led to continuous improvements. Combining LCA methodologies with other methods is being researched to overcome the above limitations (Roy et al., 2009). An example is the incorporation of water scarcity indicators into LCA which makes it possible to relate the water use impact category to local conditions (Jolliet et al., 2018). The AWARE methodology is a recent development incorporating water scarcity on a spatial scale (Boulay et al., 2015; Boulay et al., 2017).

4 Results & discussion

4.1 Overall performance

A total of 340 papers were analyzed (Figure 1) and 82 assessment methods to evaluate industrial water use were identified (see Supplementary Information 1 for an overview of the methods identified and the LCSP level of the indicators used in these methods). The SRI methodology category was not encountered in any of the 340 papers evaluating the environmental sustainability of industrial water use.

Papers matching the search criteria started appearing in 1995 and their prevalence grew up to 2018 (Figure 1). The large increase in KPIs and CI papers in 2018 is due to a large number of papers combining methods in 2018. In 26% of the papers the assessment methods used matched SSIs criteria, but performance is not uniform across the OECD methodology categories (Figure 2). In relation to the total number of papers in each category, the MEFA category performs the best with regards to SSI use (42%) while LCA performs the worst (16%) (Figure 2). Paper using LCA methods are the most prevalent (160 out of 340) and use level 4 indicators in 74% of the papers. The prevalence of papers using LCA methods, with level 4 indicators, causes overall performance to be at level 4 (39%, Figure 2).

The methods used in the majority of papers (74%) are either not suitable to assess water use at the SSIs level due to methodological limitations, or there is a lack of ambition to reach this level of assessment. The overall growth rate of papers using indicators which reach the level of SSIs is lower than papers not using SSIs (Figure 3). This is of concern because it shows that evaluating water use in relation to the carrying capacity of ecosystems (using SSIs) is not yet assimilated within the research community on the topic of industrial water use. Decision making based on level 1-4 assessments can lead do degradation of ecosystems, and the associated ecosystem services they provide.

The possibility to use SSIs is closely linked to the availability of data. The unavailability of accurate data across all spatial scales requires a trade-off between ‘precision’ and ‘applicability’ (Berger and Finkbeiner, 2010). Level 5 assessment methods (SSIs) require extensive data on human activities, as well as the carrying capacity of the local environment affected by human activities. In relation to SSIs data unavailability poses the following problem: should researchers use SSIs (level 5) with insufficient data with the possibility of arriving

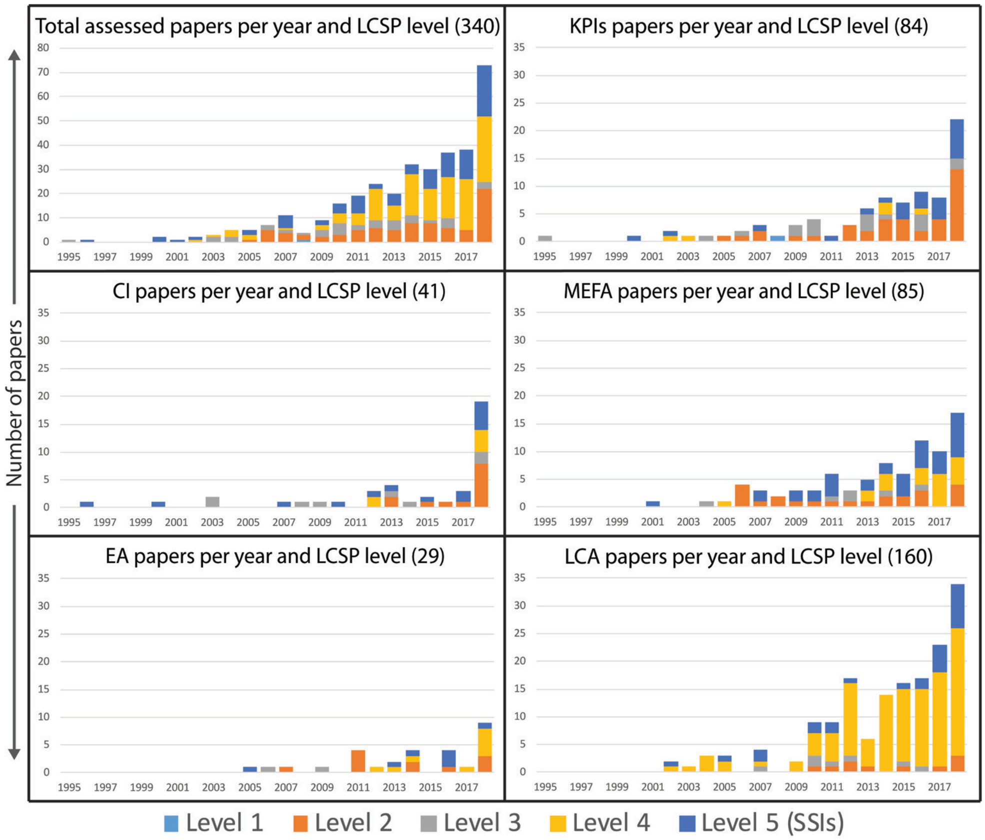

Figure 1 - Lowell Center for Sustainable Production (LCSP) indicators (Veleva et al., 2001) performance of included papers for assessing the sustainability of industrial water use. Papers are evaluated according to the LCSP levels: Facility Compliance/conformance indicators (Level 1), Facility Material Use and Performance indicators (Level 2), Facility Effects indicators (Level 3), Supply Chain and Product Life-Cycle indicators (Level 4), Sustainable Systems Indicators (SSI) (Level 5). Papers are categorized according to the OECD classification for assessment methods: Key Performance Indicators (KPIs), Composite Indices (CI), Material and Energy Flow Analysis (MEFA), Environmental Accounting (EA), and Life Cycle Analysis (LCA) (Organization for Economic Co-operation and Development, 2009). The numbers between brackets shows the total number of papers per OECD category.

at incorrect conclusions or use indicators with lower data requirements (levels 1-4) with the knowledge that environmental sustainability cannot be fully assessed. In either case, ecosystems are at risk of over exploitation. Further research on the interactions between data availability and the choice to use methods with SSIs is suggested for future research.

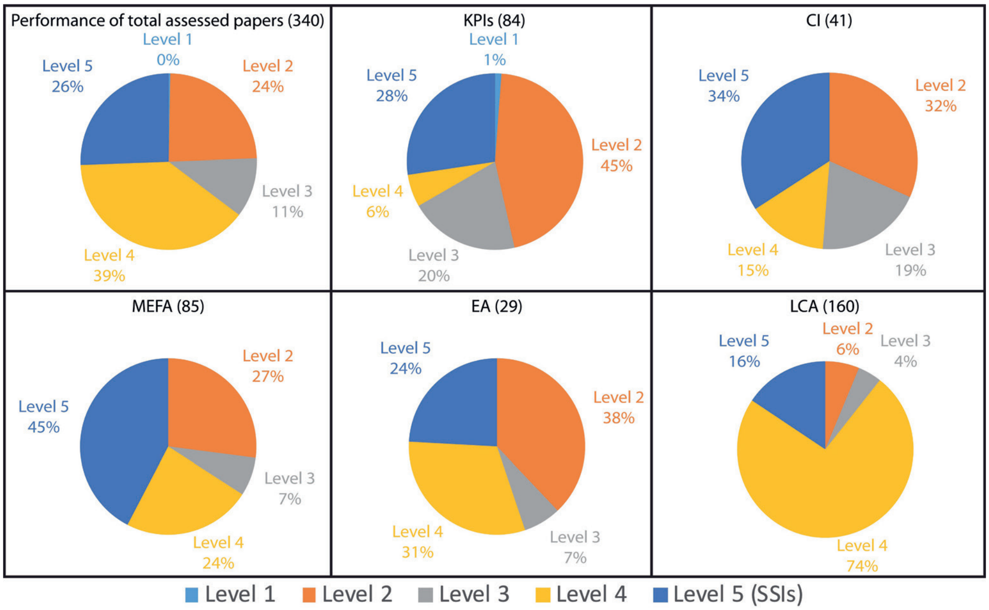

Figure 2 - LCSP indicator performance of total assessed papers and per methodology category. The performance of incorporating SSIs varies per category. The MEFA category is the most successful at incorporating SSIs. The LCA category incorporates SSIs the least. The numbers between brackets show the number of papers per OECD category.

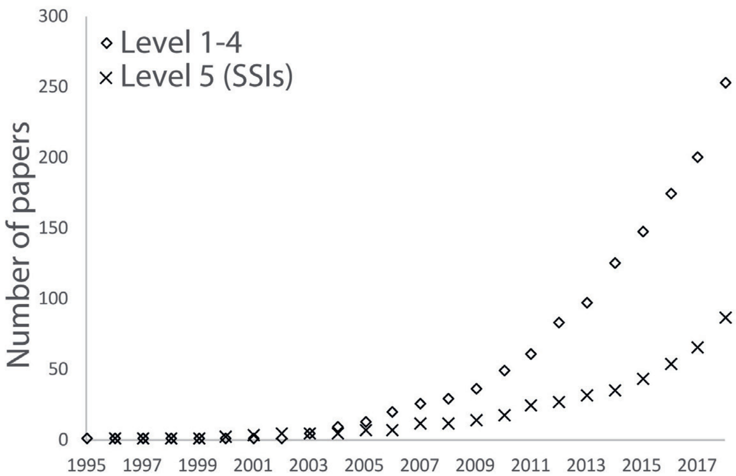

Figure 3 - Cumulative number of papers not using SSIs (Level 1-4) and cumulative number of papers using SSIs (Level 5). The number of papers using SSIs to evaluate industrial water use is growing more slowly.

Table 3 - Use of SSIs in relation to the number of methods from different categories used per paper.

Number of method categories	***Papers***	***Papers at level 5 (SSIs)***	***Percentage***
1	284	70	25%
2 or 3	56	17	30%
Overall performance	340	87	26%

In 56 papers, methods from two or three categories were combined. When methods are combined there is a higher use of SSIs (30%) compared to papers which use a single method (25%) (Table 3). The added value of combining methods from different categories is the largest for the LCA category, which increased from 16% to 33%. When MEFA and LCA are combined with each other SSIs use is the highest at 45%.

In Sections 4.2–4.6 we discuss the performance of papers in each OECD category, focusing on the methodological elements leading to the level of SSIs. In each section we first discuss the category in general, then we provide examples of papers which use SSIs and discuss why the indicators are considered SSIs. The example papers discussed in the following sections can serve as a starting point for future methodological development. Future methodological development can use the LCSP framework together with the examples provided to ensure SSIs level indicators are used or argue why indicators at the SSIs level are intentionally omitted.

4.2 Key Performance Indicators (KPIs)

KPIs were encountered in 84 papers and of those 23 papers used SSIs (28%). In 19 papers where KPIs were used, the level of SSIs was achieved without utilizing additional methods from other categories. Of the 16 papers where KPIs were combined with methods from other categories 4 used SSIs. The predominant performance of papers using KPIs is level 2 (45%, Facility Material Use and Performance indicators). KPIs generally focus on the performance and efficiency within the facility and therefore do not include the required environmental conditions outside the facility to assess system sustainability. Assessments at this level generally lead to efficiency gains instead of progress towards sustainable systems, as explained by Bakshi (2011).

Examples of KPIs at SSIs level:

Gaidajis and Angelakoglou (2016) provide a comprehensive set of indicators to assess the sustainability of industrial water use by linking water use to effects on the aquifers or water bodies from which water is taken. To meet the criteria of SSIs they combine performance indicators (withdrawal by source, m^3 $year^{-1}$) with concern indicators (aquifers/sources significantly affected by water withdrawal, water risk at national level) (Gaidajis and Angelakoglou, 2016). This approach creates effective threshold values for the indicators to be considered SSIs.

The Techno-Ecological Synergy (TES) method developed by Bakshi et al. (2015) evaluates the demand for any ecosystem service (e.g. water quality regulation or water provisioning service) against the supply of this service on each ecological scale. The TES method considers the demand site for resources to be a "black box" and evaluates whether flows in and out of the black box are in balance with the local environment. The system is considered sustainable when the renewable supply is larger than the demand at the investigated scale. The framework generates an indicator for any ecosystem service used by humans and relates the use of each service to the (renewable) availability over any spatial scale. The TES methodology was applied to evaluate and optimize a methanol transesterification process (Gopalakrishnan and Bakshi, 2018). The optimization process takes the carrying capacity of local ecosystems into account, and therefore accurately reflects the amount of economic activity which can be sustained for longer periods of time.

A modelling approach is taken by Xu et al. when optimizing water resource allocation in a coal chemical industrial park (Xu et al., 2018). They use the availability (including the uncertainty) of water resources provided by a river as a constraint to optimize water allocation. By setting the sustainable availability as a constraint the resulting optimal solution is in line with the local carrying capacity of water systems.

Aitken et al. evaluate the water use of the mining industry in Chile (Aitken et al., 2016) by relating water use to water scarcity. They calculate a water scarcity index (WSI) for a baseline scenario and in a scenario where environmental water requirements are included. Subsequently the impact of water use by mining on water scarcity are calculated. By relating the water use of individual industries to overall water availability the approach meets the criteria for SSIs. The use of WSI has also been promoted in relation to water use within the LCA community (see Section 4.6).

4.3 Composite Indices (CI)

In 14 of 41 cases (34%) the indicators used in the CI category matched SSIs criteria. Combining CI with methods from other categories occurred in 17 papers and resulted in SSIs in 4 papers (24%). CI perform better than KPIs because the focus shifts from individual processes within the system to a broader evaluation of the system.

Examples of CI at SSIs level:

Zaharia et al. used the Global Pollution Index method to evaluate the environmental impacts of economic activities in general (Zaharia, 2012) and of a specific product (Zaharia et al., 2010). The Global Pollution Index method relates the actual state of the environment, as influenced by human activities, to the ideal state of the environment. This method matches the criteria for SSIs, although quantification of environmental states is challenging and is very data intensive.

The Sustainable Process Index method was used in multiple cases: (1) by Narodoslawsky and Krotscheck (2000) to evaluate industrial production in general; (2) by Gwehenberger and Narodoslawsky (2007) to evaluate the sugar industry; and (3) by Moser (1996) to evaluate several industrial case studies (e.g. biological instead of chemical production, renewable instead of fossil based production). The Sustainable Process Index measures the land area required to sustainably produce a product or to perform any other activity. The unit of measurement is land area per year and is the sum of the land area required to create all inputs (e.g. raw material production, waste assimilation, or rainwater harvesting). This method is considered to use SSIs since the threshold value for this method is the amount of land area available.

The Water Security Sustainability evaluation is proposed by Nie et al. Their evaluation uses several indicators which relate water use to water availability (Nie et al., 2018). The combination of indicators used that meet the criteria for SSIs are: water resources vulnerability index, water resources demand-supply balance index, and water availability index.

4.4 Material and Energy Flow Analysis (MEFA)

MEFA methods were used in 85 papers, using SSIs in 36 (42%). This is the highest use of SSIs of the analyzed categories. MEFA is also the category with the highest growth rate of papers using SSIs. The underlying concepts of mass/energy balancing are suitable for SSIs because they can be used over any scale and can therefore be applied outside the immediate boundaries of the industrial system.

Within the MEFA category two sub-categories were identified: Water Footprint (WF) methods and energy flow analyses. WF methods require an inventory of the amount of water required for a product/service along the supply chain (Hoekstra et al., 2011b). These methods can reach the level of SSIs by quantifying the impact of human activities on the natural water cycle. Energy flow analysis converts water use into an energy requirement. For water use, this conversion is related to the amount of energy involved in the natural hydrological cycle (Bogardi et al., 2013) or the amount of energy required for desalination (Martínez et al., 2009). System sustainability is achieved when the energy embodied in water use is in balance with the availability of renewable energy.

Examples of Water Footprint (WF) at SSIs level:

WF methods were combined with spatial data by Li et al. (2018) to evaluate the water footprint of different sectors. The spatial data on water use is combined with spatial data on water scarcity (the water scarcity index). This method makes it possible to scale the assessment based on the availability and detail of spatial data. Additionally, the discharge of pollutants to water bodies (gray water footprint) is evaluated in relation to the availability of water which can assimilate pollutants. Method incorporating water scarcity with WF were also used by Huang et al. (2014) and Jeswani et al. (2015) to assess of the dairy industry.

Yeh et al. met the SSIs criteria by including the hydrological balance of water bodies as a threshold value when assessing water use for bioenergy (Yeh et al., 2011) with WF methods. The hydrological balance relates the total water renewably available in a watershed with the water used for human purposes.

Within the WF framework, the available water remaining (AWaRe) method has been developed. The AWaRe method provides an indication of the water remaining after the human and ecosystem demand has been met. This method is used by Norhtey et al. to evaluate water use in the mining industry (Northey et al., 2016; Northey et al., 2018). The AWaRe method is suitable for WF assessments but is also being adopted by the LCA community to generate more accurate assessments for the water use impact category (Boulay et al., 2015; Boulay et al., 2017).

Examples of Energy Flow Analysis at SSIs level:

De Meester et al. (2011) and Dewulf et al. (2007) evaluated human activities with the Cumulative Exergy Extraction from the Natural Environment (CEENE) method. Within the CEENE method water use is expressed in terms of the energy requirements to obtain this water. The CEENE method makes a distinction between renewable and non-renewable energy and can therefore evaluate system sustainability (Dewulf et al., 2007; Meester et al., 2011).

Emergy (*embodied* energy → emergy) accounting methods are a valuable tool to gain insights into the water-energy nexus (Sun and An, 2018). Sun and An evaluate industrial sectors in terms of their long term sustainability by comparing the renewable emergy input to the total emergy input of the sector. By including the renewable availability of emergy this method is considered to use SSIs. With appropriate system boundaries, emergy accounting methods can effectively incorporate the interaction between water use and energy use, leading to effective evaluations of the water-energy nexus.

4.5 Environmental Accounting

EA methods were used in 29 papers and used SSIs 6 times (24%). Despite the internal debates within EA research (explained in Section 3) the inclusion of SSIs is very close to the overall average (26%). EA was combined with methods from other categories 14 times but did not lead to increased use of SSIs. In two of the 14 combined papers (14%) SSIs were used.

Examples of Environmental Accounting at SSIs level:

Angelis-Dimakis et al. (2016) used the Total Value Added method to evaluate the environmental impacts of the textile dying industry. The Total Value Added method serves to assess different technological scenarios. The SSIs level is reached by relating "current freshwater use to the available freshwater resources" (Angelis-Dimakis et al., 2016).

Zarsky & Stanley (2013) utilize a "strong sustainability" (i.e. considering ecosystem services not to be substitutable (Pelenc et al., 2015)) framework to evaluate the net benefits of a mining project. The above concept is able to evaluate system sustainability because the net benefits of economic activity are related to “maintaining the resilience of essential natural life-support systems” on a local scale (Zarsky and Stanley, 2013).

The ‘environmental performance resource impact’ method proposed by Brent & Visser (2005) evaluates environmental impacts against monetary value added. This method allows manufacturers to assess the sustainability of suppliers. Meeting SSIs criteria (in the case of water use) is achieved by comparing water use to available reserves in terms of the "capacity of the natural environment to sustain further burdens". This approach yields threshold values for the maximum extraction of water resources in line with the carrying capacity of the environment (Brent and Visser, 2005).

4.6 Life Cycle Analysis

Life Cycle Analysis methods were used in 160 papers. The use of SSIs through LCA methods occurred in 25 papers (16%). In 13 out of 40 papers (33%) that combine LCA methods with methods from other categories SSIs were used. LCA is the only category in which the combination of methods increases the use of SSIs.

There are two main aspects within LCAs which can affect performance in terms of SSIs: (1) during the ‘goal and scope definition’ phase the ambition level of the research is defined and the choice to incorporate SSIs can be made, and (2) technical/data limitations in the Life Cycle Inventory and Life Cycle Impact Analysis phases (International Organization for Standardization, 2006) hampering SSIs use. The extensive experience within the LCA field, combined with data unavailability, can be the reason why level 4 indicators are used more often and SSI are intentionally used only on occasion. Often there is insufficient data to make a spatial differentiation for the impacts LCA attempts to measure (Potting and Hauschild, 2006). Within the LCA field there are long term efforts to address this issue (Bretz, 1998). In the face of data unavailability, it may be impossible to use/develop SSIs and to ensure the feasibility of a study. The ReCiPe (a LCA method) documentation states: “no models are available to express the damage [of water depletion] on the endpoint level” and uses a “midpoint indicator that simply expresses the total amount of water used” (Goedkoop et al., 2013). Bayart et al. (2010) propose that (1) the spatial information of withdrawal and discharge locations, (2) the quality of water flows, and (3) the type of water course from which water is withdrawn or discharged (e.g. wetland, aquifer, river, sea) should be included to evaluate water use through LCA methods. Other options are to incorporate the Water Scarcity Index into the water use impact category (Jolliet et al., 2018; Pfister et al., 2009), or relating water use to freshwater fish species extinction (Hanafiah et al., 2011). The increased availability and resolution of geographic data could be integrated with LCA methods to link impact categories with local conditions. This research shows that adoption of these improvements, which would allow for SSIs level assessments of water use, is still limited within the LCA methods used by industry.

Decision makers should be aware that LCA methods do not evaluate system sustainability by default. Until SSIs become predominant in LCA the consistency with which the category reaches level 4 can still be used to reduce environmental pressures. The added value of combining LCA methods with other categories is apparent, and should be further developed. Further research on LCA in the field of industrial water use should focus on (1) determining which data requirements are hampering incorporation of SSIs, and (2) raising the ambition level of assessments to evaluate system sustainability.

Examples of Life Cycle Analysis at SSIs level:

Lévová & Hauschild expanded LCA methods to account for spatial and temporal variations. The impact of textile industries on ecosystems was assessed through the ratio of water used against water availability after environmental water requirements were taken into account (Lévová and Hauschild, 2011). The inclusion of environmental water requirements allows for an evaluation of system sustainability. The approach of Lévová and Hauschild can be scaled to individual water catchments and thus allows for evaluation based on the local context.

Chiu et al. (2012) used LCA methods to assess the impact of water use for bioethanol production on the local environment by relating it to local precipitation. Precipitation can be considered an approximation for available renewable water resources (Sandra L. Postel et al., 1996), and provides the threshold value required to relate water use to the carrying capacity of the local environment (Chiu et al., 2012).

Arodudu et al. (2016) used LCA methods combined with MEFA methods to assess agro-bioenergy systems. Their method relates human resource utilization to what is retained or returned to nature (Arodudu et al., 2016). This procedure sets

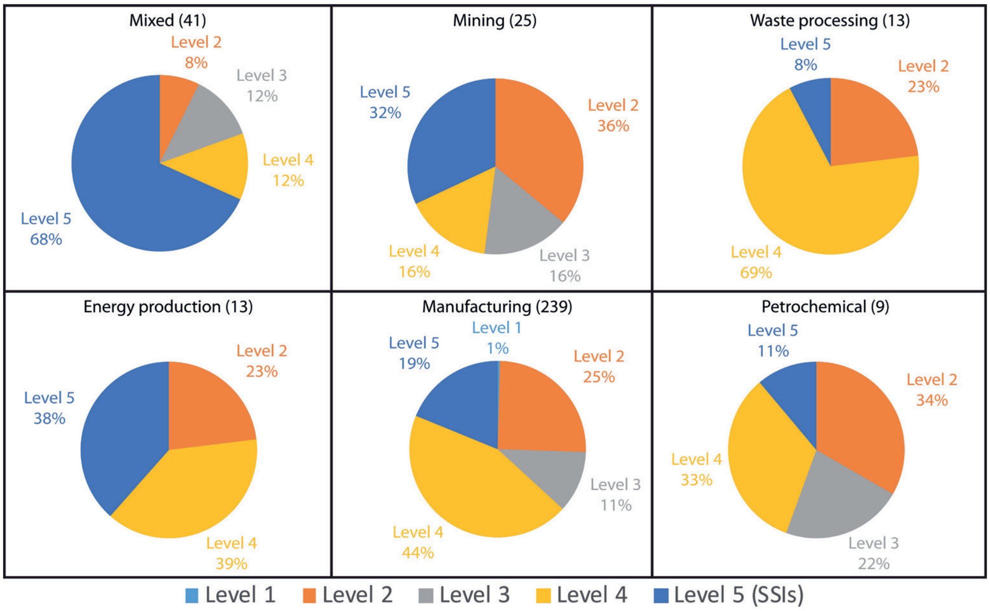

Figure 4 - Overall LCSP indicator performance per industrial sector. In papers evaluating multiple industries, the mixed category performs the best in terms of SSIs. The waste processing and petrochemical sector use the SSIs the least. The number between brackets shows the number of papers per industry.

effective threshold values which can be related to carrying capacity, and are therefore considered to be SSIs.

The overlap and interactions between methodology categories (KPI and LCI) can be seen in the work of Liu and Bakshi (2018). In this work LCA methods are combined with Techno-Ecological Synergy (TES, see Section 4.2) metrics to expand on the traditional impact categories used within LCA. This procedure adds the elements necessary to evaluate the sustainability of resource use on any scale and makes it possible to include the local characteristics of the region in which resources are used and/or emissions are discharged.

4.7 Industrial sectors and SSIs

The industrial sectors investigated in this research use SSIs to different extents (Figure 4)**.** The 'mixed' sector (where more than one industrial sector is evaluated within a single paper) is the only sector in which SSIs are used in the majority of studies (68%) compared to the other sectors (20%). This indicates that an active selection of SSIs is taking place. The holistic nature of assessments in the mixed sector steers for the selection of indicators exceeding the boundaries of a single

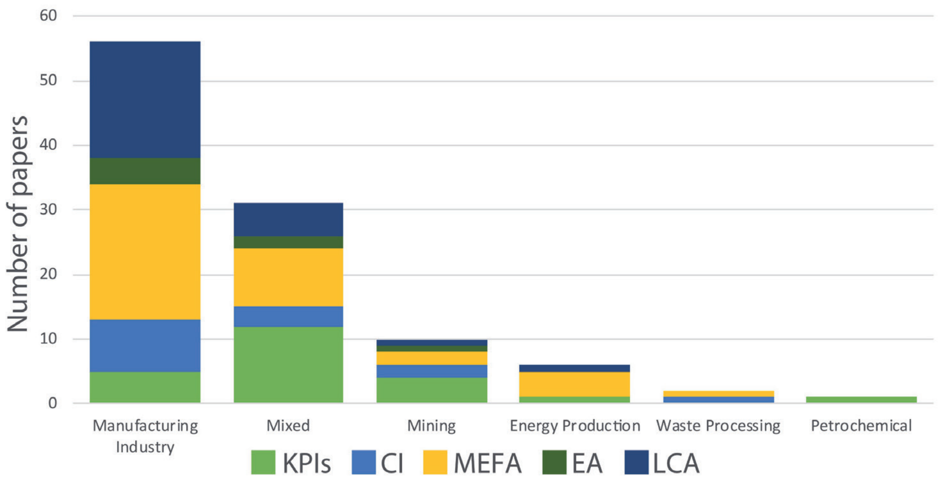

Figure 5 - Cumulative number of publications by category using SSIs level assessments per industrial sector.

company, automatically resulting in SSIs. The manufacturing industry sector uses LCA methodologies in 52% of the papers and subsequently uses level 4 indicators most often (44%). The use of level 2 indicators is most prevalent in the mining (36%) and petrochemical (34%) sectors (Figure 4) and is considerably higher than the overall use of level 2 indicators across all sectors (24%, Figure 4). The low frequency of SSIs level evaluations within the waste processing (8%) and petrochemical (11%) sectors is noteworthy but is possibly attributed to their limited prevalence in the analyzed papers. For the petrochemical industry the use of SSIs should be a high priority since this sector, at least in Europe, is the main water-using industry within the manufacturing sector (Eurostat, 2017). We suggest that further research is done to understand why the use of SSIs in assessment methods differs between industries. This understanding is needed to ensure efforts are aimed at the limiting factor for the use of SSIs. This prevents the possible situation where efforts are made to increase data availability when the limiting factor is a lack of awareness or interest to assess system sustainability. Additionally, the awareness concerning data availability can be different amongst sectors, leading to different choices for assessment methods.

Across industrial sectors the use of SSIs is attributed to different methodology categories (Figure 5). Within the manufacturing industry MEFA is used more often when reaching SSIs compared to the mixed sector. In the mixed sector most papers using SSIs do so through KPIs. The difference between these sectors is the possibility to standardize methods. The manufacturing sector can standardize methods associated with specific products, through MEFA or LCA methods, while the mixed sector needs KPIs made specifically for the for the diverse group of industries and products being assessed.

5 Conclusions

Using suitable assessment methods is needed to ensure that industrial water use remains within the carrying capacity of the local environment. Sustainable Systems Indicators (SSIs) are used in 26% of the reviewed scientific papers assessing the environmental sustainability of industrial water use. The number of papers which use SSIs has grown slower than the overall growth of papers assessing industrial water use. As a result the gap between assessments that use SSIs and do not use SSIs is increasing. In light of the projected changes in water availability, and the increasing water demand of industry, environmental assessments using SSIs is needed to create sustainable water systems (locally and globally).

Analysis of 340 scientific papers on industrial water use shows that the use of SSIs differs among assessment method categories: 28% for Key Performance Indicators, 34% for Composite Indices, 42% for Material and Energy Flow Analysis, 24% for Environmental Accounting, and 16% for Life Cycle Analysis. The use of SSIs is highest in the 'mixed' industry sector (68%) where assessment methods are designed to evaluate several industries and companies simultaneously. Evaluating several industries forces the adoption of assessment methods which extend beyond the boundaries of a single industry or facility. The mixed sector shows that deliberate selection of SSIs is possible and adoption of this practice would improve performance in other sectors.

SSIs are present in all methodological categories encountered in this research. Focusing on improving and increasing data availability for the existing assessment methods is therefore more beneficial than focusing on the development of new methods. Combining methods from different categories results in higher use of SSIs for the LCA (33%) category but shows no added value for the other categories. We suggest researchers take the criteria for SSIs into account when assessing the sustainability of industrial (water) resource use, and to take the methods already using SSIs as a starting point when improving existing or developing new methods.

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Supplementary Information

Supplementary Information 1 - Occurrence of methodologies and LCSP level achieved in reviewed papers (sorted by performance in terms of level 5). The total number of methods is larger than the number of included papers (340) because more than one method was used in several papers.

Methodology	Level 1	Level 2	Level 3	Level 4	Level 5
Life cycle impavct assessment		1	3	73	14
Emergy flow analysis					13
Life cycle assessment		7	7	82	9
Water footprint		3	1	15	7
Exergy analysis			1	1	6
Model based approach		2	1	1	5
Mass balance/flow analysis		3			4
Multi-criteria decision making		6	5	1	3
Set of separate indicators		21	5	4	3
Sustainable process index (SPI)					3
Global reporting initiative		1			2
Eco-efficiency		6	1	1	2
Global pollution index					2
Water impact index					2
Water scarcity index					2
Water evaluation and planning system (WEAP)					2
Water environment carrying capacity (WECC)					2
Techno-ecological synergy (TES)					2
Energy flow analysis		1			1
Sustainability assessment			1		1
Life cycle management (lcm)					1
Cost benefit analysis (cba)		1			1
Template for sustainable product development (TSPD)					1
Ecosystem services approach					1
Triple bottom line accounting			1		1
Ecological footprint					1
Environmental management system (EMS)		1			1
Water risk filter (WRF)					1

Aqueduct					1
India water tool (IWT)					1
Global water tool			1		1
Pollution prevention	1	1			1
Input-output		2		1	1
Wafmi					1
Industrial symbiosis					1
Peak water					1
Planetary boundaries					1
Triple value model (3V)					1
Aware					1
Water and energy use indicator (WEUI)					1
Finn's cycling index					1
Water ecotoxicity footprint (WEF)					1
Carec					1
Environmental sustainability assessment (ESA)				1	
Environmental impact assessment				1	
Iso 14001 environmental management strategy (EMS)		1			
Green productivity			1		
Hierarchical system model (HSM)				1	
Pinch analysis		4		1	
Material flow assessment/analysis		4		1	
Fuzzy expert system/logic			1		
Principal component analysis				1	
Cleaner production concept		6	2		
Eco-design		1		1	
Circular economy		1			
Eco-effectiveness		1			
Life cycle inventory		2		3	
Green degree			1		
Icheme			1		
Green metrics				1	
Best available techniques (bat)		2	3	1	
Eco-industrial approach		1			
Zero discharge		1	1		
Industrial ecosystem approach		1			
Ecological sustainability index (ESI)				1	
Material input per service unit (MIPS)		2			
Industrial sustainability index			1		

Natural step			1		
Data envelopment analysis (DAE)		2		2	
Environmental performance indicator (EPI)		1			
Environmental performance evaluation (EPE)		1			
Dpsir			1		
Doughnut model			1		
Water accounting framework		1	1		
Ipieca tool			1		
Environmental life cycle costing				1	
Water-energy-food-climate nexus index				1	
Lean manufacturing		1			
Palm oil mill sustainability index (POMSI)		1			
Vikor-qualiflex		1			
Water meta-cycle model		1			
Life cycle cost analysis				2	

Chapter 3

Water supply network model for sustainable industrial resource use

A case study of Zeeuws-Vlaanderen in the Netherlands

Abstract

Matching the regional water supply and demand can be improved by allocating local renewable water resources through decentralized water supply networks (WSNs). The feasibility of decentralized WSNs depends on the costs for the required pipeline infrastructure. The lowest cost for pipeline infrastructure depends on the local landscape characteristics. We present a model that designs decentralized WSNs to supply water with regional supply sources. The objective of the model is to include the effects of landscape characteristics on infrastructure costs and to minimize overall WSN costs. We tested the model on a case study in the fresh-water scarce region of Zeeuws-Vlaanderen in the southwestern part of the Netherlands with known (hydro)geological, geographical and climate data. The model was tested to supply a large industrial water user with groundwater resources operated within sustainable yields. The generated WSNs cover a demand between 0.5 and 5.5 million m^3 $year^{-1}$. Between 1 and 12 supply locations are needed to cover the demand. The pipeline infrastructure needed ranges from 25.1 to 114.5 km. The model determines the optimal pipeline route, the amount of water flowing over each pipeline segment, and reveals if a small increase in demand causes a relatively large increase in costs. The results can be used to determine if water transport is preferred over other options, such as wastewater re-use or desalination of saline water resources.

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1 Introduction

Many industrial processes are dependent on the availability of water; in some cases for the product itself, but often mainly for the production process. Industries largely rely on centralized water supply systems due to the general policy in the twentieth century to create large-scale infrastructure projects (Gleick, 2003). Relying on large-scale centralized systems introduces uncertainty in water supply due to the rising costs and changing availability of water resources (Schewe et al., 2014; United Nations Development Programme, 2006; World Water Assessment Programme, 2009). Projections show that rainfall patterns will change around the globe (Dore, 2005; Kitoh and Endo, 2016), that the quality of water may severely diminish due to salt water intrusion in coastal areas (Webb and Howard, 2011), and that human alterations to watersheds affect the quantity and or quality of the available water resources (Peters and Meybeck, 2000). Groundwater resources are often used in an unsustainable way, depleting water supplies and possibly leading to land subsidence and/or enhancing salt water intrusion (Foster and Chilton, 2003). New approaches are needed to use the available water resources in a sustainable way (Hoekstra, 2014, 2015; Nobel and Allen, 2000). Many efforts within industry, a sector accounting for 19% of global water withdrawals (Food and Agriculture Organization of the United Nations), focus on reducing the water demand by increasing the process efficiency and by reusing or recycling water (Klemeš, 2012). While these efforts are certainly needed, the remaining demand still needs to be supplied by extracting water from natural systems.

Alternative local sources of water, such as wastewater, harvested rainwater, surface water, and groundwater can be used to reduce dependency on remote centralized sources. The use of decentralized water supply systems is an option to alleviate future water scarcity and deal with increasing infrastructure costs (Leflaive, 2009). The use of decentralized networks provide flexibility to adjust water quality to needs of the user (Leflaive, 2009) and has the potential to increase resilience when supply is diversified (Gonzales and Ajami, 2017). A comprehensive overview of water supply network design and optimization methods was created by Mala-Jetmarova (Mala-Jetmarova et al., 2017).

Irrespective of the form of distribution, central or decentral, local extractions need to adhere to the sustainable yield of the water resource, avoid subsidence due to groundwater extraction, and prevent enhancement of salt water intrusion. The use of methods to assess all these aspects for the overall sustainability of industrial water use is currently still limited, but is needed to ensure water use remains within the limits of local water systems (Willet et al., 2019). The appropriate design and evaluation of a water supply network (WSN) based on many small scale water resources requires a model based approach. Several models exist that can be used to evaluate the regional supply and demand of conventional and alternative water resources such as: (a) the Water Evaluation And Planning System (WEAP), which can be used to evaluate water management scenarios based on a water balance accounting principle (Sieber and Purkey, 2015), (b) the WaterCress model, which simulates the quantities and qualities of water flowing through a catchment area at equal continuous time-steps (Clark and Cresswell, 2011), (c) the RIBASIM model which links hydrological conditions with the specific water users in the basin (van der Krogt), (d) or the model developed by Nobel and Allen which matches and optimizes the water reuse possibilities between industries based on their location (Nobel and Allen, 2000). These models are useful to evaluate and optimize the water supply and demand system when the water transport infrastructure is already present and the water resources to be used are defined. A modelling approach which can select the optimal configuration of supply locations, based on a WSN for which the transport infrastructure does not yet exist, was still lacking. Such a model can assist in a transition towards regional water self-sufficiency based on local renewable water sources.

A transition towards the use of local water resources requires an evaluation of the optimal network for water transport. Transporting large quantities of water usually occurs through pipelines. Pipeline construction costs depend on the local conditions and landscape features, such as land use, slope, required excavation depth, and subsurface soil type (Chee et al., 2018; Hoekstra, 2014). The objective of the model we present is to generate the lowest cost WSN based on the local landscape characteristics and the available renewable water resources. We combined geographic information system (GIS) methods, graph theory (Foulds, 1992), and mixed integer quadratic programming. The GIS methods were used to include the influence of landscape characteristics on pipeline construction costs. Graph theory was used to model the relationships between objects (Foulds, 1992; Gross and Yellen, 2006). The supply and demand locations in our model represent the objects and are referred to as nodes. The pipeline connections are the relationships between nodes and are referred to as edges. Mixed integer quadratic programming was then used to find the configuration of nodes and edges that leads to the lowest cost WSN.

In this paper, we present a modelling approach which generates the lowest cost WSN for a specific demand based on known supply locations in a region. We tested the approach on a case study in Zeeuws-Vlaanderen, in the southwestern part of the Netherlands.

2 Case study description

The was tested to generate a WSN for an industrial site in Zeeuws-Vlaanderen, the Netherlands. The current fresh water supply for the site is dependent on transport of water from outside this coastal, fresh water scarce, region. Most of the surface area of the region (733 km^2) is used for agriculture. Local fresh groundwater sources are hosted within a lithologically heterogeneous aquifer and positioned on top of deeper, more saline groundwater. In this case study, we consider a maximum chloride concentration of 1500 mg Cl^-/l as a limit for use in industry, based on an accepted classification of a fresh-saline interface (Stuyfzand, 1986). The fresh-saline groundwater distribution in the area was mapped in 2015 (Delsman et al., 2018). Calculated groundwater extractions should not cause the so-called upconing of the fresh-saline groundwater 1500 mg Cl^-/l interface in the deeper subsoil to avoid possible negative consequences for other water users (e.g. famers) in the area. We tested the model to generate a WSN with the available fresh groundwater resources in the region operated at sustainable yields. The current water supply of the industrial site is covered by importing 3 million m^3 $year^{-1}$ from outside the region. We investigate the possibility to supply between 0.5 and 5.5 million m^3 $year^{-1}$ of water with groundwater resources in the region.

3 Methodology

Transport networks, including WSNs, and their optimization have been thoroughly studied within operations research field (Mala-Jetmarova et al., 2017). A water transport network can be represented as nodes and edges (Di Nardo et al., 2014; Price and Ostfeld, 2014). The nodes represent the water demand or supply locations, and the edges represent the pipeline connections (with associated costs) between nodes. Graph theory optimization procedures can then be used to optimize the network (Sicuro, 2017). The presented model converts regional

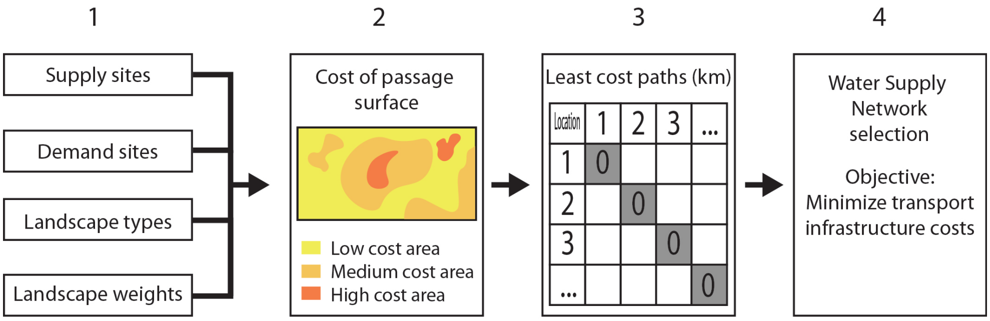


Figure 1 - Model steps to generate the water supply network with the lowest cost.

spatial data into a node and edge network, generates the lowest cost WSN based on the water demand of the user, and visualizes the result.

The model has four main steps (Figure 1): (1) Input data generation, (2) Cost of passage surface creation, (3) Least cost path determination, and (4) Water Supply Network selection.

3.1 Input data

The first step of the model compiles and generates the data required for step 2–4. In this section the components to generate the input data are described: the supply and demand sites with respect to water quantities and qualities, the landscape types and associated weights to determine the route of the pipeline infrastructure.

Supply sites: to generate a decentralized WSN, possible sources of water need to be identified. The supply site input data are the coordinates, and the amount of water which the wells can supply sustainably (m^3 $year^{-1}$).

Criteria such as the natural recharge of an aquifer (Maimone, 2004), the environmental flow requirements of an area (Poff et al., 2010), or the overall sustainable water footprint of a river basin (Hoekstra et al., 2012) can be used to determine the sustainable yield for water extractions. For this case study fresh groundwater sources in the Zeeuws-Vlaanderen region were modelled. A maximum drawdown of 50 mm (Oude Essink and Pauw, 2018) of the phreatic groundwater level (the change in water level at the extraction wells relative to the initial situation) was set as the boundary condition for the allowed extraction rate. In Zeeuws-Vlaanderen brackish and saline groundwater is present below fresh groundwater, therefore saline groundwater upconing can occur as a result of lowering the piezometric heads due to extraction and saline groundwater flowing to the extraction well. Extractions are dimensioned in such a way that the position of the 1500 mg Cl^-/l interface between the fresh groundwater above and the brackish groundwater below should not move into the groundwater extraction well (Delsman et al., 2018; Van Baaren et al., 2016)

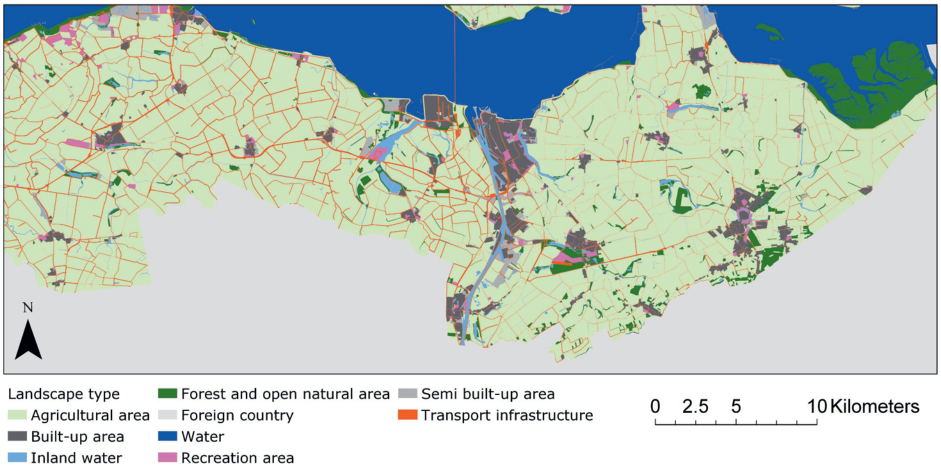
An available 3D variable-density groundwater flow model coupled with a salt transport model (Van Baaren et al., 2016) was used to provide the necessary data on hydraulic conductivities (Stafleu et al., 2011) and the groundwater salinity distribution expressed as mg Cl^- up to a depth of ~140m below mean sea-level (MSL) (Delsman et al., 2018; Van Baaren et al., 2016). The 100 x 100m resolution model uses the MODFLOW (Michael G. McDonald and Arlen W. Harbaugh, 1988) based computer code MOCDENS3D (Bakshi, 2011; Zacharias et al., 2003) and consists of 40 model layers to reproduce the movement of groundwater salinity in the vertical direction accurately enough. Stresses in the model on the groundwater system includes six different surface water types (sea and estuarine waters, lakes, canals, (small) rivers, water courses up to ditches), seasonal natural groundwater recharge from the National Hydrological Instrument (Lange et al., 2014), a shallow drainage system, and existing groundwater extraction wells. The surface water and drainage systems (seasonal water level, and with a certain resistance to the groundwater system) are inserted into the model using an accurate Digital Elevation Model ('Actueel Hoogtebestand Nederland' (AHN, (Actuel Hoogtebestand Nederland, 2020)), resolution 5 x 5m); boundary conditions (in the sea and at the hinterland) complete the model (Van Baaren et al., 2016). To obtain an estimate of fresh groundwater availability, the depth of the fresh-saline groundwater 1500 mg Cl^-/l interface was determined for the study area. The resulting interface served as an initial estimate of the potential availability of fresh groundwater locations. As the movement of groundwater is a dynamic process, sustainability constraints need to be placed on extraction rates. Determining the extraction locations and associated rates was done in two steps: (1) obtaining an initial selection of extraction coordinates based on the hydraulic properties of the subsoil (Stafleu et al., 2011) in combination with an analytical formula which estimates the maximal extraction without upconing of the fresh-saline groundwater 1500 mg Cl^-/l interface into the extraction well (Dagan and Bear, 1968), and (2) calculating the phreatic groundwater level drawdown for given extraction rates based on the super-positional effect of the extraction well clusters. The drawdown is based on hydrogeological parameters of a semi-confined groundwater system and the extraction rates (calculated with the so-called Formula of De Glee) of the wells (Bruggeman, 1999).

Upconing of saline groundwater can be approximated using analytical methods such as discussed in (1964; Dagan and Bear, 1968; Schmork and Mercado, 1969), where a *critical rise* of the interface can be calculated. The maximum sustainable extraction rate for the case study is set to the rate before saline groundwater will experience an abrupt rise towards the well screen. This rise is given by the model of Bear and Dagan (1964), and was calculated using fresh-saline groundwater interface depths, resulting in maximum extraction rates (*Qmax*) in m^3 day^{-1} per grid cell (see Supplementary Information 1). Cells with extractions that are too small (*Qmax* < 500 m^3 day^{-1}) were removed. The remaining locations were extracted as points and finally grouped into clusters with extraction wells 100 meter apart. This step serves as an initial selection but does not yet consider the summed (superposed) effect of clustered extraction wells on the overall drawdown of the phreatic groundwater level.

Saline groundwater upconing is related to drawdown, therefore the latter was also quantified using an analytical method in a second step. Pumping rates were optimized for minimal summed drawdown and maximum extraction rates considering interference, the summed effect, of neighboring extraction wells. The outcome allows the user to quantify the fresh groundwater extractable in m^3 $year^{-1}$ for a given maximum drawdown.

The relationship between the maximum accepted drawdown and the maximum extraction rate is linear; reducing the maximum accepted drawdown by half yields half the extraction rate (see Supplementary Information 1). Through this property the effect of altering the accepted drawdown, as a possible sustainability criteria, on the optimal WSN can be explored. This analytical approach provides a first estimate of the sustainable yield at a specified groundwater drawdown. The presented approach can be expanded with additional criteria to ensure overall sustainability of the groundwater system (Loáiciga, 2002; M. Sophocleous, 1997, 2000).

Demand sites: the spatial location (coordinates) of the demand site(s) and their demand (m^3 $year^{-1}$) for a specified quality of water. For the case study in Zeeland a single industrial user is used as the demand location. The demand quality is set



to a maximum of 1500 mg Cl^-/l. The model was built to accept multiple demand sites.

Landscape types: The type of landscape and land use influence the costs of placing pipeline infrastructure (Feldman et al., 1995; Marcoulaki et al., 2012). We use a landscape type map of the study area to find the pipeline routes with the lowest cost (Figure 2). The landscape types used in this work correspond to publicly available data for the Netherlands (Centraal Bureau voor de Statistiek, 2012).

Landscape weights: To determine the pipeline routes with the lowest cost, the different landscape types were weighted to reflect the cost of placing pipeline infrastructure within them. The weights assigned to the landscape types reflect the relative differences in costs between the landscape types. For example, the costs associated with placing pipeline infrastructure in a built-up area are high relative to an agricultural area. The list of included landscape types can be expanded based on data availability and importance of specific landscape types in a region (e.g. industrial areas or groundwater extraction areas).

3.2 Cost of passage surface

The lowest cost for a pipeline between two locations does not necessarily correspond to a straight line (Feldman et al., 1995). Feldman et al. (Feldman et al., 1995) showed that the use of spatial data in the form of a cost of passage

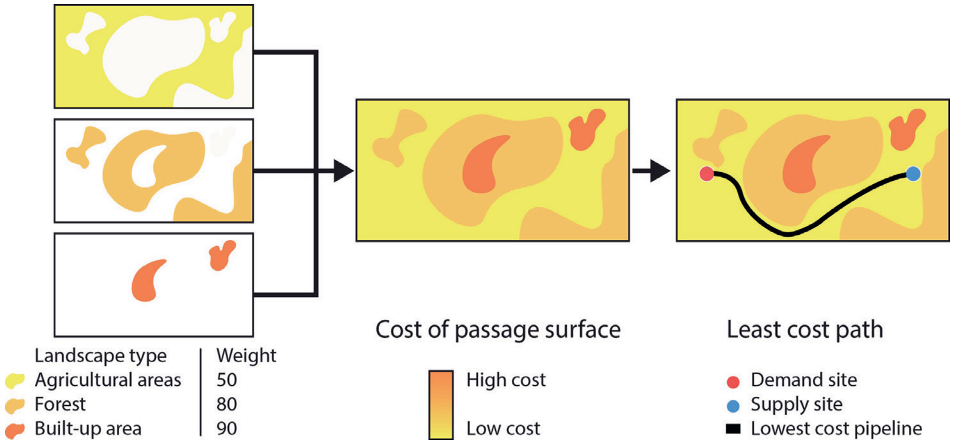


Figure 3 - Procedure showing the combination of landscape types into a cost of passage surface and into the least cost path between the water supply and demand location. Due to the different costs to place pipeline infrastructure in each landscape type, the least cost pipeline is not a straight line, but avoids the forest and built-up areas.

surface based on land use can reduce pipeline construction costs by 14%; even when the total length of pipeline increases by 21% as a consequence.

A cost of passage surface is a raster in which each cell value represents the costs of traversing that cell and can be based on any type of costs. For the case study the costs refer to the placement of pipeline infrastructure. In this paper the weights assigned to each of the landscape types (Figure 2) were combined and overlaid using GIS software to create the general cost of passage surface for pipeline infrastructure in the area. The cost of passage surface is the input data to determine the least cost path, the route with the lowest total cost to connect two locations, in this case with pipeline infrastructure (Atkinson et al., 2005; Collischonn and Pilar, 2000; Douglas, 1994).

3.3 Least cost paths

Based on the general cost of passage surface the lowest cost route for a pipeline between two locations was calculated (Figure 3). The least cost path between two locations is the shortest route between two locations according to the metric used in the cost of passage surface (Berry, 1987). Least cost path methods have been widely used for infrastructure routing (Bagli et al., 2011; Collischonn and Pilar, 2000; Douglas, 1994). To create a least cost path the cost of passage surface was converted into an accumulated cost surface for each location. The accumulated cost surfaces were then used to trace the lowest cost route between a departure and destination location (Atkinson et al., 2005). The weighting procedure (section

3.1) allows users to consider criteria with different metrics (e.g. construction costs, slope, distance to protected areas) and to have all criteria be reflected in the final least cost path (Stucky, 1998).

The steps shown in Figure 3 describe the procedure to determine the least cost path between a set of two locations. To generate the WSN with the lowest cost, an overview of all possible connections between all the demand and supply locations is needed. For each demand or supply location the least cost paths to all other locations were calculated. The resulting least cost paths, for all possible combinations of locations, were overlaid and combined into a single least cost network.

When creating the network a node was added at each location where pipelines intersect. The added nodes serve as transport hubs where flows can merge, but do not affect the overall water balance in the network. The model considers the merging of flows by calculating the required pipeline capacity, and associated costs, before and after the transport hubs. Hubs are represented by their location (coordinates) but have a demand and supply of zero.

The above procedure results in a $|V|$ *x* $|V|$ (where *V* is the set of all locations or nodes) adjacency matrix as shown in Step 3 of Figure 1. The values in the matrix represent the length (kilometers) of the lowest cost pipeline route between each starting location (*i*) and destination location (*j*). The diagonal zeros represent the fact that the distance from each location to itself is zero.

3.4 Water Supply Network selection

The mathematical representation of the optimization problem in this work is a variation of the *fixed charge network flow problem*, which is used to model many practical problems in the areas of transportation and distribution (Kim and Pardalos, 1999). The problem is characterized by the set-up costs, a fixed charge, that is incurred when an activity is performed (Balinski, 1961; Hirsch and Dantzig, 1968). For pipeline construction the fixed charges are the costs that need to be made irrespective of the size of the pipe being placed. We used a mixed integer quadratic programming (MIQP) method to solve the optimization problem and to generate the optimal WSN (Hirsch and Dantzig, 1968). The system is represented by a graph $G(V,E)$ with nodes V and edges E. The supply and demand locations are the nodes and the possible transport pipelines the edges. The set of edges

E is the result of Section 3.3. Each edge (i,j) in E, where i is the source and j is the destination, is described according to the following parameters:

- Flow $(x_{i,j})$: the amount of water being transported over the edge.
- Maximum capacity $(u_{i,j})$: the maximum amount of water which can be transported over an edge. Since the WSN is not yet built, the maximum capacity is not yet defined. This parameter makes it possible to generate WSNs incorporating (parts) of existing pipeline infrastructure.
- Fixed costs $(f_{i,j})$: the fixed costs which will be incurred to place the pipeline, irrespective of the amount of water transported.
- Cost per unit flow $(c_{i,j})$: the cost to increase the capacity of a pipeline according to the amount of water which needs to be transported.
- On/off $(y_{i,j})$: binary variable with value 1 if the pipeline connection is used, or 0 the pipeline connection is not used.
- Water demand/supply (s_i): the water demand (negative value) or supplied (positive value) to the network at each node. Transport hubs have a demand and supply of zero.

Each node has an associated water supply or water demand s_i in the network. For locations that supply water $s_i > 0$, for transport hubs that do not provide or consume water $s_i = 0$, and for water users that extract water from the network $s_i < 0$.

The costs per unit flow $(c_{i,j})$ are based on the length of the pipeline section (i,j), the result of the least cost path analysis, and the pipeline diameter required to achieve a suitable flow speed. The suitable range for flow speed, while considering a 1.5 factor for peak demands, was set between 0.5 m s^{-1} and 1.5 m s^{-1}. The fixed costs $(f_{i,j})$ are also based on the length of the associated pipeline section but are not dependent on the water flow. The capacity dependent pipeline placement costs used in the model were 0.5 € mm^{-1} diameter m^{-1}. The relation between accepted flow velocity and available pipeline diameters, generally available in increments of 100 mm, yield a stepwise behavior in terms of costs against flow (Supplementary Information 2). We approximate the stepwise behavior with a quadratic function from which the constants serve to establish the objective function for the network selection procedure according to

$$\text{minimize} \qquad TPPC = \sum_{(i,j)\in E} c_{\alpha,ij} \cdot {x_{ij}}^2 + \sum_{(i,j)\in E} c_{\beta,ij} \cdot x_{ij} + \sum_{(i,j)\in E} f_{ij} \cdot y_{ij} \qquad (1)$$

$$\text{where} \qquad c_{\alpha,ij} = \alpha \cdot L_{ij} \qquad (2)$$

$$\text{where} \qquad c_{\beta,ij} = \beta \cdot L_{ij} \qquad (3)$$

$$\text{where} \qquad f_{ij} = \varepsilon \cdot L_{ij} \qquad (4)$$

where $TPPC$ is the total pipeline placement cost for the WSN based on the adequate diameter to accommodate the required flow over each edge and L is the length of the pipeline (km) between nodes i,j generated through the least cost path analysis. The coefficients α,β and ε are the constants derived from the quadratic relationship between flow and pipeline placement costs (Supplementary Information 2). The optimization problem can be characterized as a Mixed Integer Quadratic Program due to the quadratic term in the objective function. The left and middle terms represent the sum of the costs per unit flow over each edge. The right term is the sum of the fixed costs for all the edges used. If an edge is not used there are no costs, fixed or per unit flow, associated with that edge.

The constraints of the optimization model are given by Equations (5)–(7). The first constraint ensures that the sum of the flows out of any node (left term) is smaller or equal to the sum of the flows entering the node (middle term) and the supply (right term) at the node, Equation (2) applies to every node i in the set of nodes V

$$\sum_{(i,j)\in E} x_{ij} - \sum_{(j,i)\in E} x_{ji} \le s_i \qquad \forall i \in V \qquad (5)$$

The second constraint ensures that if an edge is used, the flow should be larger or equal to zero, while at the same time it should be smaller or equal to the maximum capacity of the edge (Equation (6)). Existing pipeline infrastructure has a maximum capacity which can be incorporated in the model through parameter $u_{i,j}$. The model returns the flow over each pipeline, and therefore the capacity which needs to be installed. This constraint only applies to edges in use but is evaluated for every edge i,j in the set of edges E

$$0 \leq x_{ij} \leq u_{ij} \cdot y_{ij} \qquad \forall (i,j) \in E \qquad (6)$$

The variable y_{ij} denotes whether an edge is used or not and can take the value 0 (not in use) or 1 (in use) (Equation (7)). If the edge is used the fixed costs to place the pipeline are incurred. This variable is also evaluated for every edge i,j in the set of edges E

$$y_{ij} \in \{0,1\} \qquad \forall (i,j) \in E \qquad (7)$$

The output of the optimization yields the edgelist of the lowest cost WSN, the amount of water to be transported over each edge, and the capacity at which the supply locations should be operated.

The (MIQP) was implemented in Python and solved with the Gurobi Optimization solver.

4 Results: Zeeuws-Vlaanderen case

4.1 Regional water supply: fresh groundwater sources

The extraction location selection procedure yielded about 2000 extraction well locations from which fresh groundwater could be extracted. The possible extraction wells were grouped into 25 clusters in which individual extraction wells are at least 100m apart. Clusters close to the coastlines are dune type geological formations capturing and storing fresh rainwater. The optimized clusters including the individual extraction wells are shown in Figure 4.

The total amount of water which can be extracted from the 25 clusters, when limiting head drawdown to 50 mm, is 7.6 million m^3 year^{-1}. The spatial center of each cluster is used to generate the WSN.

4.2 Least cost pipeline network

The construction of pipeline infrastructure is preferred in areas where the construction costs are the lowest. Table 1 shows the weighted costs for pipeline infrastructure construction used in this work. The weights assigned to the different

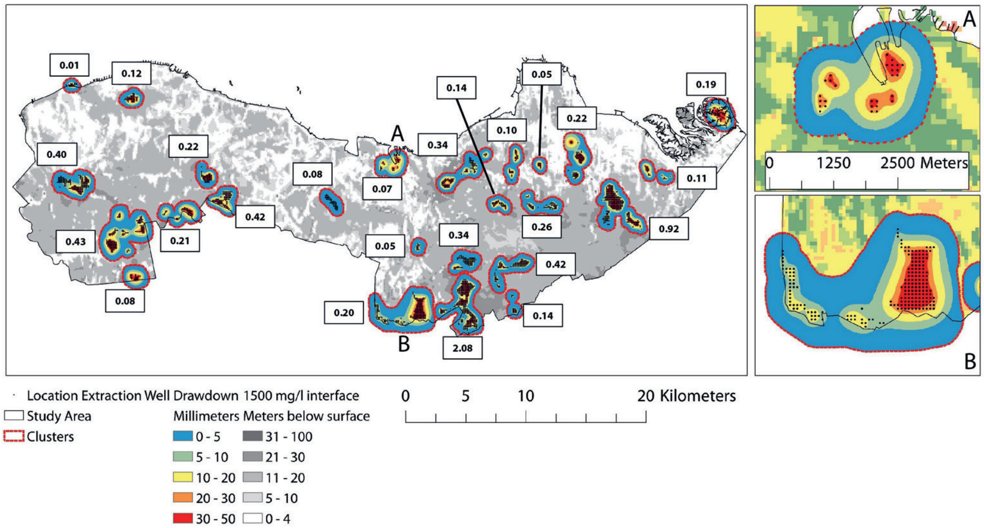


Figure 4 - Supply locations and available water supply (million m^3 year^{-1}) at optimized extraction rates when constraining maximum head drawdown to 50 mm.

categories were determined in consultation with water supply experts. A distinction was made between crossing a road or waterway as opposed to building parallel to these landscape types. The zones parallel to transport infrastructure are relatively suitable to place

pipeline infrastructure because other uses for these areas are limited. Crossing transport infrastructure should be avoided to reduce costs. In this work, we reduced the costs of pipeline infrastructure parallel to transport infrastructure by 70% compared to the original landscape type traversed.

Figure 5-A shows the combined cost of passage surface based on the landscape cost weights to place pipeline infrastructure. The areas with the lowest cost are agricultural areas along existing transport infrastructure. The original weighted cost for agricultural areas was 50 (Table 1), which is reduced by 70% in the zones parallel to existing infrastructure to yield the lowest final weighted cost of 15.

Generation of the least cost paths for all possible connections between the water supply and demand locations yielded a preliminary network with 408 edges (Figure 5-B). The preliminary number of edges did not yet account for the possibility to transport water in both directions. To include the possibility to transport water in both directions the original edges were copied and the start and

Chapter 3

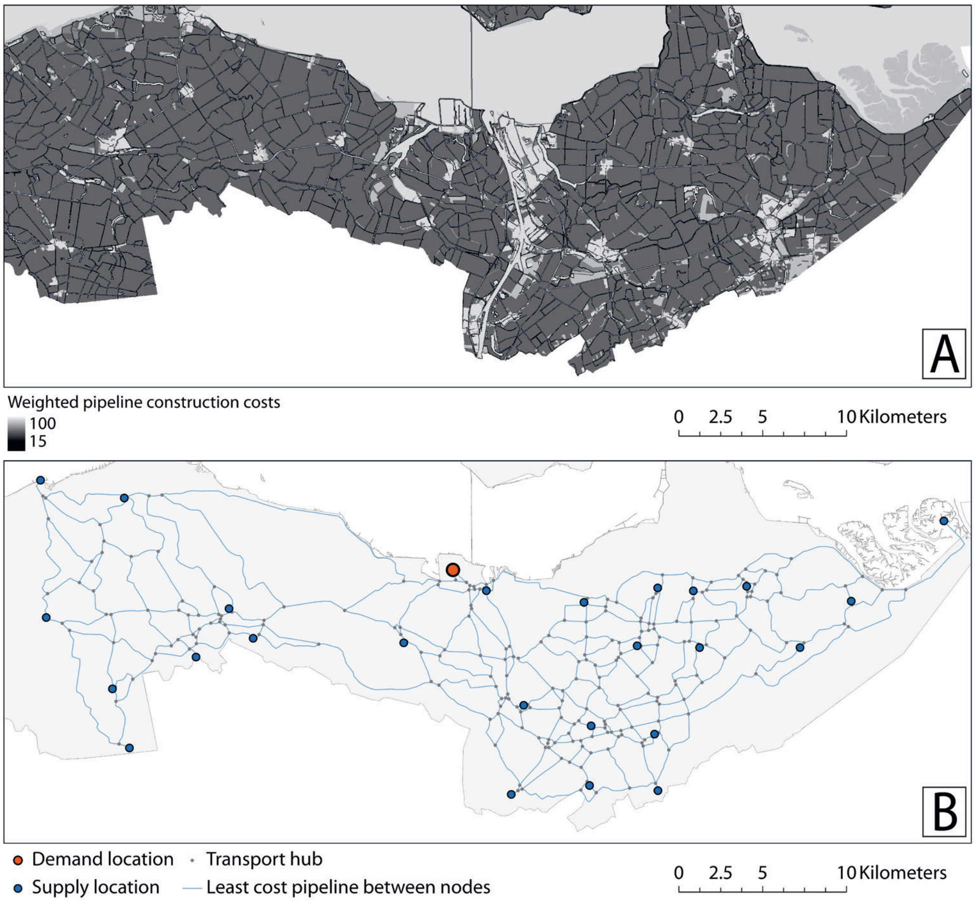


Figure 5 - Cost of passage surface with weighted costs to place pipeline infrastructure (A), lowest cost pipeline network connecting all possible pairs of supply and demand locations (B).

end points were inverted. The result is an adjacency matrix (not shown) with 816 (2 × 408) values.

The total number of nodes in the network is 269, of which 25 are the supply locations (Figure 5-B), 1 is the demand location, and 243 are transport hubs. The complete network has a total length of 1796 km, passing through different landscape types namely 21% agricultural, 1% built-up, and 1% forest and open natural areas. The remainder (76%) falls within the parallel zone alongside existing transport infrastructure or waterways. The length of pipeline traversing each landscape type is a reflection of the weights assigned to each type (Table 1). Assigning equal weights to each one would result in (unrealistic) straight lines between nodes.

Table 1 - Relative cost weight for pipeline construction.

Landscape feature	***Cost weight 1-100***
Agricultural areas	50
Built-up area	90
Inland water (crossing)	90
Forest and open natural area	80
Foreign country	100
Water (crossing)	90
Recreation area	60
Semi built-up area	80
Transport infrastructure (crossing)	75

4.3 Lowest cost water supply network

The model creates the lowest cost WSN specific to the demand of the user and the available water supply (Figure 6). Pipeline diameter and flow velocity are shown in Supplementary Information 3 and Supplementary Information 4.

We discuss the WSNs *I–VII* of Figure 6 in order of increasing demand below:

I. The optimal WSN to supply the starting demand of 0.5 million m^3 $year^{-1}$ uses three supply locations and is 25.1 km long.

II. The WSN configuration changes considerably because the supply locations of I, while being closer, cannot cover the demand of 0.6 million m^3 $year^{-1}$. The optimal WSN uses the most southern supply location as the single supply source.

III. Demand reaches 2.1 million m^3 $year^{-1}$, exceeding the 2.08 million m^3 $year^{-1}$ available at the most southern location. A small supply location close to the existing route is added to the WSN to cover the demand. The inclusion of the small supply location reduces the capacity at which the southern supply locations is operated, and reduces the diameter of the pipeline up to the point where the pipelines merge.

IV. The optimal WSN shifts to the east to include a supply location with more water to cover the demand. The inclusion of this new location reduces the capacity at which the southern well is operated from 2.05 (in *III*) to 1.8 million m^3 $year^{-1}$.

V. The optimal WSN still includes the most southern supply location but now also includes the second largest supply location in the area with a supply of 0.92 million m^3 $year^{-1}$. The second largest supply location

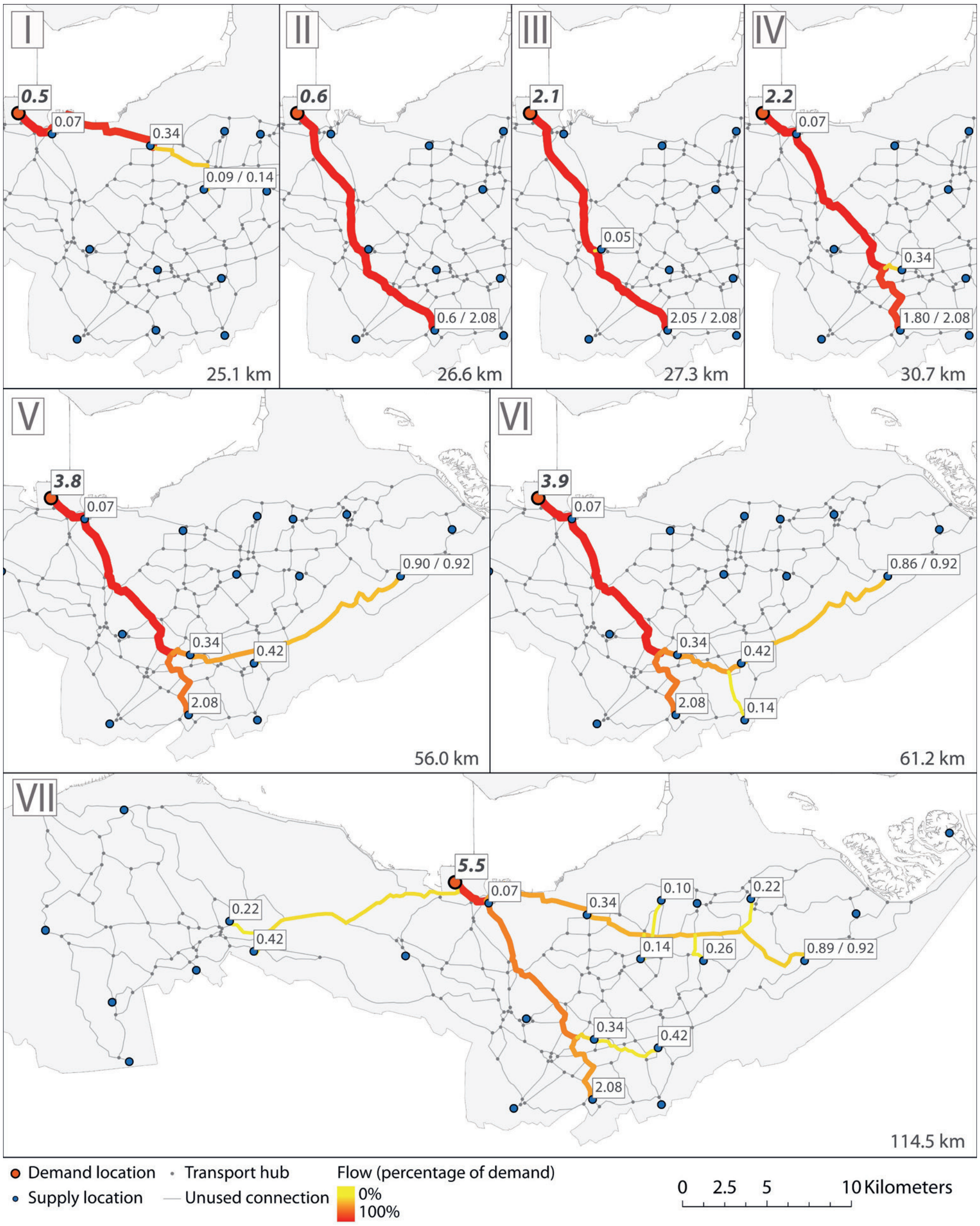


Figure 6 - Optimal WSN for a demand of 0.5 (I) 0.7 (II), 2.1 (III), 2.2 (IV), 3.8 (V), 3.9 (VI), and 5.5 (VII) million m^3 year^{-1} and a maximum accepted drawdown of 0.50 m at each supply location. The labels show the amount of water supplied by each well. Labels with two values indicate that a well is operated below maximum capacity (water supplied / maximum capacity). Labels in bold indicate the demand location. The value in the bottom right corner of each frame indicates the total pipeline length for the WSN.

is operated at 98% capacity (0.90 million m^3 $year^{-1}$) because demand is still below the maximum water availability.

VI. The optimal WSN is rearranged to include the southern supply source with 0.14 million m^3 $year^{-1}$. The capacity at which the most eastern supply location is operated is lowered to 93% (0.86 million m^3 $year^{-1}$).

VII. The optimal WSN has a different configuration compared to VI to supply the maximum investigated demand of 5.5 million m^3 $year^{-1}$. The most eastern supply site with a supply 0.92 million m^3 $year^{-1}$ is approached with a new branch of the network directly going east, instead of expanding the branch from the south-east as in *V* and *VI*.

In general, the optimal WSN configuration results from operating the supply location furthest from the demand location at the lowest possible capacity. This can reduce the amount of water supplied by a specific well when demand increases and new supply locations are added to the WSN (an example of this occurs during the transition from *III* to *IV*). By reducing the operating capacity of the furthermost supply location the pipeline diameter which needs to be installed over the complete network is minimized, leading to reduced costs.

As the demand increases the costs of the optimal WSN increases with steps to reflect the shifts in WSN configuration (Figure 7). In Figure 7 the costs of the WSNs *I*–*VII* of Figure 7 are annotated, and the optimal WSN costs for a drawdown of 75 mm are shown for comparison. The steps in costs arise from the need to add new supply locations to the WSN each time demand exceeds the maximum capacity of a set of supply locations.

At each step increasing the diameter (capacity) of pipelines is no longer sufficient to cover the demand and additional pipelines to new supply locations are needed. The addition of a new pipeline connection incurs the fixed costs, which causes the steps in costs. In the lower demand range, up to *VI,* the steps in costs for adding supply locations are more pronounced. At higher demand ranges the cost steps become less pronounced because the total number of supply locations required to cover the demand is larger. When many supply location are needed subtle changes in the network are possible to minimize costs, making the steps less pronounced. A linear increase in costs, as occurs between a demand of 0.7 *(II)* and 2.0 million m^3 $year^{-1}$ (at 50 mm drawdown), indicates that the only added

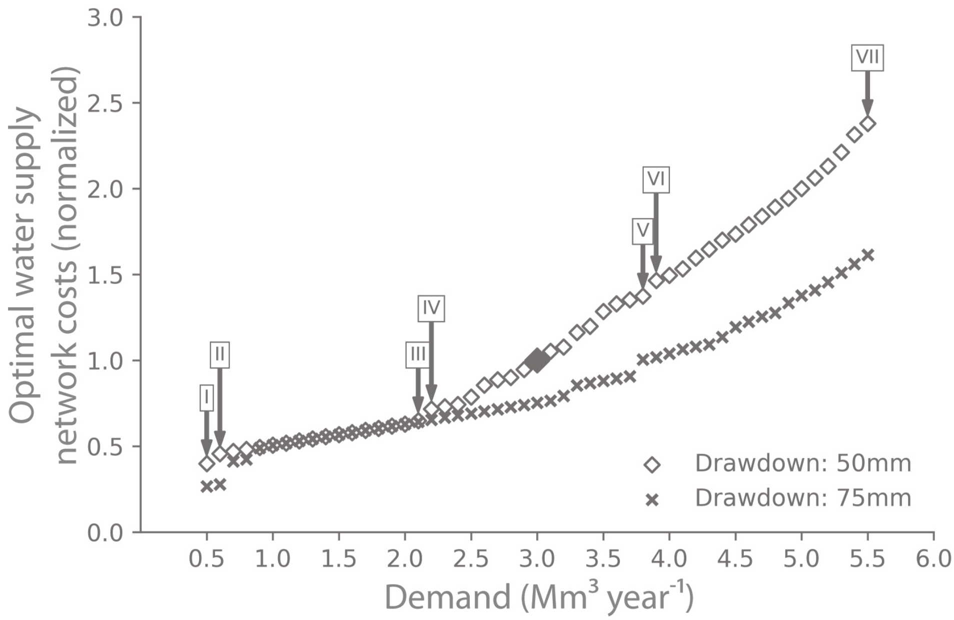


Figure 7 - Optimal water supply network costs in relation to demand of the water user. Costs are normalized based on the WSN costs for a demand of 3.0 million m^3 year^{-1} and a drawdown of 50 mm (indicated with the filled square). Normalization was done according to $NormalizedWSNcost(D) = WSNcost(D)/WSNcost\ (3.0\ million\ m^3\ year^{-1}, 50\ mm\ drawdown)$ *where D is the demand. The normalization data point is indicated with an enlarged marker.*

costs occur from adding additional capacity (increasing pipeline diameter) to the network.

5 Discussion

5.1 Modelling approach

Over the last decades water resources management has increasingly relied on computer models (Srdjevic et al., 2004). The model in this study adds to the existing modelling toolbox by offering the possibility to generate and evaluate decentralized water supply networks. These networks are based on local fresh (and in the future saline) water resources as a base for enhancing regional water self-sufficiency. The model accepts any supply location if the spatial location and the available amount of water are provided. This allows the evaluation of water supply networks in which surface water, rainwater, wastewater, brackish or saline water are used as decentralized supply sources. The complexity of the optimization problem, in terms of the number of network configurations which can cover the demand, increases exponentially as the number of supply locations increases. The presented model is therefore particularly suited to assist in the design process for decentralized water supply networks with many smaller supply locations adhering to maximum sustainable yields.

Reducing the overall water demand of a user is directly related to a reduction in the amount of water which needs to be transported. The stepwise behavior of the WSN costs reveals tipping points where reductions in demand can significantly influence the WSN configuration and costs. The model can be used to compare the costs of transport with the costs for demand reduction through the implementation of water saving technologies, or through an increase of water re-use. Depending on the local landscape and water supply sources either option may be favorable. For example: the costs for desalination have been decreasing over the years (Ziolkowska, 2015) which can make water supply networks based on small scale local brackish sources preferable over long distance transport of high quality water.

The cost of pipeline infrastructure depends on many factors (Clark et al., 2002), and can vary with a factor of 25 based on the methods and materials used (Selvakumar et al., 2002). As long as the same cost function for placing pipeline infrastructure is applicable to the complete case study area the model will generate the lowest cost WSN. The WSN can also be optimized based on other criteria than monetary costs. A cost function in terms of carbon dioxide emissions or energy use will yield the optimal WSN in terms of the respective cost function metric.

5.2 Sustainable water use

Self-sufficiency and sustainability can be enhanced by harvesting alternative local renewable resources (Agudelo-Vera et al., 2012a; Agudelo-Vera et al., 2012b). The model we present generates the optimal network to connect supply and demand within the boundaries of sustainably available water resources on any scale. Considering sustainable water availability over all relevant scales is needed to ensure overall long term sustainability (Bakshi, 2011; Bakshi et al., 2015). Long term sustainability of the decentralized WSN requires adherence to the catchment's water budget (Zacharias et al., 2003) and ensuring that the cumulative effect of local extractions do not negatively alter the entire drainage basin (Peters and Meybeck, 2000).

In the case study the maximum phreatic water level drawdown was set to a single value for all well clusters. Determining and applying specific drawdown values for each location, based on criteria applicable to the local context, is suggested for future research. Land subsidence as a consequence of draining peatlands (Hoeksema, 2007) is such an additional criteria for specific low-lying areas in the Netherlands. In other areas the maximum phreatic water level drawdown should be sensible with the presence of water intensive crop areas. Drawdown values and subsequent extraction rates can be matched with these local conditions at a very high spatial resolution. For this study it was decided that the analytical methods to determine water extraction rates are sufficient to identify possible supply locations and show the functionality of the modelling approach. Validating the extraction rates through a 3D numerical groundwater flow model (Faneca Sànchez et al., 2012; Oude Essink et al., 2010; Van Baaren et al., 2016) with an adequate resolution is suggested as a future step.

5.3 Context specific application

The case study presents a single set of weights for the landscape types in the region based on contact with water transport infrastructure experts. Involving local stakeholders to determine the weights makes the model results more context specific. Methodologies such as multi-criteria evaluations can be applied to spatial data to determine which areas are more or less suited for a certain purpose (Eastman, 2005). Each set of favored criteria will yield a specific cost of passage surface, which will in turn yield a specific WSN configuration. By defining and assigning the cost weights for each landscape type in consultation with local stakeholders the model generates water supply networks tailored to the local context.

Publicly available spatial data on landscape types limited to the Netherlands was used to demonstrate the workings of the model. Spatial data from other countries, Belgium for this case study, can be incorporated to assist with the transboundary nature of integrated water resources management (Rahaman and Varis, 2005). Consultation with local stakeholders can increase the number of landscape types included in the model because the categories of the national dataset are limited. The manual addition of no-go areas (such as Natura 2000 areas (Ministerie van Landbouw, Natuur en Voedselkwaliteit, 2020), or local heritage sites) makes results more site specific, and complements the generic spatial data relevant for pipeline construction costs.

6 Conclusions

This study presents a modelling approach to generate decentralized water supply networks based on the local landscape characteristics and water availability of a region. We add a novel approach to the modelling toolbox for regional water planners by incorporating spatial data and the effect of landscape types on the costs to place pipeline infrastructure, in combination with an optimization procedure based on a water balance between supply and demand. Water supply networks optimized to the local context can be generated by incorporating these spatial aspects. Representing the water network as nodes and edges makes it possible solve the complex optimization problem with mixed integer quadratic programming. The model was used for a case study in Zeeuws-Vlaanderen, in the south of the Netherlands, to supply an industrial zone with regional fresh groundwater as an alternative to importing fresh water from outside the region. The model generates: (1) the pipeline configuration for the lowest cost water supply network, (2) the amount of water flowing over each pipeline in the network, and (3) the capacity at which the supply locations should be operated. The model can be extended with other conventional and alternative water sources such as brackish water resources and wastewater treatment plant effluents. In that case treatment costs to achieve adequate quality and related costs need to be included. Decision makers can use the model to evaluate scenarios with varying supply and demand settings, and to identify the points at which sudden increases in transport network costs occur.

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Supplementary Information

Supplementary Information 1 - Maximum extraction rate calculation per well based on Bear and Dagan and Bruggeman (Bear and Dagan, 1964; Bruggeman, 1999).

$$Qmax \leq 2\pi\alpha k_x \vartheta d^2$$

Where

$Qmax =$ *maximum extraction rate (M^3 T^{-1})*

$\alpha =$ *relative density difference between fresh and saline water (-), 0.025*

k_x = *horizontal hydraulic conductivity (L T^{-1})*, 10^{-5} m s^{-1}

d = *distance between the well screen and the fresh-saline interface (L)*

ϑ =*factor that takes into account uncertain behavior of fresh and saline water under extraction wells in real cases* (-)*, 0.6*

Calculations are based on extractions undertaken at the surface. For this situation d = depth to fresh-saline groundwater interface from surface and that the horizontal hydraulic conductivity (k_x) was homogenous. Using the Dutch Geological Survey (DGN-TNO) it was found that the most commonly encountered sediment type within the study area is fine sand. For this research the hydraulic conductivity was set to 10^{-5} m s^{-1}.

The De Glee Formula represents the exact axial-symmetric solution for the extraction of groundwater with a constant discharge from a semi-confined aquifer by means of a fully penetrating well (Bruggeman, 1999);

$$\Delta h = \frac{Q}{2\pi kD} K_0\left(\frac{r}{\lambda}\right)$$

Where

Δh = *phreatic water level drawdown (L)*

Q = *the groundwater extraction rate (m³ T⁻¹)*

k = *hydraulic conductivity of the aquifer (L T⁻¹)*

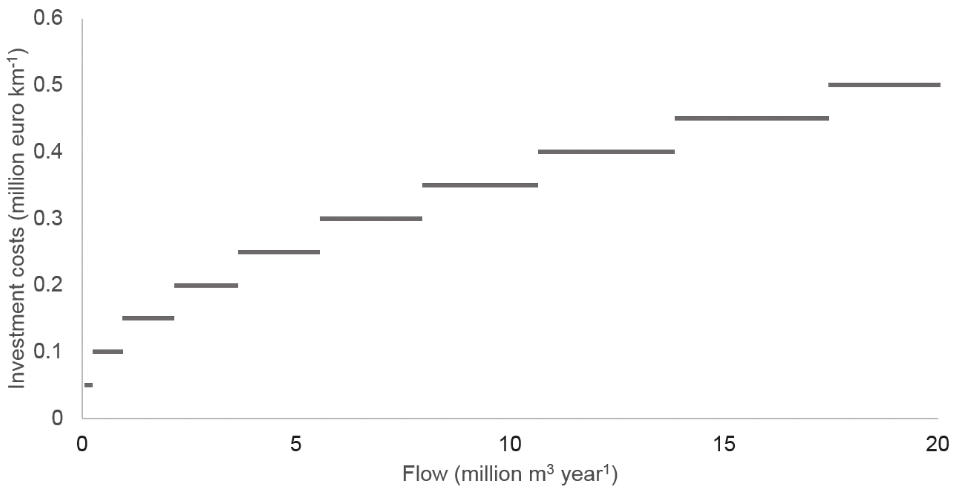
D = *thickness of the aquifer (L)*

r = *radius to the center of the well (L)*

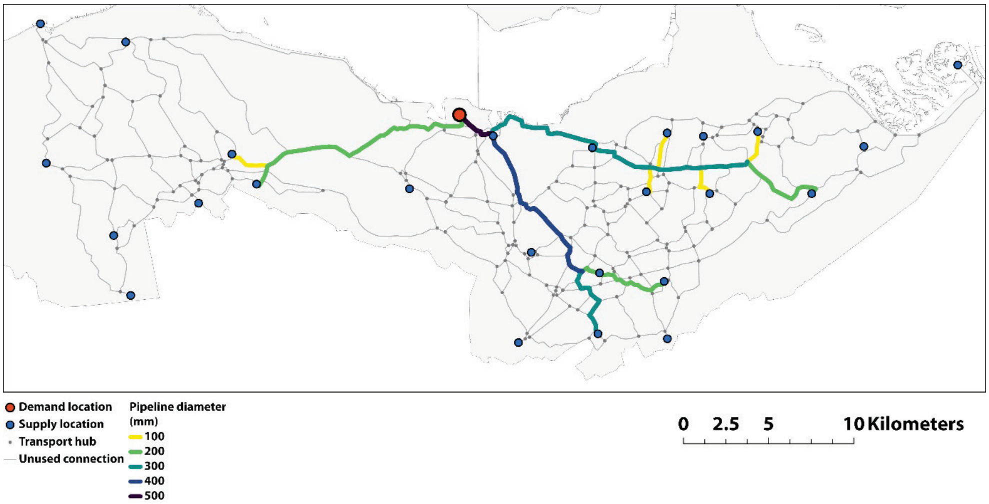
$\lambda = \sqrt{kDc}$ = *characteristic length (L), where c = the hydraulic resistance of the aquitard (T)*

$K_0(x)$ = *the modified Bessel Function of the second kind, order zero.*

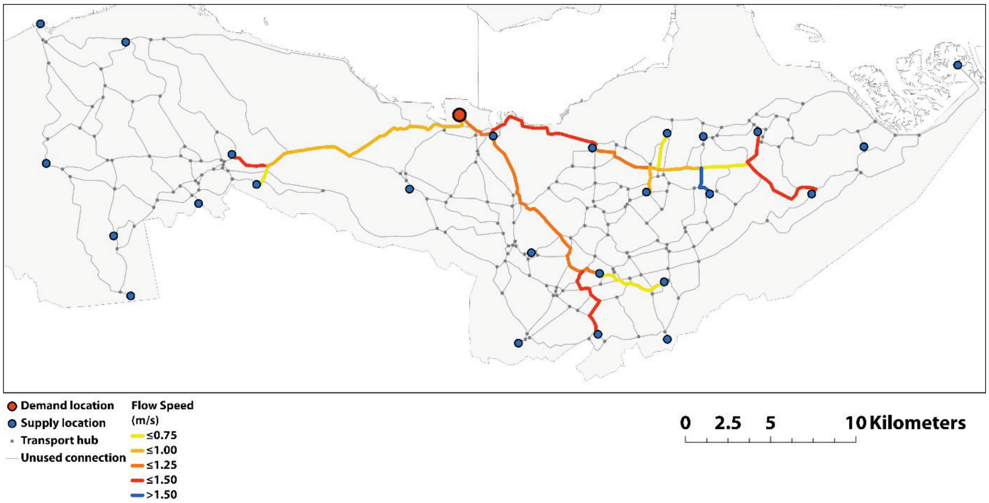
Supplementary Information 2 - Pipeline placement costs based on flow requirements and a cost of 0.5 € mm^{-1} diameter m^{-1}. Each plateau represents an available pipeline diameter, starting at 100 mm with increments of 100 mm, in which the flow velocity is within the optimal range (0.5 m s^{-1} and 1.5 m s^{-1}). The relationship between investment costs per unit distance in relation to the flow are approximated with a quadratic function ($Investment\ Costs = a \cdot Flow^2 + b \cdot Flow + c$).



Supplementary Information 3 - Pipeline diameters for the optimal WSN for a demand of 5.5 Million m^3 $year^{-1}$.



Supplementary Information 4 - Water flows velocities ($m\ s^{-1}$) for the optimal WSN with a demand of 5.5 Million m^3 $year^{-1}$. The instance in which the flow velocity is outside the 0.5 and 1.5 $m\ s^{-1}$ range (1.59 $m\ s^{-1}$, indicated with blue) occurs because increasing pipeline diameter from 100 mm to 200 mm would lead to a flow velocity of 0.4 $m\ s^{-1}$.



Chapter 4

WaterROUTE: a model for cost optimization of industrial water supply networks when using water resources with varying salinity

Abstract

Water users can reduce their impact on scarce freshwater resources by using more abundant regional brackish or saline groundwater resources. Decentralized water supply networks (WSN) can connect these regional groundwater resources with water users. Here, we present WaterROUTE (Water Route Optimization Utility Tool & Evaluation), a model which optimizes water supply network configurations based on infrastructure investment costs while considering the water quality (salinity) requirements of the user. We present an example simulation in which we determine the optimal WSN for different values of the maximum allowed salinity at the demand location while supplying 2.5 Mm^3 $year^{-1}$ with regional groundwater. The example simulation is based on data from Zeeuws-Vlaanderen, the Netherlands. The optimal WSN configurations for the years 2030, 2045 and 2110 are generated based on the simulated salinity of the regional groundwater resources. The simulation results show that small changes in the maximum salinity at the demand location have significant effects on the WSN configuration and therefore on regional planning. For the example simulation, the WSN costs can differ by up to 68% based on the required salinity at the demand site. WaterROUTE can be used to design water supply networks which incorporate alternative water supply sources such as local brackish groundwater (this study), effluent, or rainwater.

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1 Introduction

Global water consumption has increased more than fivefold in the 20th century and is expected to keep growing in the 21st century (Gleick, 2003; Shiklomanov, 1998). The combination of population growth (United Nations et al., 2019; Vörösmarty et al., 2000), overextraction (UN Water - FAO, 2007), contamination (UNEP, 2016), and hydrological changes due to climate change (Bates et al., 2008; Vörösmarty et al., 2000) will threaten water security around the world. Water scarcity is projected to increase (Hanasaki et al., 2013) and is increasingly considered a systemic risk to human welfare and biodiversity (Mekonnen and Hoekstra, 2016). New concepts for human water supply are needed to alleviate water scarcity for humanity and nature.

Industrial activities constitute a small fraction of the global water footprint (4.4%) (Hoekstra and Mekonnen, 2012) but have a high local water use intensity. Industrial facilities are generally located close to an abundant water source or large quantities of water are transported towards the industrial site to cover the demand. Historically, industries rely on centralized water supply infrastructures to transport water (Domènech, 2011; Gleick, 2003). The use of alternative local water resources can reduce the environmental impact of industrial water supply and requires a transition to decentralized water supply systems. Decentralized systems can alleviate environmental impacts while also reducing costs (investment, operational, network maintenance) and provide greater supply security (Domènech, 2011; Leflaive, 2009; Piratla and Goverdhanam, 2015). Decentralized systems can provide water from local surface water and groundwater sources such as local fresh water, rainwater, treated wastewater effluents, and brackish water (the focus of this study). The use of several supply sources creates the possibility for delivering water -after mixing- at the desired quality (Leflaive, 2009) and can lower costs by using local water supply sources to reduce total transport distance. This study focuses on delivering the desired quality when mixing groundwater with different salinities.

Optimizing the layout of a water supply network (WSN) is needed to minimize the high investment costs for piping infrastructure (Plappally and Lienhard, 2013). The costs for placing piping infrastructure depend on sub-soil characteristics, the land use where pipelines are to be placed, local policies, and property rights (Chee et al., 2018). Considering the differences in local pipeline construction costs at a high spatial resolution can significantly reduce overall capital investment costs (Feldman et al., 1995; Zhou et al., 2019).

The great number of potential pipeline connections in decentralized systems requires model-based approaches to generate cost effective designs. Model-based approaches are extensively used in the area of Integrated Water Resources Management (IWRM) (Medema et al., 2008). The system level analysis of IWRM is valuable for regional scale planning since it evaluates economic, environmental and social benefits simultaneously (Haasnoot et al., 2012; Savenije and van der Zaag, 2008). For an overview of the licensed and open source models available to decision makers in IWRM see: Awe et al., 2019; Clark and Cresswell, 2011; Sieber and Purkey, 2015; Sonaje and Joshi, 2015.

In this study we present WaterROUTE (Water Route Optimization Utility Tool & Evaluation), a model that adds new functionality to the previously developed WSN model (Willet et al., 2020). The original WSN model generates regional water supply networks only based on water quantity requirements. In the work presented here, the previously developed WSN model is extended to include water quality, specifically in terms of salinity. The addition of water quality as a design criterion for water supply networks is crucial to design regional decentralized water supply networks. The inclusion of water quality makes the delivery of water at the desired quality possible by mixing. In this study WaterROUTE is used to demonstrate how brackish/saline groundwater resources, exploited at sustainable yields, can serve as potential alternative water resources for industrial use. Brackish water resources can ensure a sustainable water supply when combined with optimal network layouts and desalination (Caldera and Breyer, 2017; Reddy and Ghaffour, 2007). For the first time, to our knowledge, we present and apply a modeling approach to create water supply network layouts with optimal pipeline routing at a high spatial resolution, connecting supply sources with different salinities, which also accounts for pipeline placement costs.

WaterROUTE optimizes water supply network configurations according to site-specific demands for water quality and quantity with water supply sources that have different and variable water qualities. With this functionality we connect regional hydrological modeling with planning of water supply infrastructure. The model generates the optimal network configuration and quantity of water needed from each supply source to satisfy the (industrial) demand without trespassing sustainable limits for water extractions. WaterROUTE is a valuable tool for IWRM and regional planning in areas where maximum sustainable yields of aquifers need to be enforced. Areas of particular interest are freshwater scarce areas with intensive industrial activities for which lower quality water can be used and where alternative (ground)water resources are available. We present and example simulation with regional brackish groundwater resources as the alternative water source for an industrial site.

2 Methodology

WaterROUTE is an optimization and visualization model which calculates optimal water supply network configurations. The optimization model mixes water streams with different qualities to supply a single demand location with a desired water quality. Mixing of water is a new and essential functionality to design decentralized water supply networks that use alternative water resources with different qualities.

In WaterROUTE, water supply and demand sites are represented as vertices and pipeline connections are represented as edges. The vertex and edge representation of (water) transport networks is commonly used for optimization (Mala-Jetmarova et al., 2017) and was previously used for network design without mixing in Willet et al. (2020).

WaterROUTE requires two inputs: the available water sources in a region and a preliminary network from which the optimal network configuration is selected. The preliminary network is created by determining the lowest cost routes between demand and supply locations using geographic information systems (GIS) methods. The inputs are processed by the WaterROUTE optimization model to yield the network configuration with the lowest cost for a specific water demand at the demand location (Section 2.1 - 2.6). The outputs are then visualized with GIS software for evaluation and decision making. An overall representation of WaterROUTE[1] is shown in Figure 1.

[1] Software used for the input data: MODFLOW (version: MODFLOW-96), MOC3D (version: 1.1 05/14/9), MOCDENS3D (adaptation to MOC3D as described in [Oude Essink (2001); Oude Essink et al. (2010)]
Software used for the preliminary network layout and visualization: ArcGIS Pro (build number: 2.4.19948)
Software used for the optimization: Python (version: 3.7.9), Gurobi (version: 9.0.3).

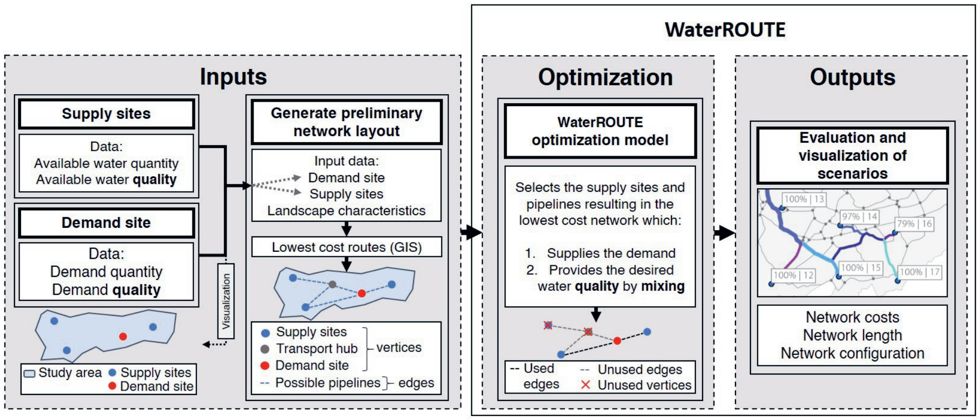

Figure 1 - The model framework of WaterROUTE.

2.1 Formulation and parameters

The WaterROUTE optimization model is a variation of the fixed charge network flow problem (FCNFP) (Hirsch and Dantzig, 1968; Kim and Hooker, 2002). In this study, we alter the original FCNFP formulation to include water quality parameters as a constraint. The water quality parameter included in this study is the salinity (the chloride concentration) of groundwater. Water may mix throughout the network, yet the water reaching the demand location must not exceed the maximum salinity defined by the user.

The WaterROUTE optimization problem is described as a planar mathematical system represented by vertices (V_i) and edges (E_{V_i,V_j}). Vertices represent supply locations, demand locations, and transport hubs/junctions. Edges represent the possible pipeline connections between vertices. Each vertex (V_i) has a chloride concentration (c_i) and an associated water supply or demand (s_i). Three situations can be distinguished for each vertex:

- when $s_i > 0$, vertex V_i is a water source, s_i is the volume of water available, and c_i is the chloride concentration of the available water;
- when $s_i < 0$, vertex V_i is a demand location, s_i is the volume of water to be supplied, and c_i is the maximum chloride concentration for the water;
- when $s_i = 0$, vertex V_i is a transport hub/junction in the network where water can mix.

Edges (E_{V_i,V_j}) transport water from vertex V_i into vertex V_j. Each edge (E_{V_i,V_j}) has two variables: flow of water ($x_{i,j}$) and flow of product ($p_{i,j}$), the product is the

Table 1 - Overview of parameters used to formulate the optimization problem with mixing and quality constraints.

Parameter	Description
V_i	Vertex i represents the source or demand location i
$E_{i,j}$	Edge i,j represents the pipeline connection between vertex i (V_i) and vertex j (V_j)
s_i	Water supply ($s_i > 0$) or demand ($s_i < 0$) at vertex i (m^3 day^{-1})
c_m	Maximum allowed concentration at the demand location ($mgCl^-$ L^{-1})
c_i	Product concentration at vertex i if $s_i > 0$ or target concentration $c_i \leq c_m$ if $s_i < 0$ at vertex i ($mgCl^-$ L^{-1})
$x_{i,j}$	Flow of water through edge i,j (decision variable in the optimization problem) (m^3 day^{-1})
$p_{i,j}$	Flow of product (chloride) through edge i,j ($mgCl^-$ day^{-1})
$u_{i,j}$	Maximum flow capacity of pipeline section (edge) i,j (m^3 day^{-1})
$t_{i,j}$	The maximum allowed product concentration for water flowing through pipeline i,j ($mgCl^-$ L^{-1})
$r_{i,j}$	Pipeline investment costs per meter (€ m^{-1}) per unit flow (m^3 day^{-1}) → (€ m^{-1} / m^3 day^{-1}) (based on a maximum flow velocity of 1.5 m s^{-1})
$l_{i,j}$	The length of the pipeline represented by edge i,j

amount of chloride (in $mgCl^-$ day^{-1}). The total product is determined based on the concentration and amount of water extracted from each supply vertex. Each edge has an associated cost per unit flow per km ($r_{i,j}$), and a length in km ($l_{i,j}$). Additional parameters are the maximum flow ($u_{i,j}$) and maximum product capacity ($t_{i,j}$) over each edge. We define a maximum allowed concentration (c_m) that is used to constrain the final quality of the supplied water. Table 1 gives an overview of the parameters in the WaterROUTE optimization problem formulation.

2.2 Objective function

The WaterROUTE optimization problem minimizes the total investment costs for pipeline placement (TPPC, Total Pipeline Placement Costs). The TPPC is the sum of the costs of the individual pipeline segments required for the complete water supply network. Due to the limited number of available pipeline diameters the pipeline investment costs (r_{ij}) increase with steps depending on the flow required. The interaction between the available pipeline diameters, flow requirements, and flow velocity leads to investment costs which increase with a stepwise pattern (see Supplementary Information 1). A stepwise increase in costs is referred to as a stairwise arc cost function (Bornstein and Rust, 1988; Du and Pardalos, 1993; Holmberg, 1994). In this study, pipeline diameters with increments of 100 mm and a maximum flow velocity of 1.5 m s^{-1} are used. The steps in the cost function

Table 2 - Pipeline investment costs for a flow between 0 and 5.5 Mm^3 year^{-1} (0–15068 m^3 day^{-1}) based on design guidelines for water distribution networks (Mesman and Meerkerk, 2009). Investment costs were determined in consultation with experts in the field of water distribution in the Netherlands.

k	λ_{ij}^k	Flow over edge x_{ij} (m^3 day^{-1})	Pipeline diameter (mm)	Investment costs r_{ij}^k (€ m^{-1})
	0	0	0	0
1	548	$0 < x_{ij} \leq 548$	100	50
2	2466	$548 < x_{ij} \leq 2466$	200	100
3	5753	$2466 < x_{ij} \leq 5753$	300	150
4	9863	$5753 < x_{ij} \leq 9863$	400	200
5	15068	$9863 < x_{ij} \leq 15068$	500	250

were determined for a flow range between 0 and 5.5 Mm^3 year^{-1} by increasing the flow with steps of 0.1 Mm^3 year^{-1} with a peak factor of 1.5 (Supplementary Information 1). The stepwise behavior is incorporated in the objective function, given by

$$\text{minimize} \qquad TPPC = \sum_{(i,j)\in E} f_{ij}(x_{ij}) \tag{1}$$

The stepwise costs for placement of new pipelines $f_{ij}(x_{ij})$ are defined by

$$f_{ij}(x_{ij}) = \begin{cases} 0 & x_{ij} = 0, \\ r_{ij}^k l_{ij} & \lambda_{ij}^{k-1} < x_{ij} \leq \lambda_{ij}^k \end{cases} \qquad \text{with } r_{ij}^k \text{ and } \lambda_{ij}^k \text{ as defined in Table 2} \tag{2}$$

where x_{ij} is the flow, and λ_{ij}^k represent the breakpoints in the cost function based on the flow in the pipeline. When there is no flow over an edge ($x_{ij} = 0$) no investment costs are incurred (resulting in $f_{ij}(x_{ij}) = 0$) and the edge is considered unused. The possible pipeline diameters are represented with an index $k = 1$ to $k = 5$. The length of the pipeline segment is l_{ij}, and r_{ij}^k are the investment costs per meter (Table 2).

2.3 Constraints: water quantity and pipeline capacity

The amount of water extracted from any vertex should be smaller than or equal to the total amount of water available at that vertex, and is ensured by

$$\sum_{(i,j)\in E} x_{ij} - \sum_{(j,i)\in E} x_{ji} \leq s_i. \qquad \forall i \in V \tag{3}$$

which ensures the water balance at each vertex. We apply this constraint to every vertex i in the set of vertices V.

Edges can be assigned a flow of 0, meaning the edge is not used, but the flow should not exceed the maximum capacity (u_{ij}) of the edge, which is ensured by

$$0 \leq x_{ij} \leq u_{ij} \qquad \forall (i,j) \in E \qquad (4)$$

which represents the allowed minimum and maximum flow over each edge. The maximum capacity over the edges in the preliminary network is equal to the demand volume of the demand site because existing pipelines are not included in the example simulation. If existing pipelines are re-used the maximum capacity over an edge depends on the size of the existing pipeline section. We apply the constraint to every edge.

The sum of the water flows exiting a vertex should be equal to the sum of the water flows entering the vertex if the vertex is a transport hub ($s_i = 0$)

$$\sum_{(i,j)\in E} x_{ij} - \sum_{(j,i)\in E} x_{ji} = 0 \qquad \forall i \in V; s_i = 0 \qquad (5)$$

which ensures that the outgoing flow (x_{ij}) is equal to the incoming flow (x_{ji}) for all transport hubs ($s_i = 0$).

Supply sites located in the middle of the network can perform a dual function: providing water to the network while also serving as a transport hub (see Figure 2).

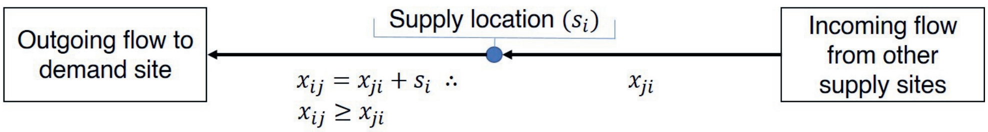

Figure 2 - Dual function of a supply site: supply location and transport hub. The outgoing flow must be larger or equal to the incoming flow.

The water flowing out from any supply vertex needs to be larger or equal to the water flowing towards the supply vertex and is ensured by

$$\sum_{(i,j)\in E} x_{ij} - \sum_{(j,i)\in E} x_{ji} \geq 0 \qquad \forall i \in V; s_i > 0 \qquad (6)$$

The sum of the water flows out (x_{ij}) from a supply site vertex $(s_i > 0)$ must be greater than or equal to the sum of the water flows entering (x_{ji}) the vertex.

2.4 Constraints: water quality

WaterROUTE generates network layouts that supply water with a specific maximum concentration at the demand site. For mixing of water flows up to a maximum concentration we formulate the constraints in Equation (7)-(11). These constraints control the amount of product (p_{ji}) flowing over an edge $(E_{i,j})$.

The amount of product (mass) extracted from a supply vertex must be equal to the amount of water (volume) extracted from that vertex times the concentration (mass/volume) at that vertex if the vertex is a source $(s_i > 0)$. We ensure this with

$$\sum_{(i,j)\in E} p_{ij} - \sum_{(j,i)\in E} p_{ji} = \left(\sum_{(i,j)\in E} x_{ij} - \sum_{(i,j)\in E} x_{ji}\right) c_i \qquad \forall i \in V; s_i > 0 \qquad (7)$$

The constraint in Equation (7) ensures that the water extracted from a supply vertex $(\sum x_{ij} - \sum x_{ji})$ times the concentration at the vertex (c_i) is equal to the product extracted $(\sum p_{ij} - \sum p_{ji})$.

The amount of product extracted from any supply vertex must be lower than or equal to the amount of product extractable from that vertex

$$\sum_{(i,j)\in E} p_{ij} - \sum_{(j,i)\in E} p_{ji} \leq s_i \cdot c_i \qquad \forall i \in V;\ s_i > 0 \qquad (8)$$

The product available at a supply vertex is determined by multiplying the concentration at the vertex by the amount of water available $(s_i \cdot c_i)$

Similar to the water flows for a supply site functioning as a transport hub, the sum of the product flows towards the vertex must be lower than or equal to the sum of the product flows exiting the vertex. This is achieved with

$$\sum_{(i,j)\in E} p_{ij} - \sum_{(j,i)\in E} p_{ji} \geq 0 \qquad \forall i \in V;\ s_i > 0 \qquad (9)$$

where $\sum p_{ij}$ is the outgoing product flow and $\sum p_{ji}$ is the incoming product flow.

The product flow (mgCl$^-$ day^{-1}) towards the demand site ($s_i < 0$) divided by the water volume (m^3 day^{-1}) towards the demand vertex must be lower or equal to the maximum allowed concentration. We ensure this with

$$\sum_{(i,j)\in E} p_{ij} - \sum_{(j,i)\in E} p_{ji} \geq \left(\sum_{(i,j)\in E} x_{ij} - \sum_{(i,j)\in E} x_{ji} \right) c_i \qquad \forall i \in V;\ s_i < 0 \qquad (10)$$

which is similar to Equation (7), but the equality condition is replaced by an inequality condition and Equation (7) is only applied to the demand location ($s_i < 0$). If an exact target concentration is required, the inequality condition in Equation (10) is replaced by an equality condition.

If an edge is used the product flow should be larger than zero and the product flow must not exceed the maximum allowed concentration for water in the pipeline (t_{ij})

$$0 < p_{ij} \leq t_{ij} \cdot x_{ij} \qquad \forall (i,j) \in E \qquad (11)$$

which can be used for the expansion of existing networks where the product concentration needs to be limited for certain pipelines.

2.5 Formulation overview and outputs

The complete formulation for the WaterROUTE optimization problem is written as

minimize	Objective function: TPPC of Equation (1)
subject to	Flow conservation: constraints (3), (5), (6)
	Physical bounds: constraints (4), (11)
	Product conservation: constraints (7), (8), (9), (10).

Solving the optimization problem yields the lowest cost WSN that supplies water with a concentration lower than or equal to the maximum allowed concentration at the demand location. The output of the problem is the water flow ($x_{i,j}$) over each edge of the preliminary network layout. Edges that are assigned a flow of zero (see Equation (2) and Table 2) are not in use and do not contribute to the TPPC.

2.6 Special case: minimum salinity network determination

When the desired water quality is set to the minimum salinity achievable for a certain demand (see Supplementary Information 3) the supply sources can be determined before the network configuration optimization. Supply sites are ordered by increasing salinity and the cumulative water availability and associated salinity are calculated. The set of clusters which can supply the demand at the minimum salinity is determined from the cumulative water and salinity list. Clusters not in the set are removed from the WaterROUTE optimization model inputs and the optimal network is determined by omitting the water quality constraints. This procedure reduces calculation time considerably for large networks.

3 WaterROUTE example simulation inputs

WaterROUTE is demonstrated by generating water supply networks to supply an industrial site (DOW Terneuzen, in Zeeuws-Vlaanderen, the Netherlands) with local groundwater. The WaterROUTE model is used to investigate the effect of varying the maximum chloride concentration (mgCl$^-$ L^{-1}) reaching the industrial site on the optimal WSN layout. WaterROUTE is used to generate water supply networks for 2030, 2045 and 2110 to account for changes in groundwater salinity, and a static demand of 2.5 Mm^3 year^{-1}. The inputs for the example simulation are the available local groundwater sources (Section 3.1) and the preliminary network layout between the demand and supply locations (Section 3.2).

3.1 Groundwater salinity and availability

The groundwater in the example simulation comes from several well clusters identified based on the fresh-salt groundwater interface as well as the transmissivity, which affects the possibility to extract water, of the groundwater system in the region (see Willet et al., 2020). The regional groundwater system has been extensively monitored, mapped and modelled in the past and shows the presence of fresh groundwater resources on top of groundwater with a higher salinity (Delsman et al., 2018).

A submodel of an existing, calibrated, 3D variable-density groundwater flow and coupled salt transport model is used to simulate changes in groundwater salinity and piezometric heads over time, for the period 2020-2110 (Van Baaren et al., 2016). The submodel covers Zeeuws-Vlaanderen, the Netherlands, and has the dimensions 70 km west-east by 28 km north-south by 143 m thick. The 3D groundwater model uses the MODFLOW (Michael G. McDonald and Arlen W. Harbaugh, 1988) based computer code MOCDENS3D (Faneca Sànchez et al., 2012; Oude Essink et al., 2010). It uses 40 model layers (with grid cell thicknesses varying from 0.5 m to 10 m with increasing depth) to reproduce the movement of groundwater salinity in the vertical direction; resulting in over 7.8 million grid cells. Changes in groundwater salinity are simulated by advection and hydrodynamic dispersion. Complex geology (horizontal and vertical hydraulic conductivities) (Stafleu et al., 2011) and the mapped groundwater salinity (via intensive airborne electromagnetics (Delsman et al., 2018)) are inserted in the model. Stresses to the groundwater system consist of seasonal natural groundwater recharge (from de Lange et al., 2014), six surface water types (sea and estuarine waters, lakes, canals, (small) rivers, watercourses up to ditches), a shallow drainage system, and groundwater extraction wells (retrieved from a database of the Water Board Scheldestromen). The surface water and drainage systems are inserted into the model using an accurate Digital Elevation Model (Actuel Hoogtebestand Nederland, 2020) (resolution 5*5 m). Boundary conditions (the sea, the estuary, and the Belgian hinterland) complete the existing 3D groundwater model (Van Baaren et al., 2016).

The original 3D variable-density groundwater flow and coupled salt transport model has been calibrated based on a database of piezometric heads (calibration was done in Van Baaren et al., 2016). The model has been published in a Deltares report (Van Baaren et al., 2016). The final calibration set of piezometric heads consisted of 606 observations for the entire area of the province of Zeeland from the database of dinoloket.nl, over the period 1-1-1991 up to 31-12-2000. The effect of the groundwater density in the observation wells on the heads was considered (Post et al., 2007). We used the code PEST, the most widely used calibration software for groundwater in the world (Doherty, 2005). Parameters that have been changed during the calibration are the horizontal hydraulic conductivity of the aquifers, the vertical hydraulic conductivity of the aquitard, the hydraulic resistance from/to the surface water system and finally the groundwater recharge. The results for Zeeuws-Vlaanderen are as follows: the median of the difference between the calculated minus the measured heads changes from 0.18 m to -0.009 m and the average absolute difference between the calculated minus the measured heads changes from 0.29 m to 0.24 m. We believe these differences are good enough calibration results. Validation of the model has not been performed as the entire dataset was believed to be needed for the calibration.

In this study, the 3D groundwater model simulates the effect of multiple brackish groundwater extractions (used as the alternative water supply source) over the well clusters on the groundwater salinity over time and the piezometric heads in the vicinity of well clusters. In Willet et al. (2020), analytical equations were used to estimate the upconing of the interface between fresh and saline groundwater (Dagan and Bear, 1968) and the drawdown of the phreatic groundwater level (Bruggeman, 1999). The numerical 3D groundwater model incorporates hydro(geo)logical details of the local setting (the heterogeneous salinity distribution, interaction with the surface water system, geology), includes changes in groundwater salinity due to extraction wells, and thus produces more accurate results than the previously used analytical methods. The same locations of the 2079 extraction wells in the 25 well clusters identified in Willet et al. (2020) were used. The number of extraction wells per well cluster varies, from a minimum of 10 to a maximum of 331. The extraction wells are positioned at least 100 m from each other to limit strong drawdown superposition. For further details on well placement and extraction rates see Supplementary Information 2.

The surface water boundary is modelled with a fixed salinity concentration and does not change over the entire simulation period. There is not enough surface water salinity data to insert a seasonal varying surface water salinity boundary condition (though the model can do so; a seasonal varying surface water head boundary was modeled). Several surface water features in the Zeeuws-Vlaanderen region are draining from the groundwater system or are not active in summer. The fresh groundwater recharge is likely a dominant source of fresh water that enters the wells, given that small water courses and ditches are the main surface water phenomena in this region.

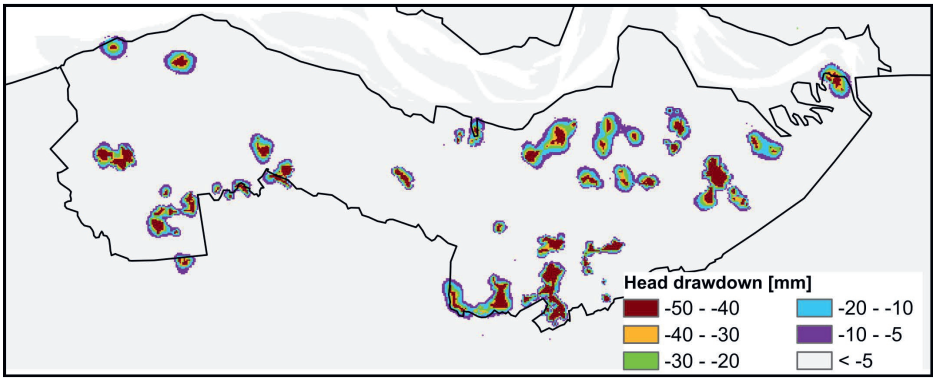

Figure 3 - Modelled drawdown of the piezometric head per well cluster, caused by 2079 extraction wells distributed over 25 well clusters. The maximum drawdown is 50 mm wherever extraction wells are positioned.

To meet environmental targets (e.g. Natura 2000) and to limit drought effects, the maximum drawdown of the phreatic groundwater level is set to 50 mm (Figure 3). The exact maximum allowed groundwater extraction rate per well was determined iteratively while meeting the maximum drawdown of the phreatic groundwater level. In the first iteration step, the starting groundwater extraction rates as used in Willet et al. (2020) are taken. Within ten iteration steps, the changes in groundwater extraction rates become negligible. The 3D groundwater model considers interferences in piezometric head and groundwater salinity over time of nearby extraction wells. The overall salinity of a well cluster is determined based on the sum of the salt ($mgCl^{-}$ day^{-1}) extracted from all wells in the well cluster and the sum of the water (m^3 day^{-1}) extracted from all wells in the well cluster.

The available groundwater from all well clusters in the study area is 6.119 Mm^3 $year^{-1}$ while having a maximum drawdown of 50 mm. Changes in precipitation patterns and the associated effects on groundwater availability were not included. The overall combined salinity of all 2079 wells over 25 well clusters is 472 $mgCl^{-}$ L^{-1} in 2020. In 2020, there are two well clusters (in the north-west and center of the study area) which are significantly more saline (Figure 4). Operating all well clusters at the maximum extraction rate increases the salinity of most clusters.

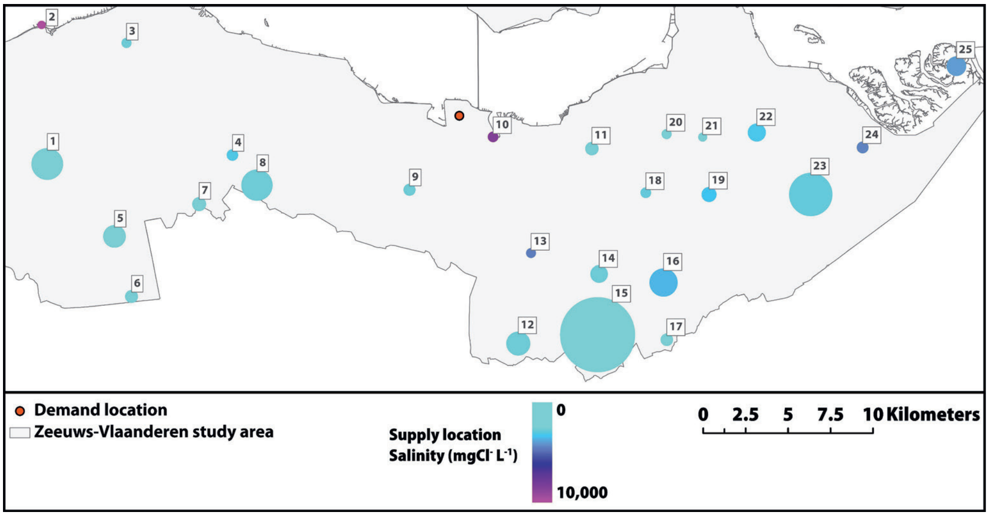

Figure 4 - Modelled groundwater supply locations in Zeeuws-Vlaanderen and salinity in 2020. Labels represent the well cluster numbers. The diameter of the marker represents the amount of water available. Most water is available at well cluster 15 (1.43 Mm^3 $year^{-1}$), and the least at well cluster 2 (0.01 Mm^3 $year^{-1}$).

The average chloride concentration increases from 472 $mgCl^-$ L^{-1} in 2020 to 852 $mgCl^-$ L^{-1} in 2030, 981 $mgCl^-$ L^{-1} in 2045, and 1095 $mgCl^-$ L^{-1} in 2110 (see Supplementary Information 4 for details on water availability at each well cluster). When water extractions start, the salinity of well clusters changes quickly within (on average) 10 years but stabilizes over time when a new equilibrium in the subsoil is reached (see Supplementary Information 5). For some well clusters, a significant decrease in salinity (i.e. freshening), occurs because fresh water from the surface water system moves towards the extraction point when groundwater is extracted (clusters 10, 13, 16, and 19, see Figure 5). Well cluster 24 first becomes more saline between 2020 and 2030 and then becomes slightly fresher up to 2110. The salinization or freshening rate of well clusters is not uniform for all clusters, and therefore, the optimal WSN configuration with the lowest costs is specific for each period and demand quality.

3.2 Preliminary network layout

The preliminary network layout is the complete set of possible pipelines connecting all the supply and demand locations in the study area. The WaterROUTE optimization model selects the subset of pipelines with the lowest total costs for a specific demand at the demand site. The selected subset is the optimal WSN configuration for a specific scenario. The preliminary network layout in this study represents a water supply network which still needs to be built but

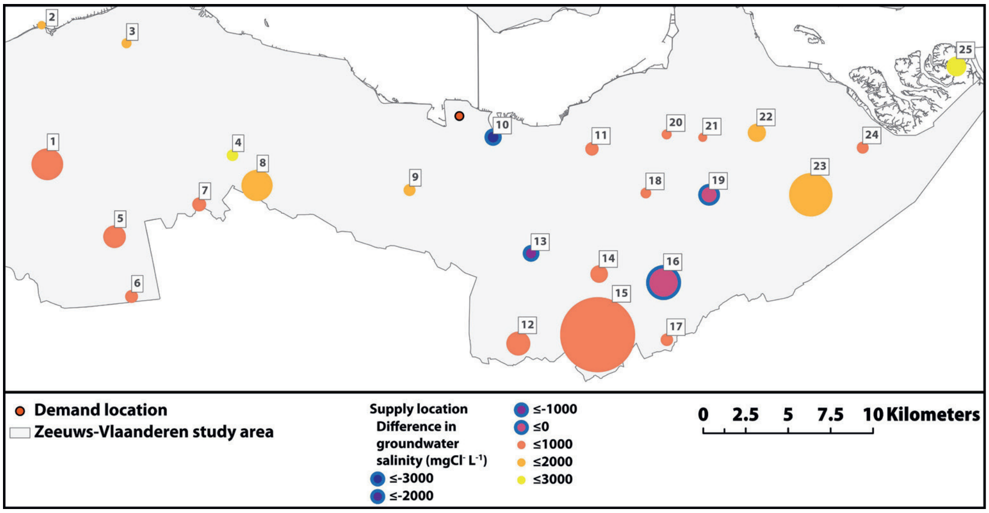

Figure 5 - Modelled changes in groundwater salinity for well clusters in Zeeuws-Vlaanderen between 2020 and 2110 based on the extraction rates in Supplementary Information 4. These changes vary between -3412 mgCl$^-$ L^{-1} (water becoming fresher, well cluster 10) and 2785 mgCl$^-$ L^{-1} (water becoming more saline, well cluster 25). A blue outline indicates the well cluster becomes fresher. Labels represent the well cluster numbers. The diameter of the marker represents the amount of water available.

the same methodology can be applied for an existing (to be expanded) water supply network. The preliminary network for the Zeeuws-Vlaanderen region was generated following the steps as outlined in Willet et al. (2020), using lowest cost route methods with GIS software. The main steps to generate the preliminary network layout are:

(1) Creating a cost of passage surface based on local land-use types in collaboration with water supply experts (see Willet et al., 2020). A cost of passage surface is needed to include the local spatial data in the network optimization problem. Including local spatial data is important since the costs for placing pipeline infrastructure depend on the local land-use and subsurface characteristics (Feldman et al., 1995).

(2) Tracing the lowest cost route between each possible combination of supply and demand locations based on the cost of passage surface. The resulting network serves as the preliminary network layout for optimization. The use of lowest cost route methods is common for infrastructure routing (Atkinson et al., 2005; Collischonn and Pilar, 2000; Douglas, 1994).

The preliminary network has a total of 408 pipeline segments and 243 transport hubs to connect the 25 groundwater supply locations and the single demand location (see Supplementary Information 7).

4 Results

WaterROUTE is used to generate the optimal water supply network configuration for five demand scenarios in the Zeeuws-Vlaanderen region for the years 2030, 2045, and 2110 (a total of 15 simulations). In each scenario the salinity of the water reaching the demand location differs while the demand volume is kept the same at 2.5 Mm^3 $year^{-1}$. The scenarios are:

1. The minimum possible salinity for water reaching the demand location
2. No salinity requirements for water reaching the demand location

After determining the salinity range in scenario 1 and 2 three intermediate scenarios are simulated:

3. A salinity of 375 $mgCl^-$ L^{-1} or lower for water reaching the demand location
4. A salinity of 400 $mgCl^-$ L^{-1} or lower for water reaching the demand location
5. A salinity of 425 $mgCl^-$ L^{-1} or lower for water reaching the demand location

4.1 Network configurations for a minimum salinity at the demand location

The lowest possible salinity is determined by sorting well clusters in order of increasing salinity and by calculating the cumulative salinity based on the available water (see Supplementary Information 6). The set of the well clusters included in the WSN differs between 2030, 2045, and 2110 because the salinization/freshening rate is not equal for all well clusters. The minimum possible salinity for a demand of 2.5 Mm^{-3} $year^{-1}$ at the demand location is 246 $mgCl^-$ L^{-1} in 2030, 287 $mgCl^-$ L^{-1} in 2045, and 318 $mgCl^-$ L^{-1} in 2110.

Supplying water at the lowest possible salinity requires supply networks covering almost the complete study area (Figure 6). Such extensive networks are needed when high quality water is not available close to the demand site. The main difference between the 2030 simulation and the simulations of 2045 and 2110 is the use of well cluster 1. The salinity of well cluster 1 increases at a faster rate than other well clusters and is excluded from the minimum salinity network in

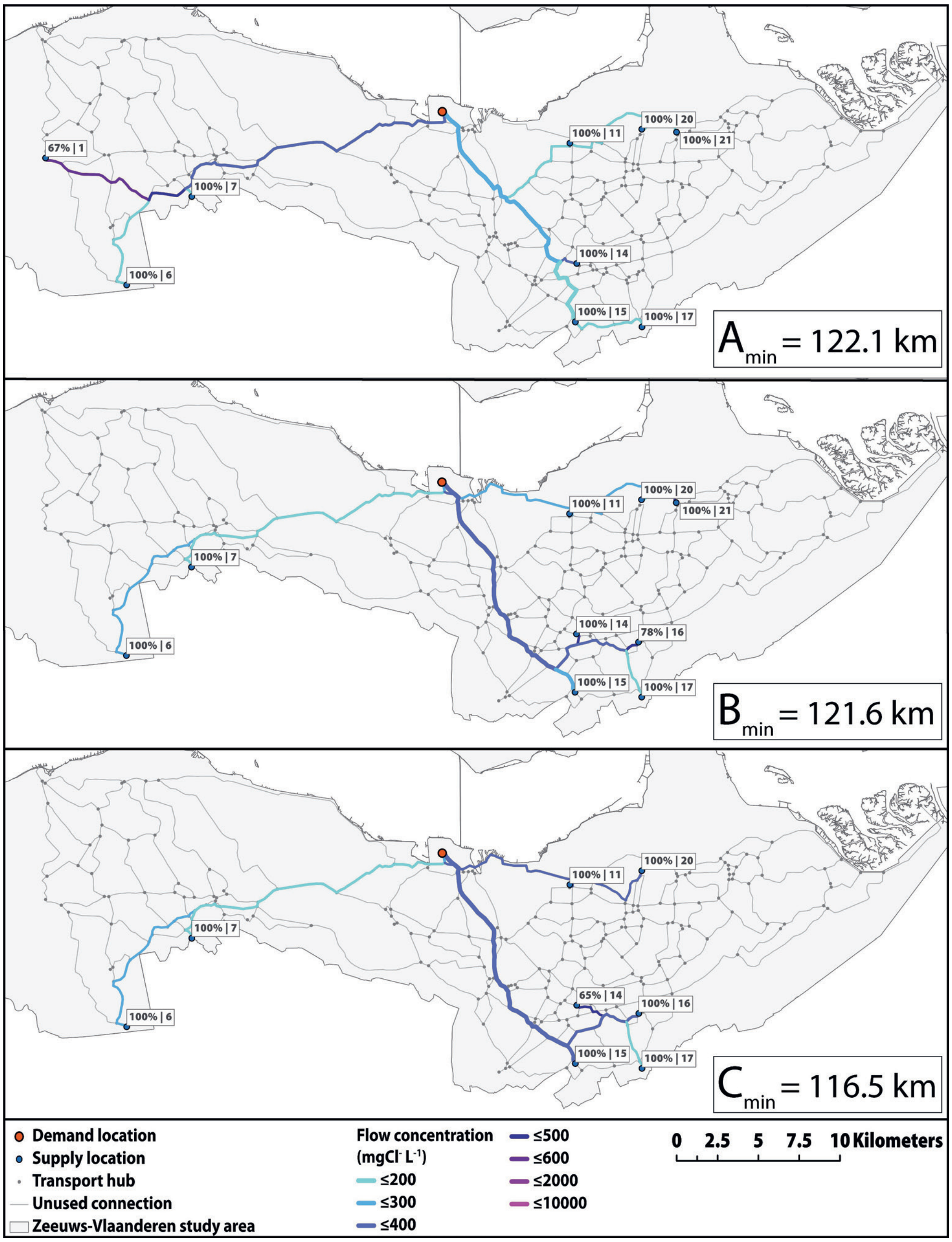

Figure 6 - Optimal network configurations for the lowest possible salinity in 2030 (A_{min}, 246 mg Cl^- L^{-1}), 2045 (B_{min}, 287 mg Cl^- L^{-1}) and 2110 (C_{min}, 318 mg Cl^- L^{-1}). The well cluster labels show the rate (relative to water availability) at which the well clusters are operated and the well cluster number (operation rate | well cluster number).

favor of well cluster 16 in 2045 and 2110. Well cluster 21 also has a relatively high rate of salinization and is excluded in the 2110 network.

4.2 Network configurations without salinity requirements at the demand location

Networks without a salinity requirement have an identical configuration, total length (46.9 km), and costs in 2030, 2045, and 2110 (Figure 7). The configuration is identical because the water quantity which can be extracted from each well cluster is considered constant. Due to salinization the resulting chloride concentrations at the demand location are 491 $mgCl^- L^{-1}$ in 2030, 510 $mgCl^- L^{-1}$ in 2045 and 529 $mgCl^- L^{-1}$ in 2110. The chloride concentration increase is 38 $mgCl^- L^{-1}$ (±8% [2]) and is low compared to the overall 243 $mgCl^- L^{-1}$ (29% [3]) increase for the complete study area. The low salinization of the water supplied by the WSN is caused by freshening of well clusters 10, 13, and 16.

The extraction rate from well cluster 14 is capped at 97% corresponding to a flow of 548 $m^3 day^{-1}$ with a pipeline diameter of 100 mm (see Table 2). Increasing the flow of this cluster would require a pipeline diameter of 200 mm, leading to higher costs. The amount of water that can be extracted from well cluster 10 is flexible and can be increased from 98% to 100% without increasing or decreasing the network investment costs. This flexibility can be used to provide slightly more water but leads to water with higher salinity at the demand location.

4.3 Network configurations for a salinity at the demand location of 375 $mgCl^- L^{-1}$, 400 $mgCl^- L^{-1}$, and 425 $mgCl^- L^{-1}$ or lower

The optimal network configurations for different periods and salinities at the demand site are shown in Figure 8. Small changes in demand quality (25 $mgCl^- L^{-1}$) affect the optimal configuration of the water supply network. The general trend is that the length, complexity, and costs of the supply network increase when groundwater with a lower salinity is required at the demand location. This trend is the most pronounced for the 2110 simulation; the optimal network for a demand quality of 425 $mgCl^- L^{-1}$ is 17.2 km shorter than for a demand of 375 $mgCl^- L^{-1}$ (see Figure 8 and Table 3). The salinization of well clusters leads to longer networks and increasing costs over time.

[2] (529 $mgCl^- L^{-1}$ - 491 $mgCl^- L^{-1}$) / 491 $mgCl^- L^{-1}$= 8%
[3] (1095 $mgCl^- L^{-1}$ - 852 $mgCl^- L^{-1}$) / 852 $mgCl^- L^{-1}$= 29%, see last row of Supplementary Information 6

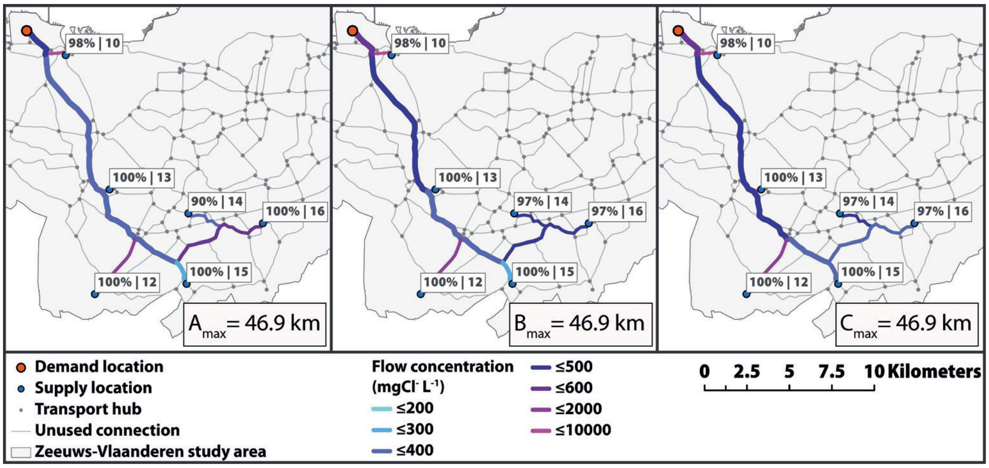

Figure 7 - Optimal network configurations for networks without salinity requirements at the demand location in 2030 (A_{max}, 491 $mgCl^{-}$ L^{-1}), 2045 (B_{max}, 510 $mgCl^{-}$ L^{-1}) and 2110 (C_{max}, 529 $mgCl^{-}$ L^{-1}). The well cluster labels show the rate (relative to water availability) at which the well clusters are operated and the cluster number (percentage | well cluster number).

The networks A_2, A_3, and B_3 (see Figure 8) share the same configuration. This network configuration has a length of 51.8 km and is suitable between 2030 and 2045 for a salinity up to 425 $mgCl^{-}$ L^{-1}. The difference with the network configuration without a salinity requirement at the demand location (Section 4.2) is the addition of well cluster 17. Well cluster 17 is added because it provides enough fresh groundwater to reach the desired salinity.

The networks A_1, B_2, and C_3 (see Figure 8) also share the same configuration. This network configuration of 51.6 km is 0.1% more expensive than the 51.8 km network (A_2, A_3, and B_3). A shorter network can have higher costs depending on the specific pipeline diameters which need to be used. The salinity of the groundwater supplied by this network is lower than the required salinity of the demand site for any of the periods shown in Figure 8. For example, the chloride concentration of groundwater provided by network A_1 is 337 $mgCl^{-}$ L^{-1} instead of the maximum allowed concentration of 375 $mgCl^{-}$ L^{-1}. This is possible due to the constraint in Equation (10) which ensures that the salinity of groundwater reaching the demand location is lower than or equal to the demand salinity. A network which supplies groundwater with a lower salinity than the demand salinity, the case for A_1, B_2, and C_3, only occurs when the lowest cost network happens to yield a lower salinity.

Chapter 4

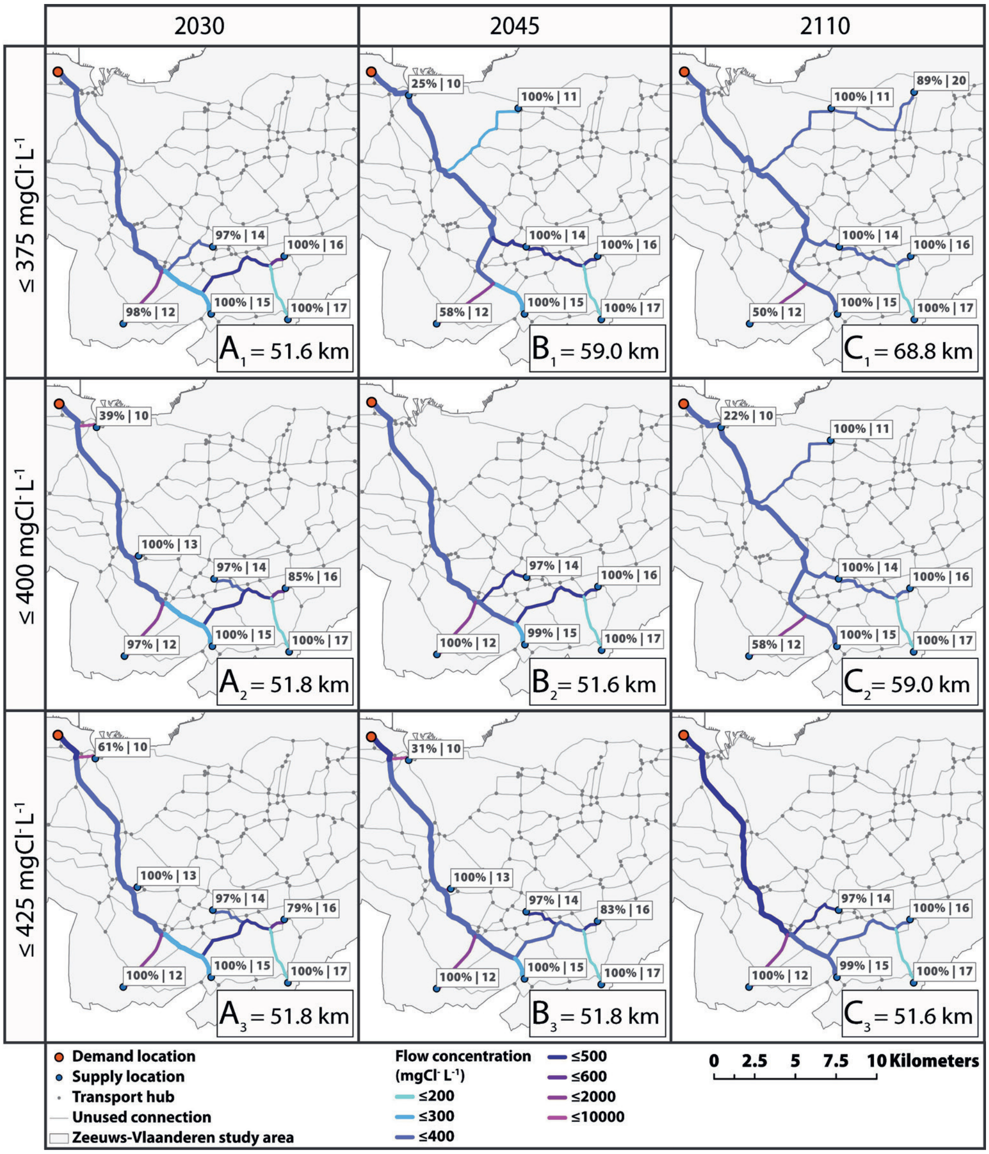

Figure 8 - Optimal network configurations for the transport of water with a maximum salt concentration at the demand location of 375 mgCl- L-1, 400 mgCl- L-1, and 425 mgCl- L-1 in 2030, 2045, and 2110. The well cluster labels show the rate (relative to water availability) at which the well clusters are operated and the well cluster number (percentage | well cluster number).

The networks B_1, and C_2 (see Figure 8) share the same configuration. This network configuration has a length of 59.0 km and is needed for a demand salinity up to 375 $mgCl^{-1}$ by 2045. The C_1 network is created by connecting cluster 20 to the B_1/C_2 network resulting in a 68.8 km network.

Table 3 - Network length and costs. Costs are shown as a percentage in relation to the network without a salinity requirement at the demand site.

Network	Network length (km) | Network costs[a]		
	2030	**2045**	**2110**
Minimum	122.1 | 168%	121.6 | 159%	116.5 | 153%
≤ 375 mgCl⁻ L⁻¹	51.6[b] | 104%	59.0 | 107%	68.8 | 114%
≤ 400 mgCl⁻ L⁻¹	51.8[b] | 104%	51.6 | 104%	59.0 | 107%
≤ 425 mgCl⁻ L⁻¹	51.8 | 104%	51.8 | 104%	51.6 | 104%
No salinity requirement	46.9 | 100%	46.9 | 100%	46.9 | 100%

[a] Costs are normalized based on the scenario in which there is no salinity requirement at the demand site
[b] Costs for the 51.6 km network are higher than the 51.8 km network due to the specific pipeline diameters needed

For a detailed description of the characteristics of the network configurations see Supplementary Information 8 to Supplementary Information 10.

4.4 Network costs in relation to salinity and time

As the maximum allowed salinity at the demand site increases, the length and costs of the WSN decrease (Table 3, from top to bottom). Increasing the maximum allowed salinity increases the number of well clusters which can be used in the network. A larger number of usable well clusters increases the probability that well clusters located close to the demand location can be used. The possibility to choose well clusters close to the demand location results in shorter networks. Shorter networks generally have lower costs, with some exceptions (see Section 4.3).

In general, the WSN costs increase when the same water quality needs to be supplied further in the future (Table 3, from left to right, except for the minimum salinity network). This is the result of the salinization of the well clusters in the study area. Salinization of well clusters results in fewer clusters which can contribute to the network for a specific demand salinity. As a result, longer networks which transport fresh water from further away are needed.

The optimal network configuration for a specific region depends on the local groundwater availability and the groundwater salinization/freshening dynamics. Salinization and freshening of specific well clusters can lead to unexpected WSN costs. For the Zeeuws-Vlaanderen simulation this is reflected in the optimal network configuration for the minimum possible salinity at the demand location when only using groundwater. Based on the modeled changes in groundwater salinity in Zeeuws-Vlaanderen the minimum salinity network for 2110 has lower costs compared to 2045 and 2030.

5 Discussion

5.1 WaterROUTE for regional planning

The modelling approach presented in this study expands the functionality of the WSN model (Willet et al., 2020) with the possibility to mix water and further expands the modelling toolbox on which Integrated Water Resources Management is reliant (Srdjevic et al., 2004). Determining the most cost-effective network for a specific quality at the demand site needs to consider different water qualities and water quantities at the supply sites. Input data on water quantity and water quality is supplied by existing and tested external hydrological models. WaterROUTE processes these inputs and makes it possible to explore water supply network options when the water quality of regional supply sources changes over time. It shows how small changes in the maximum allowed salinity of water reaching the demand location cause significant changes in the configuration of the water supply network. This knowledge is useful for regional planning purposes.

WaterROUTE can also be used to plan network expansion by using the characteristics of an existing supply network as inputs. For existing networks, the capacity of the existing pipelines is fixed but using these pipelines does not require new investments. Other characteristics of existing networks can also be incorporated. For example, if existing networks contain segments with iron pipelines a maximum salinity constraint for these pipeline sections can prevent corrosion when using saline/brackish water resources.

The possibility to include several demand locations, instead of a single demand location, for decentralized water supply network design and regional planning is relevant for areas where multiple water users compete for the same water resources. The addition of multiple demand locations, with different water demand quantities and qualities, introduces non-convex quadratic constraints to the optimization model and requires a problem formulation where several water flows of different qualities can flow over the same trajectory in parallel pipelines. Developing an effective problem formulation for multiple demand sites is suggested for future research.

5.2 Alternative water sources for industrial use

Decentralized supply networks making use of alternative water sources can be a solution to cope with future changes in water availability around the world. Decentralization of water supply can enhance water reuse possibilities (Leflaive, 2009) and can have advantages over centralized systems (Domènech, 2011; Leflaive, 2009; Piratla and Goverdhanam, 2015). Supplying industrial sites with alternative regional water resources requires data on the availability of alternative sources, now and in the future. WaterROUTE is a tool that can evaluate the feasibility of using these alternative sources and their corresponding decentralized supply networks at a high spatial resolution. Modeled brackish groundwater is used as the alternative water supply in the Zeeuws-Vlaanderen example simulation. Other alternatives, such as treated wastewater, rainwater, desalinated seawater, or surface water, can also be evaluated with WaterROUTE.

The formulation of the optimization problem in WaterROUTE is based on an overall mass balance of water and a product. The product used in the Zeeuws-Vlaanderen simulation is chloride. Other water quality parameters than chloride can also be used. Another possibility is to investigate multiple products simultaneously by adding new variables and constraints for each of the additional products to the basic model framework. This functionality is useful when evaluating other local alternative water sources such as rainwater and treated wastewater from industries, urban areas, and agriculture. When adding additional quality parameters non-linear and non-additive relationships between products should be accounted for. For example, two water steams originally free of microbial activity, the first due to a lack of nutrients, the second due to a lack of organic carbon, can lead to bacterial growth when mixed. The addition of these complex interactions is only possible when they can be accurately predicted mathematically but can lead to computational problems if relationships are non-linear. The fields of industrial ecology (Hond, 1999) and circular urban metabolism (Agudelo-Vera et al., 2012) can benefit from such additions for analysis and design. Within industrial ecology, specifically industrial symbiosis, providing water at a specific quality (fit for purpose) has been proposed to alleviate water shortages (Bauer et al., 2019).

5.3 Supply sources and sustainability

Groundwater extractions have inevitable consequences on local groundwater hydrology. Limiting the amount of groundwater extracted to renewable rates is one step towards sustainable exploitation of local water resources. WaterROUTE is suitable for designing water supply networks which respect sustainable extraction rates. This functionality is needed for regional planning that aims to anticipate on the expected changes in water availability (Hanasaki et al., 2013), salinization of (ground)water resources (H.D. Holland and K.K. Turekian, 2003; UNEP, 2016), and the overall need to match resource utilization with the local/global carrying capacity (Bakshi et al., 2015). Within industrial water use the connection between local carrying capacity and evaluation methods for water use is still lacking (Willet et al., 2019). WaterROUTE provides a link between the physical (hydrological) modeling of water resources and regional planning of water supply networks. Through this link the costs for mismanagement of scarce water resources, e.g. overextraction leading to salinization requiring longer supply networks, becomes apparent.

In this study, the maximum groundwater extraction rates are made dependent on a maximum drawdown of the phreatic groundwater level for the complete region. It is proposed to replace regional values for maximum salinization and phreatic groundwater level drawdown by well cluster specific values in future research. Using well cluster specific values reveals the effect of sustainability thresholds at a higher spatial resolution on WSN design. Other possible criteria for groundwater extractions are the vulnerability of local ecosystems to salinization (Castillo et al., 2018; Herbert et al., 2015) and the susceptibility of soils to sodification (Minhas et al., 2019) (a nearly irreversible process).

The results of WaterROUTE show that in most scenarios not all well clusters are used, or well clusters are exploited below their maximum capacity. WaterROUTE does not yet consider the effects of partial extractions on the complete groundwater system. The simulations performed for this study suggest that interference between well clusters can be neglected for the Zeeuws-Vlaanderen area because well clusters are far enough apart. In other areas interference may occur and simulating the effects of partial extractions on groundwater salinity and drawdown to verify the feasibility of the network design is suggested. Simulating the effects of a network design on groundwater and subsequently updating the network design creates a dynamic interaction between the optimization model and the groundwater model. Such a dynamic interaction is relevant in areas where water extractions at one well cluster can affect other well clusters but is currently computationally infeasible.

The WaterROUTE model can also assist in designing regional water supply networks which counteract saltwater intrusion from the sea by using the WSN to recharge aquifers when fresh surface water is abundant. Smart groundwater extractions can lead to freshening of groundwater resources by attracting fresh water from the surface water systems instead of saline groundwater from below the extraction point. Coupling the operation of decentralized water supply networks with locations where this form of freshening is possible can lead to regional benefits besides water supply. Fresh water resources can be stored during the wet season to be retrieved at a later moment with Aquifer Storage and Recovery (ASR) (Maliva et al., 2006). Correct timing of extractions can make the stored water available for use without affecting the fresh-salt groundwater interface in the subsoil while being a cost effective option compared to other water supply alternatives (Oude Essink et al., 2018; Vink et al., 2010; Zuurbier et al., 2012). WaterROUTE is needed to design the supply network in which ASR sites are embedded.

5.4 Interactions with desalination

WaterROUTE can, in future work, be combined with desalination models to evaluate the potential for local supply networks in combination with (mild) desalination. Desalination of lower quality water provided by shorter and less expensive networks can be preferable over extensive networks which provide high quality water. The Zeeuws-Vlaanderen simulation shows that up to 2030 the 375 $mgCl^{-} L^{-1}$ network is not significantly more expensive than the 400 $mgCl^{-} L^{-1}$ or 425 $mgCl^{-} L^{-1}$ network. Supplying water at 375 $mgCl^{-} L^{-1}$ in 2110 leads to a significant increase in costs. Instead of expanding the supply network (mild) desalination can be applied to achieve the desired quality. Desalination technology improvements and optimization of treatment train design allow for treatment of a wide range of saline streams (McGovern et al., 2014). Several modeling approaches exist to design treatment trains optimized for a specific input stream (Skiborowski et al., 2012; Wreyford et al., 2020). Coupling a treatment train model which calculates the lowest treatment train costs, such as DESALT (Wreyford et al., 2020), with the costs for water transport can yield better overall system configurations. The performance of such systems can be evaluated through Multi-Criteria Decision Making techniques such as Data Envelopment Analysis (Belmondo Bianchi et al., 2020). Determining the optimal location for desalination systems (at the user, at the individual supply sites, or at mixing locations) within decentralized networks has implications for the energy system and is a next step within the water-energy nexus research field (Hussey and Pittock, 2012).

6 Conclusions

WaterROUTE is a valuable tool for planning and design of water supply networks using local alternative water sources. WaterROUTE designs water supply networks that deliver water at the specified quality and quantity of the user based on the modeled or known availability of water resources in a region. The model is used in an example simulation to show how the dynamics of groundwater resources can be connected to the regional design and planning of water supply networks. Long-term scenarios can be generated which help to anticipate on changes in (fresh)water availability. WaterROUTE is demonstrated with a simulation for Zeeuws-Vlaanderen, the Netherlands, and shows that a small decrease in demand quality (a chloride concentration increase from 375 $mgCl^{-}$ L^{-1} to 400 $mgCl^{-}$ L^{-1} in 2110) results in a decrease of the supply network placement costs by 7% for a demand of 2.5 Mm^{3} $year^{-1}$. Delivering higher quality water leads to higher costs because longer networks are needed. The length of the water supply network for the Zeeuws-Vlaanderen simulation varies between 46.9 km and 122.1 km based on the water quality required at the demand location. The WaterROUTE model shows that costs can be up to 68% higher to supply water with the lowest possible salinity compared to a demand with no salinity constraint in the Zeeuws-Vlaanderen simulation. The best network configuration depends on the specific water quality demand of the user, the local water availability, and the time horizon over which planning occurs. As water quality requirements become more stringent, optimal network selection becomes more complex and modeling tools such as WaterROUTE are needed to assist decision makers in designing cost-effective decentralized water supply networks. WaterROUTE can, in future work, be expanded, and can be used to determine the optimal balance between water transport and water treatment/desalination, the use of aquifer storage and recovery within decentralized networks, and the creation of decentralized water supply networks based on the exchange of water between urban, industrial, and agricultural areas. Through these applications WaterROUTE can assist in coping with regional water scarcity over time by connecting demand sites with local supply sources.

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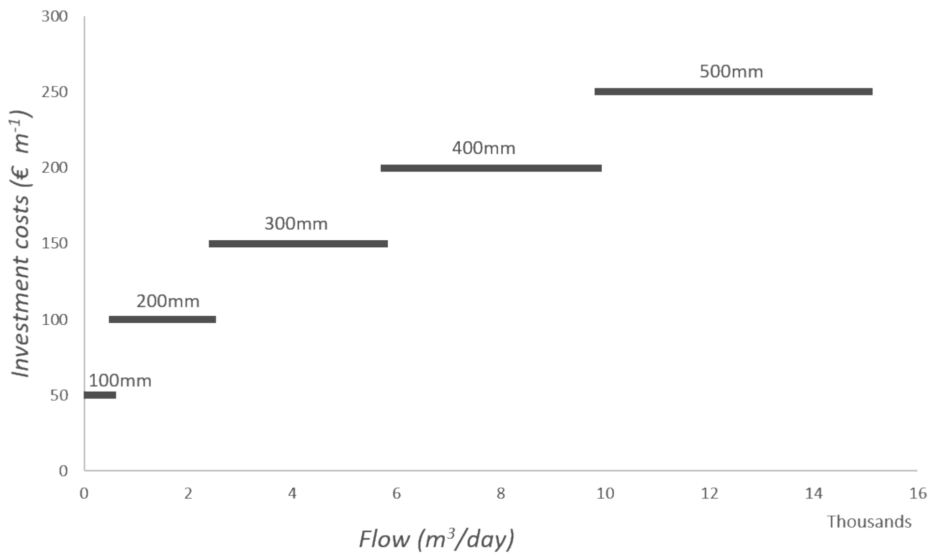
Supplementary Information

Supplementary Information 1 - Pipeline placement costs based on flow requirements and a cost of 0.5 € mm^{-1} diameter m^{-1}. Each plateau represents an available pipeline diameter, starting at 100 mm with increments of 100 mm, in which the flow velocity is within the optimal range (0.5 m s^{-1} and 1.5 m s^{-1}).



Supplementary Information 2 - Procedure for well placement and drawdown determination.

Methodology to determine the extraction and drawdown of well clusters in Zeeuws-Vlaanderen

The distribution of well clusters over the Zeeuws-Vlaanderen region and number of extraction wells was one-to-one adopted from Willet et al. (2020). We use a 100 m spaced well cluster grid as the model has also a spatial model cell distribution of 100 m.

The choice was made to optimize the extractions, rather than optimizing the well placement based on extraction possibilities, since the extraction wells will likely affect each other within a well cluster. In an iterative process the extraction rate per extraction well is adapted until the maximum drawdown of the phreatic groundwater level in a well cluster is at maximum 50 mm. The procedure is as follows:

1. The model starts with rates at each extraction well that are retrieved from Willet et al. (2020).

2. The model is run for one year to determine a steady-state piezometric head distribution.

3. The drawdown of the phreatic groundwater level at each well cluster due to the extraction well scheme is assessed by comparing the piezometric head distribution with a model without extraction wells. If the drawdown at an extraction well is more than 50 mm, the extraction rate is reduced; if it is less, the extraction rate is increased. This fraction is equal to 0.05 (piezometric head without extraction wells minus piezometric head with extraction wells).

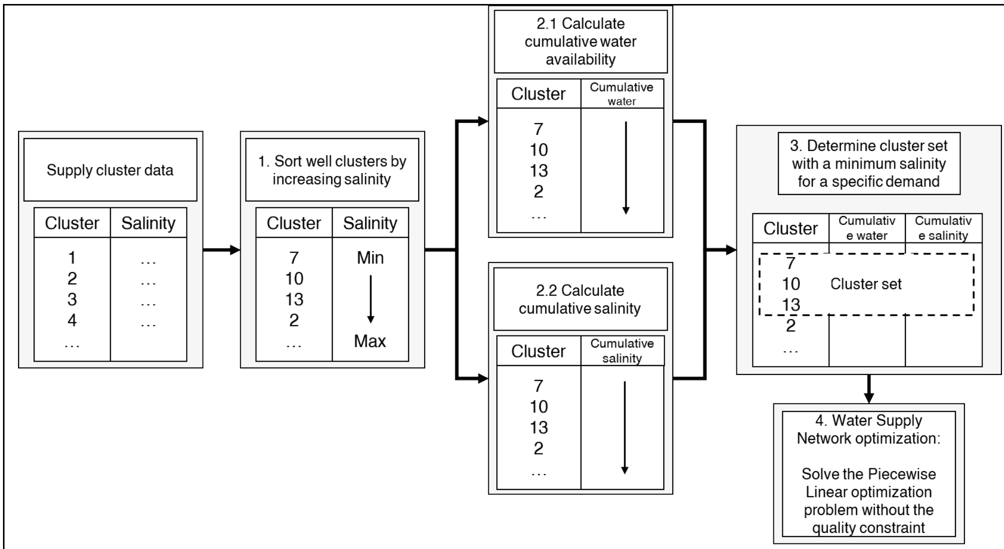
4. The model is run again, and the procedure is repeated for in total ninety-nine times. In general, after thirty iterations the total groundwater extraction rate does not change significantly anymore (and differs less than 0.1% from the value after ninety-nine iterations).

This procedure yields an approximation for the optimized extraction scheme over the extraction wells per well clusters over the entire region. In this approach, we neglect the effect that the groundwater salinity change has on piezometric heads; this is acceptable as we are dealing with only fresh to light brackish groundwater in the extraction wells.

5. The model is run again with the optimized extraction well scheme for the period 2020–2110 to determine the change of the chloride concentration over time. Every 10 days, the average chloride concentration that belongs to each well in each well cluster is determined (we account for the rate per well as they differ). In most wells, the average chloride concentration increases due to upconing, but the increase is small as the extraction rate per well is quite modest (the maximum drawdown is only 50 mm).

Reference: Willet, J., King, J., Wetser, K., Dykstra, J.E., Oude Essink, G.H.P., Rijnaarts, H.H.M., 2020. Water supply network model for sustainable industrial resource use a case study of Zeeuws-Vlaanderen in the Netherlands. Water Resources and Industry 24, 100131.

Supplementary Information 3 - Procedure to generate minimum salinity networks.

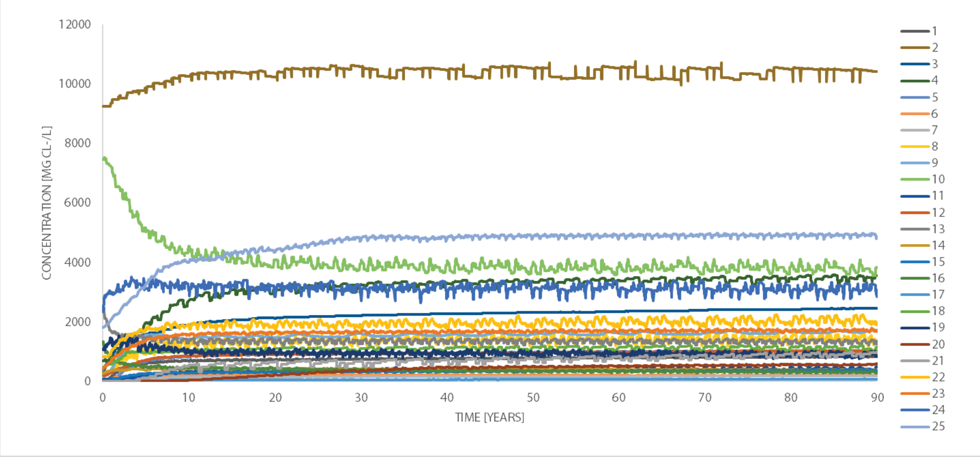


1. The well cluster data is sorted by increasing salinity in step 1.
2. In step 2.1 and 2.2 the cumulative water availability and salinity are determined.
3. The cumulative water available at cluster 2 in the figure is given by the sum of water from well clusters 7, 10, 13, and 2.
4. The cumulative salinity is determined by the sum of the total amount of salt from each well cluster divided by the total amount of water.
5. Based on the water demand at the demand site the minimum possible salinity can be determined by looking up the volume in the combined table from 2.1 and 2.2. This yields the cluster set which can provide the minimum possible salinity for that level of demand. This cluster set is used for the optimization procedure.
6. The optimization model is used to determine the optimal network layout. The quality constraints are disabled because the amount of water coming from each cluster has already been determined.

Supplementary Information 4 - Water extraction rate and average chloride concentration per cluster in 2020, 2030, 2045, and 2110.

Cluster	Extraction rate (mm^3 $year^{-1}$)	Salinity ($mgCl^-$ L^{-1})			
		2020	**2030**	**2045**	**2110**
1	0.508	2	519	637	747
2	0.010	9243	9828	10164	10353
3	0.046	212	1454	1825	2195
4	0.079	684	1761	2518	3134
5	0.315	0	553	756	926
6	0.107	75	173	201	213
7	0.130	1	82	118	153
8	0.498	174	922	1171	1351
9	0.088	188	1223	1391	1543
10	0.059	7464	5449	4641	4052
11	0.117	78	187	287	375
12	0.343	196	638	786	923
13	0.046	2518	1523	1424	1365
14	0.206	263	394	411	402
15	1.432	8	210	266	325
16	0.436	1327	570	486	382
17	0.099	0	23	38	57
18	0.060	415	899	1002	1087
19	0.154	1068	1193	1068	968
20	0.046	0	7	98	382
21	0.024	0	175	410	668
22	0.220	818	1593	1779	1934
23	0.757	414	1247	1469	1630
24	0.086	2331	3186	3181	3147
25	0.253	1816	3160	3863	4602
TOTAL	6.119	472	852	981	1095

Supplementary Information 5 - Simulated well clusters concentrations 2020–2110. Each line represents one well cluster.

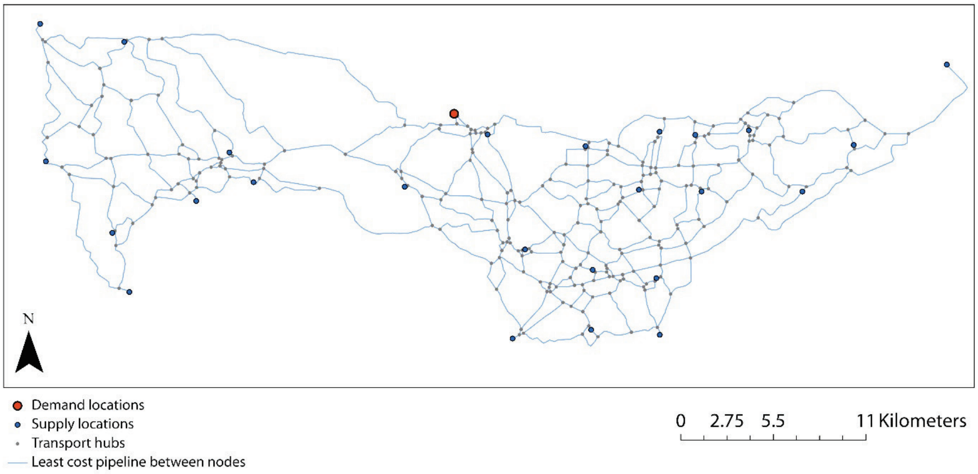


Supplementary Information 6 - Cumulative water salinity (mgCl⁻ L^{-1}) and cumulative water availability (Mm^{-3} $year^{-1}$). The dark shaded rows indicate that covering a demand of 2.5 Mm^{-3} $year^{-1}$ requires water up to and including the shaded cluster.

2030			**2045**			**2110**		
Cluster	***Salinity***	***Water***	***Cluster***	***Salinity***	***Water***	***Cluster***	***Salinity***	***Water***
20	6	0.05	17	38	0.10	17	57	0.10
17	17	0.15	20	57	0.15	7	112	0.23
7	48	0.28	7	86	0.28	6	144	0.34
6	83	0.38	6	118	0.38	15	290	1.77
21	88	0.41	15	235	1.81	11	296	1.89
11	110	0.52	11	238	1.93	20	298	1.93
15	184	1.96	21	240	1.96	16	313	2.37
14	204	2.16	14	256	2.16	14	320	2.57
1	264	2.67	16	295	2.60	21	324	2.60
5	294	2.98	1	351	3.11	1	393	3.11
16	329	3.42	5	388	3.42	12	446	3.45
12	357	3.76	12	424	3.76	5	486	3.76
18	366	3.82	18	433	3.82	19	505	3.92
8	430	4.32	19	458	3.98	18	514	3.98
19	456	4.48	8	537	4.48	8	607	4.48
9	471	4.56	9	554	4.56	13	614	4.52
23	581	5.32	13	562	4.61	9	632	4.61
3	589	5.37	23	690	5.37	23	773	5.37
13	597	5.41	22	733	5.59	22	819	5.59
22	636	5.63	3	742	5.63	3	830	5.63
4	651	5.71	4	767	5.71	4	862	5.71
25	758	5.96	24	802	5.80	24	896	5.80
24	792	6.05	25	930	6.05	10	928	5.86
10	837	6.11	10	966	6.11	25	1080	6.11
2	852	6.12	2	981	6.12	2	1095	6.12

Chapter 4

Supplementary Information 7 - Preliminary network over which flows are optimized. The network was generated using least cost path methods as described in: Willet, J., King, J., Wetser, K., Dykstra, J.E., Oude Essink, G.H.P., Rijnaarts, H.H.M., 2020. Water supply network model for sustainable industrial resource use a case study of Zeeuws-Vlaanderen in the Netherlands. Water Resources and Industry 24, 100131.



Supplementary Information 8 - Network configurations for a salinity at the demand location of 375 mgCl⁻ L⁻¹ or lower.

The optimal networks for a maximum salinity of 375 $mgCl^- L^{-1}$ vary significantly between 2030, 2045, and 2110 (Figure 1). This is reflected in the length of the required network which increases from 51.6 km to 68.8 km (Table 1), an increase of 33%, from 2030 to 2110. The main difference between the scenarios is the addition/exclusion of well clusters and the configuration to connect well clusters 14, 16 and 17 to the rest of the network. The differences in the networks in chronological order are:

- 2030 (Figure 1, A_1) to 2045 (Figure 1, B_1): well clusters 10 and 11 are added to the network. Well cluster 11 is needed for its low salinity. Well cluster 10 has a high salinity, 4641 $mgCl^- L^{-1}$, but is added to the network to ensure the demand is covered. Adding well cluster 10 to the network makes it possible to reduce the flow from cluster 12 to 548 $m^3 day^{-1}$, which reduces the required pipeline diameter from cluster 12 to junction 12|15. Cluster 14 needs to be operated at 100% instead of 97%, requiring an increase in pipeline diameter. The addition of cluster 11 to the network moves the main branch of the network to the east.
- 2045 (Figure 1, B_1) to 2110 (Figure 1, C_1): salinization of the well cluster requires expansion of the network. Cluster 20 is added to the network to reach the desired water quality, and well cluster 10 is excluded. The operation capacity of cluster 12 is further reduced from 58% to 50%. This reduction is purely needed to reach the desired water quality at the demand location.

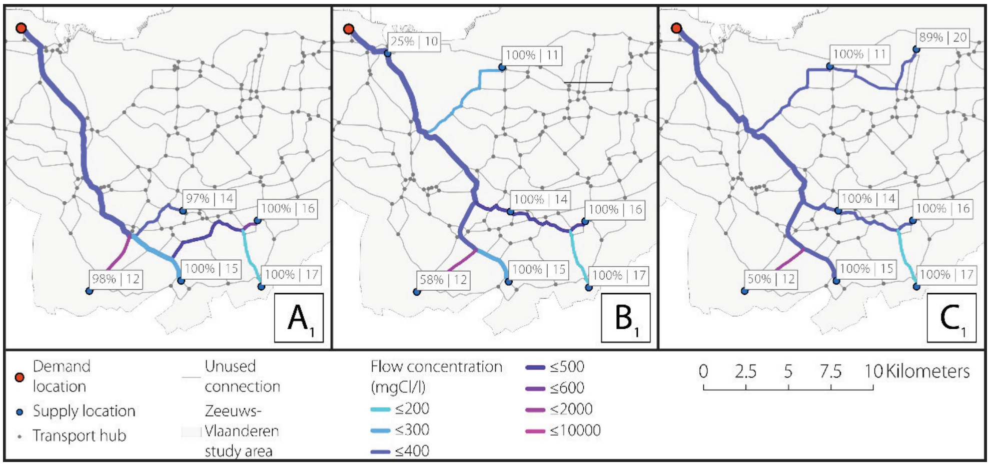


Figure 1 - Optimal network configurations for a maximum of 375 $mgCl^- L^{-1}$ in 2030 (A, 337 $mgCl^- L^{-1}$), 2045 (B, 375 $mgCl^- L^{-1}$), and 2110 (C, 375 $mgCl^- L^{-1}$). The labels show the rate (relative to water availability) at which the well clusters are operated and the cluster number (percentage | cluster number).

The water supplied by the 2030 network reaches the demand location with a concentration of 337 $mgCl^- L^{-1}$ instead of 375 $mgCl^- L^{-1}$ (Table 1). This indicates that a network with lower costs than a network which provides 375 $mgCl^- L^{-1}$ exists. The specific combination of water availability and water quality at each cluster at this specific point in time makes this possible. The difference in quality over time is highest for the 2030 network (73 mgCl$^-$ L^{-1}) and lowest for the 2045 network (58 mgCl$^-$ L^{-1}).

Table 1 - Cost and salinity effects of using 375 mgCl$^-$ L^{-1} networks at different periods.

375 mgCl^{-1} L^{-1} NETWORK (NETWORK | COSTS | LENGTH)	APPLIED IN 2030	APPLIED IN 2045	APPLIED IN 2110
	(mgCl$^-$ L^{-1})	(mgCl$^-$ L^{-1})	(mgCl$^-$ L^{-1})
A_1 | 100% |51.6 km	337	376	410
B_1 | 103% | 59.0 km	344	375	402
C_1 | 110% | 68.8 km	306	341	375

Supplementary Information 9 - Network configurations for a salinity at the demand location of 400 mgCl$^-$ L^{-1} or lower.

Networks for a maximum salinity at the demand location of 400 mgCl$^-$ L^{-1} have similar costs and configurations for 2030 and 2045. Achieving the same salinity in 2110 requires a different network configuration (Figure 2). The length of the networks reduces from 51.8 km in 2030 to 51.6 km in 2045 and increases to 59.0 km in 2110. The differences in the networks in chronological order are:

- 2030 (Figure 2, A_2) to 2045 (Figure 2, B_2): well clusters 10 and 13 can be removed from the network by increasing the capacity at which cluster 16 is operated from 85% to 100%. Cluster 16 is crucial for the network because salinity significantly decreases over time. Cluster 14 is connected to the rest of the network by going west (2045) instead of east (2030). This change is needed to avoid increasing the pipeline capacity at the junction of cluster 15 with clusters 14|16|17.
- 2045 (Figure 2, B_2) to 2110 (Figure 2, C_2): cluster 10 and 11 are added to the network. Cluster 14 is operated at 100% instead of 97% which changes the configuration of the network. Cluster 12 is operated at 58% to reduce the required pipeline diameter and cluster 10 is used to provide the remaining water.

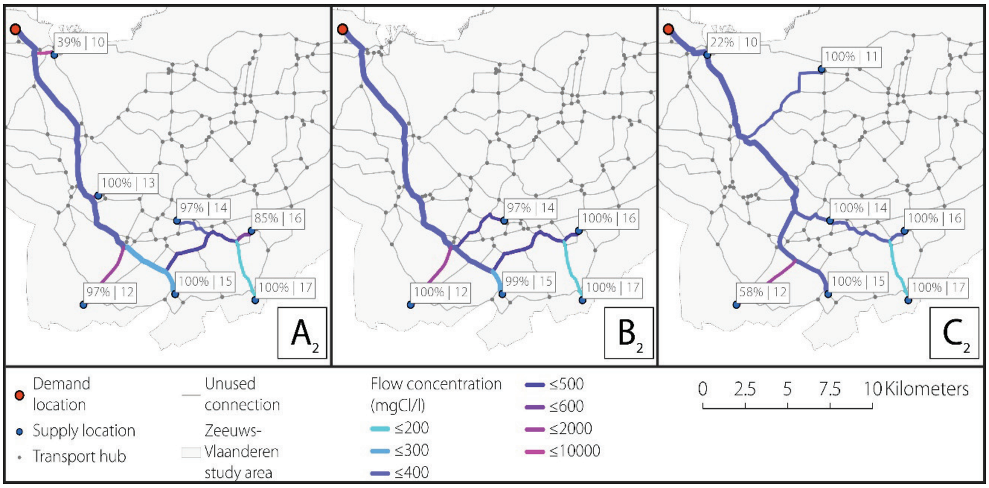


Figure 2 - Optimal network configurations for a maximum of 400 mgCl$^-$ L^{-1}in 2030 (A, 400 mgCl$^-$ L^{-1}), 2045 (B, 378 mgCl$^-$ L^{-1}) and 2110 (C, 400 mgCl$^-$ L^{-1}). The labels show the rate (relative to water availability) at which the well clusters are operated and the cluster number (percentage | cluster number).

The 2110 network supplies water with the smallest difference in salinity over time (59 mgCl$^-$ L^{-1}, Table 2). The 2045 network supplies water with a concentration of 378 mgCl$^-$ L^{-1} instead of 400 mgCl$^-$ L^{-1}. Flexibility off all networks is limited by the maximum capacity of the pipelines in combination with water availability at the supply sites. For the 2030 network increasing the water supplied by clusters 14 or 16 requires increasing pipeline capacity, while increasing extractions from clusters 10 or 12 has a high impact on water quality. The 2045 network operates most clusters at, or close to, maximum capacity. The 2110 network operates all low salinity clusters at 100% capacity.

Table 2 - Cost and salinity effects of using 400 $mgCl^{-}$ L^{-1} networks at different periods.

400 $mgCl^{-1}$ L^{-1} NETWORK (NETWORK | COSTS | LENGTH)	**APPLIED IN 2030**	**APPLIED IN 2045**	**APPLIED IN 2110**
	($mgCl^{-}$ L^{-1})	($mgCl^{-}$ L^{-1})	($mgCl^{-}$ L^{-1})
A_2 | 100% | 51.8 km	400	432	462
B_2 | 100% | 58.1 km	339	378	412
C_2 | 104% | 59.0 km	341	372	400

Supplementary Information 10 - Network configurations for a salinity at the demand location of 425 mgCl$^-$ L^{-1} or lower.

The networks for 425 mgCl$^-$ L^{-1} are the same in 2030 and 2045 but changes for 2110 (Figure 3). The networks for 425 mgCl$^-$ L^{-1} practically have the same costs (Figure 3). Freshening of cluster 16 makes it possible to reach the desired water quality over time while keeping costs at the same level. In 2110 clusters 10 and 13 are removed from the network because cluster 16 is operated at a higher capacity. The differences in the networks in chronological order are:

- 2030 (Figure 3, A_3) to 2045 (Figure 3, B_3): The network configuration remains the same. Cluster 16 is operated at a higher capacity to reach the desired salinity while cluster 10 is operated at a lower capacity.
- 2045 (Figure 3, B_3) to 2110 (Figure 3, C_3): cluster 10 and 13 are removed from the network. Cluster 16 is operated at 100% capacity instead of 86%. Cluster 14 connects to the main branch going west instead of east. This configuration change is needed to avoid increasing pipeline capacity at the junction of cluster 15.

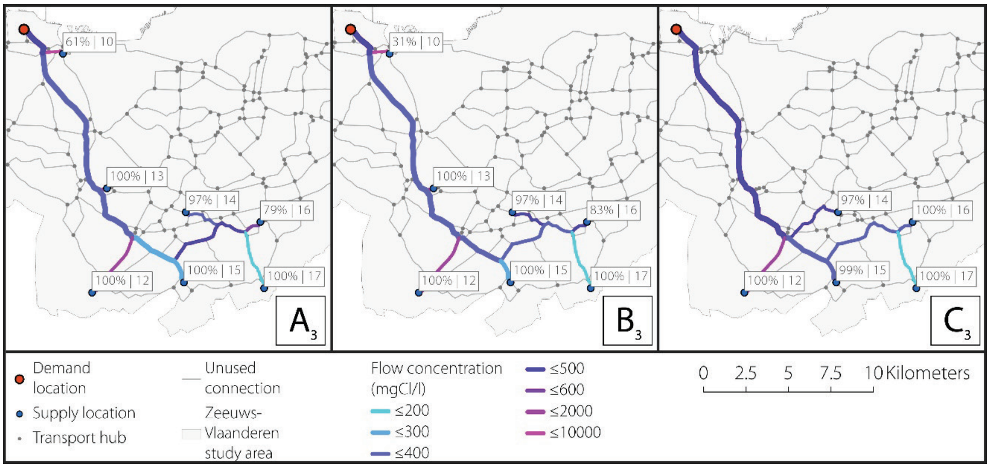


Figure 3 - Optimal network configurations for a maximum of 400 mgCl$^-$ L^{-1}in 2030 (A, 400 mgCl$^-$ L^{-1}), 2045 (B, 378 mgCl$^-$ L^{-1}), and 2110 (C, 400 mgCl$^-$ L^{-1}). The labels show the rate (relative to water availability) at which the well clusters are operated and the cluster number (percentage | cluster number).

The 2030 network has the smallest difference in water quality when applied in a different period (58 mgCl$^-$ L^{-1}). The 2110 network supplies water at 412 mgCl$^-$ L^{-1} instead of 425 mgCl$^-$ L^{-1} because this leads to a lower cost network. The 2110 network is the most efficient because all clusters are operated close to or at maximum capacity (cluster 15 can provide 1% more water, cluster 14 cannot provide more water without increasing pipeline capacity).

Table 3 - Cost and salinity effects of using 425 mgCl$^-$ L^{-1} networks at different time periods.

425 mgCl^{-1} L^{-1} NETWORK (NETWORK | COSTS | LENGTH)	APPLIED IN 2030	APPLIED IN 2045	APPLIED IN 2110
	(mgCl$^-$ L^{-1})	(mgCl$^-$ L^{-1})	(mgCl$^-$ L^{-1})
A_3 | 100% | 51.8 km	425	454	483
B_3 | 100% | 51.8 km	391	425	457
C_3 | 100% | 51.6 km	339	378	412

Chapter 5

Decentralized water supply network optimization using harvested rainwater and groundwater as alternative water sources

Abstract

Industry can cope with freshwater scarcity by using alternative regional water sources, such as harvested rainwater, brackish groundwater, or treated wastewater effluent. The design of a water supply network (WSN) using multiple alternative water sources requires modelling tools to optimize the network layout and to minimize costs. In this study we present new modelling tools for WSN optimization where storage is needed to make effective use of intermittent water sources, such as harvested rainwater. We test these modelling tools by optimizing water supply networks using both harvested rainwater and groundwater. Using rainwater and groundwater simultaneously requires location specific data about infrastructure costs. A modified Yield After Spillage model is used to generate location specific infrastructure costs for rainwater storage basins. The infrastructure costs for the placement of groundwater wells depend on the number and depth of wells in a well cluster. WSN optimization is demonstrated by simulating several scenarios for an industrial water demand site in the south of the Netherlands. The results of the simulations show that harvested rainwater and groundwater are competitive in terms of costs. The use of rainwater or groundwater depends on the vicinity to the demand location and the amount of water available. By making use of harvested rainwater the regional availability of alternative water resources is increased, which reduces WSN costs by 42% on average. The modelling tools developed in this study can be adapted to any other regionally available water source, which is constant or intermittent, in decentralized water supply networks.

This chapter is under preparation for publication as:

Willet, J.; Wetser, K.; Dykstra, J. E.; Rijnaarts, H.H.M.: Decentralized water supply network optimization using harvested rainwater and groundwater as alternative water sources.

1 Introduction

Increasing water scarcity around the world (Hanasaki et al., 2013) forces human communities to reconsider the way in which water is sourced and used. Exploiting water resources beyond the rate at which they can be sustainably replenished leads to ecosystem degradation and welfare loss (Mekonnen and Hoekstra, 2016). The transition towards sustainable water supply systems requires a paradigm shift in the way water supply systems are designed and operated.

Industry is reliant on water and is a sector where water shortages can have significant financial impacts. The industrial sector is generally reliant on centralized water supply infrastructures (Domènech, 2011; Gleick, 2003) and is one of the first where water supply is reduced in case of drought (Rijkswaterstaat, 2020). A transition towards decentralized water supply systems can increase water supply security (Domènech, 2011; Leflaive, 2009; Piratla and Goverdhanam, 2015) in times when changes to precipitation patterns and water availability are expected (IPCC, 2021; Trenberth, 2011). Using multiple alternative water resources (e.g. surface water, groundwater, brackish water, rainwater, wastewater) is a possible approach for such a transition.

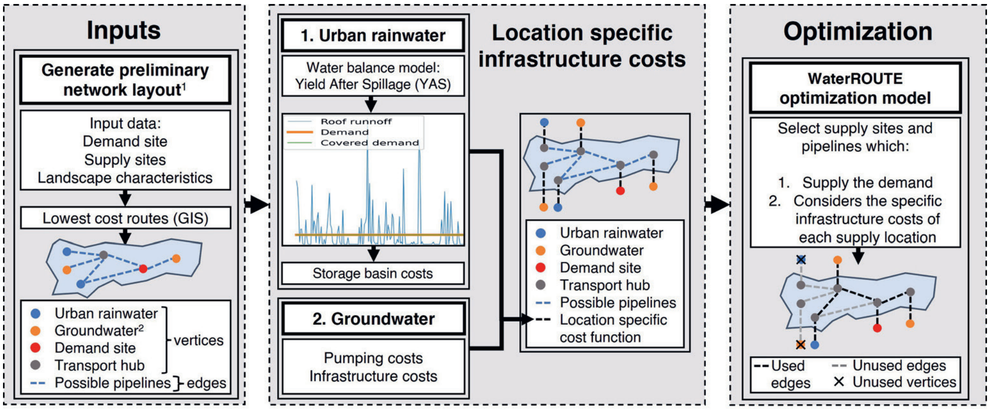
One of the potential alternative water resources for industry is harvested rainwater from urban areas. Rainwater harvesting can increase the self-sufficiency of urban areas (Agudelo Vera, 2012a) and can reduce the drinking water needs for individual homeowners (Campisan et al., 2017; Campisano and Lupia, 2017). A secondary benefit of urban rainwater harvesting is that runoff is reduced or captured, which reduces the risk of water nuisance and flooding (Chan and Bras, 1979; Sample and Liu, 2014). Expected changes in precipitation patterns (higher intensities) are likely to increase the risk of flooding in urban areas if preventive measures are not taken (Ashley et al., 2005; Schreider et al., 2000). The potential benefits of urban rainwater harvesting are constrained by the purposes for which rainwater can be used. Domestic rainwater use is limited to purposes for which the quality of rainwater is suitable (Campisano et al., 2017). The limited usability of rainwater in cities results in surpluses which can be exported (Agudelo Vera, 2012a) for use in industry.

Harvesting rainwater from urban areas requires the installation of water storage facilities and sewerage systems in which rainwater is collected separately from domestic wastewater. Storage facilities are needed because rainwater availability is intermittent. Storage makes it possible to overcome the temporal mismatch in rainwater supply and industrial demand. Several modelling approaches have been developed to optimize the sizing and design of RWH storage facilities (Sample and Liu, 2014). The presence of contaminants in harvested rainwater depends on the catchment surface but in general rainwater is of good quality (H.J. Liefting et al., 2020). Separated sewer systems are needed to prevent contamination of high quality rainwater with domestic wastewater to avoid unnecessary treatment costs. The implementation of separated sewers also reduces the risk of sewer overflows with untreated wastewater to surface waters, and can make it easier to deal with high intensity rainfall events (J.G. Langeveld, 2019).

Water transport infrastructure is needed to deliver groundwater and rainwater harvested in cities to the industrial facilities where it can be used. The placement and operation of infrastructure to transport water resources is costly (Plappally and Lienhard, 2013) and varies depending on location specific circumstances (Chee et al., 2018; Feldman et al., 1995; Zhou et al., 2019). The high complexity of the water system and water supply network design requires modelling approaches to aid decision makers (Medema et al., 2008). We refer to the work of Awe et al., 2019, Clark and Cresswell, 2011, Sieber and Purkey, 2015, and Sonaje and Joshi, 2015 for an extensive overview of models/modelling approaches in the field of water resources management.

One of the modelling approaches for water supply network design is WaterROUTE (Willet et al., 2020; Willet et al., 2021). WaterROUTE was developed to assist decision makers in the design of decentralized water supply networks which make use of alternative water resources on a regional scale. WaterROUTE optimizes the layout of decentralized water supply networks based on the location specific costs for water transport infrastructure.

The goal of this study is to develop modelling methods to design decentralized water supply networks where storage is needed to deal with temporal variations in water availability. Harvested rainwater is a potential water source for which storage is needed. The possibility to use storage was not yet part of WaterROUTE and is investigated in this study. Besides including storage WaterROUTE is adapted to use multiple types of alternative water resources simultaneously: rainwater and groundwater. Each alternative water source has different costs due to specific infrastructure requirements. For example, using groundwater requires borehole and pumping infrastructure while using rainwater requires storage infrastructure. In this study the functionality of WaterROUTE is expanded by including these



¹See Willet et al., 2020 for details
²See Willet et al., 2021 for details

Figure 1 - Model framework of WaterROUTE using location specific cost functions for urban rainwater and groundwater as supply sites.

variations in infrastructure costs in the optimization of decentralized water supply networks. The new functionality is demonstrated by generating water supply networks using rainwater harvested from urban areas together with groundwater for a large industrial site in the south of the Netherlands.

2 Methodology

In this research modelling tools are developed and added to WaterROUTE to optimize the configuration of decentralized water supply networks for industry that use harvested rainwater and groundwater. Optimization is based on minimizing the capital and operational costs of the network from an economic perspective. Rainwater and groundwater are available at several locations in the study area. At each water supply location the infrastructure requirements – and the costs – are different depending on the amount of water available. The differences in local costs must be included in the optimization procedure to determine the best overall network configuration.

In this extended WaterROUTE framework we take the water availability from different water sources in a region and a preliminary set of pipelines as inputs. The output is a selection of pipelines from the preliminary set which forms the lowest cost water supply network (WSN) based on the demand of the water user. The overall structure of the WaterROUTE model used in this study is shown in Figure 1. The optimization problem is presented in Section 2.1, the procedure to determine rainwater availability and storage costs is presented in Section 2.2. The

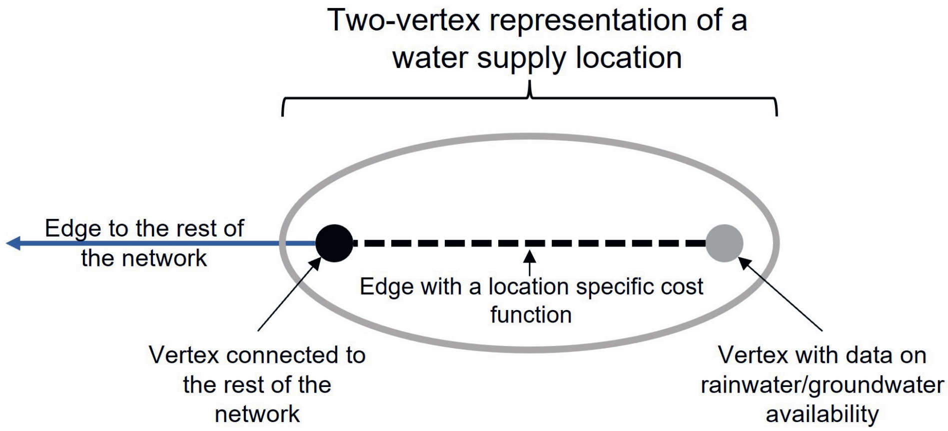


Figure 2 - Two-vertex representation of a groundwater or urban rainwater harvesting location in WaterROUTE.

availability of groundwater in the region (see Willet et al., 2021 for details), and the generation of the preliminary network (see Willet et al., 2020 for details) are additional model inputs and are briefly explained in Section 2.3.

2.1 WaterROUTE optimization model

2.1.1 Optimization problem formulation

In WaterROUTE water supply networks are represented with vertices (V) and edges (E_{V_i,V_j}) in a planar mathematical system (see Willet et al., 2020; Willet et al., 2021). Supply locations, demand locations, and transport hubs are represented with vertices and the pipeline connections between them are represented with edges. The model operates based on the principle of a water balance throughout the network to distribute water and to match supply and demand.

In previous studies using WaterROUTE the water supply locations were modelled as a single vertex. In this study rainwater harvesting locations and groundwater extraction locations are modelled as two-vertex elements to allow for location specific cost functions to be included (Figure 2). In these two-vertex elements one vertex functions as the physical location with the associated data on water availability, the other vertex functions as the connection with the water supply network. The edge connecting the two vertices is used to represent the location specific costs for rainwater storage or groundwater extraction, which we will discuss in Section 2.1.1.

Table 1 - WaterROUTE parameters used to formulate the optimization problem with multiple types of water supply sources.

Parameter	***Description***
V_i	Vertex i represents the source or demand location i
$E_{i,j}$	Edge i,j represents the connection between vertex i (V_i) and vertex j (V_j)
s_i	Water supply ($s_i > 0$) or demand ($s_i < 0$) at vertex i (m^3 day^{-1})
$x_{i,j}$	Flow of water over edge i,j (decision variable in the optimization problem) (m^3 day^{-1})
$r_{i,j}$	Pipeline investment and operation costs per meter (€ m^{-1}) per unit flow (m^3 day^{-1}) → (€ m^{-1} / m^3 day^{-1}) (based on a maximum flow velocity of 1.5 m s^{-1})
$l_{i,j}$	The length of the pipeline represented by edge i,j
$u_{i,j}$	Maximum flow capacity of pipeline section (edge) i,j (m^3 day^{-1})

Water can be transported from vertex V_i into vertex V_j over edge $E_{V_i,V_j} \rightarrow E_{i,j}$. Within the set of edges $E_{i,j}$ we distinguish three subsets:

- $E_{i,j}^{p}$: edges representing pipeline (p) connections between physical locations. Using these edges incurs the pipeline costs $(r_{i,j})$ based on the length $(l_{i,j})$ of the pipeline.
- $E_{i,j}^{c}$: edges between the two-vertex representation of groundwater well clusters (c). Using these edges incurs the infrastructure costs and pumping costs for the operation of a specific well cluster.
- $E_{i,j}^{h}$: edges between the two-vertex representation of urban rainwater harvesting sites (h). Using these edges incurs the infrastructure costs for the placement of water storage basins at the urban area.

The WaterROUTE optimization model determines the amount of water that should be transported over each edge $(E_{i,j})$ to minimize the total costs of the water supply network. The amount of water transported over an edge is represented with the decision variable $x_{i,j}$. The decision variable $(x_{i,j})$ is used in the objective function of the optimization problem (Section 2.1.2). The parameters for the WaterROUTE optimization problem used in this study are shown in Table 1 and we discuss these parameters in the coming sections.

2.1.2 Objective function

The WaterROUTE implementation in this study minimizes the investment and operational costs of water supply networks (WSNcosts, Water Supply Network costs). To make the comparison between different types of infrastructure for groundwater and rainwater possible the lifetime capital costs and the lifetime operational costs are used. We use a 25-year lifetime for infrastructure to calculate the total capital and operational costs. The initial infrastructure investment costs are covered with a 25-year loan at a 3% interest rate and operational costs consist of the pumping costs for pipes and wells with an electricity price of 0.2 € kWh^{-1}. The lifetime costs of using water from different sources are approximated with piecewise linear functions in the objective function, given by

$$\text{minimize } WSN\text{costs} = \sum_{(i,j)\in E^p} P_{ij}(x_{ij}) + \sum_{(i,j)\in E^c} W_{ij}(x_{ij}) + \sum_{(i,j)\in E^h} H_{ij}(x_{ij}) \qquad (1)$$

The first term – $\sum_{(i,j)\in E^p} P_{ij}(x_{ij})$ – of the objective function represents the costs for the pipelines. Due to a limited number of possible pipeline diameters and general design criteria for water distribution networks (Mesman and Meerkerk, 2009) a maximum flow velocity within pipes of 1.5 m s^{-1} and a peak factor[1] of 1.5 is used. The lifetime pipeline costs for different flows are shown in Supplementary Information 1 and are implemented in the objective function with

$$P_{ij}(x_{ij}) = \begin{cases} 0 & x_{ij} = 0, \\ r_{ij}^k(x_{ij}) \cdot l_{ij} & \lambda_{ij}^{k-1} < x_{ij} \leq \lambda_{ij}^k \end{cases} \quad \text{with } r_{ij}^k \text{ and } \lambda_{ij}^k \text{ as defined in Table 2} \qquad (2)$$

in which the flow in the pipeline is x_{ij} and λ_{ij}^k are the bounds on the cost function for a specific amount of flow. The costs over an edge where there is no flow are 0 ($x_{ij} = 0$). The index k represents the individual linear segments of the cost function based on the available pipeline diameters. The total costs for a pipeline segment is obtained by multiplying the lifetime costs per meter – calculated with $r_{ij}^k(x_{ij})$ – by the length of the pipeline segment l_{ij}. For example, the lifetime costs for a 100 m pipeline transporting 0.22 Mm^3 year^{-1} is determined with the second row of Table 2, in this row k is 1 and l_{ij} is 100 m, which results in $r_{ij}^1(0.22) \cdot 100\ \text{m} = (236 \cdot 0.22 + 75)\ € \ \text{m}^{-1} \cdot 100\ \text{m} = €\ 12692$

[1] The peak factor is used to ensure pipelines have a large enough capacity during peak demand periods. For example, the capacity of a pipeline which is expected to transport 100 m^3 hour^{-1} with a peak factor of 1.5 is designed at 150 m^3 hour^{-1} (1.5×100 m^3 hour^{-1}). The pipeline diameter is based on a flow velocity of 1.5 m s^{-1} during the peak demand.

Table 2 - Lifetime pipeline costs for a flow between 0 and 13 Mm^3 $year^{-1}$ based on a 25-year loan for investments at 3% interest and energy costs for pumping of 0.2 € kWh^{-1}.

k	λ_{ij}^k	***Flow over edge*** x_{ij} **(Mm^3 $year^{-1}$)**	***Lifetime costs*** $r_{ij}^k(x_{ij})$ ***(€ m^{-1})***
	0	0	*0*
1	0.3	$0 < x_{ij} \leq 0.3$	$236 \cdot (x_{ij}) + 75$
2	1.0	$0.3 < x_{ij} \leq 1.0$	$114 \cdot (x_{ij}) + 112$
3	2.1	$1.0 < x_{ij} \leq 2.1$	$74 \cdot (x_{ij}) + 152$
4	3.6	$2.1 < x_{ij} \leq 3.6$	$56 \cdot (x_{ij}) + 190$
5	5.9	$3.6 < x_{ij} \leq 5.9$	$42 \cdot (x_{ij}) + 239$
6	7.9	$5.9 < x_{ij} \leq 7.9$	$38 \cdot (x_{ij}) + 266$
7	*10.7*	$7.9 < x_{ij} \leq 10.7$	$31 \cdot (x_{ij}) + 318$
8	*13.0*	$10.7 < x_{ij} \leq 13$	$25 \cdot (x_{ij}) + 380$

The height difference between nodes is not considered in the formulation of the optimization problem in this study because the study area of the example simulation is characterized by minimal height differences. In areas with larger height differences additional pumping costs can be added to the objective function based on the flow and the height difference which needs to be overcome over each edge.

The second term – $\sum_{(i,j)\in E^c} W_{ij}(x_{ij})$ – in the objective function represents the lifetime costs for well clusters based on the investment costs for the wells and the pumping costs based on the depth of the wells. Every well cluster (c) in the study area has a different number of wells resulting in well cluster specific investment requirements depending on the amount of water extracted, given by

$$W_{ij}(x_{ij}) = \begin{cases} 0 & x_{ij} = 0, \\ (P_c + I_c) \cdot \left(\dfrac{x_{ij}}{x_{c,\max}}\right) + CW_{c,\text{fixed}} & 0 < x_{ij} \leq x_{c,\max} \end{cases} \tag{3}$$

where P_c are the pumping costs (for well cluster c) if all water from the well cluster is used, I_c are the infrastructure costs if all water in the well cluster is used, x_{ij} is the amount of water extracted from the well cluster, $x_{c,\max}$ is the maximum amount of water which can be extracted from the well cluster, and $CW_{c,\text{fixed}}$ are the fixed costs to place the first well.

Table 3 - Parameters for well placement and operational costs.

Parameter	Value	Description
pe	84%	Pump efficiency
me	90%	Motor efficiency
ep	0.2	Electricity price (€ kWh^{-1})
G	25	Gravel (€ well^{-1})
D	25	Depth of wells (m)
P	50	Well borehole placement costs (€ m depth^{-1})
f	2.78×10^{-7}	kWh per joule (kWh J^{-1})
v	2	Investment factor for well cluster pipelines

The total pumping costs P_c for well cluster c over 25 years is determined with

$$P_C = \sum_{i=1}^{|W_c|} \frac{x_{i,c} \cdot g \cdot D_{i,c}}{pe \cdot me} \cdot f \cdot ep \tag{4}$$

where $|W_c|$ is the set of wells in well cluster c, $x_{i,c}$ is the maximum water extraction (kg) from well i in well cluster c over 25 years, g is the acceleration due to gravity, $D_{i,c}$ is the depth of well i in well cluster c, pe is the pump efficiency, me is the motor efficiency. These parameters return the lifetime energy use (in joule) for the operation of the well clusters. The conversion of energy use to costs is done with ep (the price of electricity in € kWh^{-1}) and f (kWh J^{-1}). In this study the amount of water extracted by each well in a single well cluster is the same and is based on the total water availability in the well cluster divided by the number of wells in the well cluster. The parameters used to calculate the well cluster costs in this study are shown in Table 3.

Individual wells have a depth of 25 meters and are lined with gravel to ensure clogging of the well is minimized. The total infrastructure costs I_c for well cluster c over 25 years are determined with

$$I_C = \sum_{i=1}^{|W_c|} \left(\frac{r \cdot v \cdot (D_{i,c} \cdot P + G)}{1 - (1+r)^{-n}} \right) \cdot n \tag{5}$$

where I_c are the lifetime infrastructure costs for well cluster c in euro per 25 years, r is the interest rate (0.03 = 3%), $D_{i,c}$ is the depth of well i in well cluster c, P are the well placement costs in relation to the depth of the well in € m depth^{-1}, G are the costs for the gravel liner in € well^{-1}, and n is the number of years of the loan

(25 years). The investment factor v is used for the pipeline costs in a well cluster based on the costs for borehole placement. The value for v is set at 2 in this study based on consultation with experts in the field of water infrastructure.

The fixed costs to start exploiting a well cluster $(CW_{c,\text{fixed}})$ are € 3661 for all well cluster in this study. These costs are the costs to drill the first well ($D_{1,c}$), and are calculated with

$$cw_{c,\text{fixed}} = \left(\frac{r\left(D_{1,c} \cdot P + G\right)}{1-(1+r)^{-n}}\right) \cdot n \tag{6}$$

The third term – $\sum_{(i,j)\in E^h} H_{ij}(x_{ij})$ – in the objective function is the sum of the lifetime costs for the storage basins required to capture the rainwater harvested from each urban area h and is calculated with

$$H_{ij}(x_{ij}) = \begin{cases} 0 & x_{ij} = 0, \\ (gw_h + lc_h) \cdot \left(\dfrac{x_{ij}}{x_{h,\max}}\right) + CH_{h,\text{fixed}} & 0 < x_{ij} \le x_{h,\max} \end{cases} \tag{7}$$

where gw_h are the lifetime costs for the ground/construction work of the storage infrastructure for urban area h, lc_h are the costs for the land area required for the storage basin, x_{ij} is the flow of water from the storage basin towards the water supply network, $x_{h,\max}$ is the maximum flow of water from the storage basin to the water supply network, and $CH_{h,\text{fixed}}$ are the fixed costs incurred when placing a storage basin.

In this research, an open storage basin with a depth of 3 m with a liner and a lifetime of 25 years is used. Data from literature was used to establish the variable costs for ground/construction work of such systems depending on the storage volume (L.M. Curtis, M.M. Nelson, P.L. Oakes, 2001; stowa, 2014). The total lifetime costs are given by

$$gw_h = \left(\frac{r \cdot sc \cdot V_h}{1-(1+r)^{-n}}\right) \cdot n \tag{8}$$

where sc are the costs per cubic meter of storage capacity, set at 2.4 € m^{-3}, V_h is the storage capacity in m^3 corresponding to the maximum amount of water which can be harvested from urban area h, r is the interest rate, and n is the lifetime of the storage basin in years.

The fixed costs for storage basin placement (ch) are set at € 15,000 based on the values reported in L.M. Curtis, M.M. Nelson, P.L. Oakes, 2001; stowa, 2014. Over a 25-year loan period these costs are € 29335, given by

$$CH_{h,fixed} = \left(\frac{r \cdot ch}{1-(1+r)^{-n}}\right) \cdot n \tag{9}$$

Besides the ground/construction works we consider the costs for the (agricultural) land required to place the storage basin. Based on a basin depth of 3 m the costs for land are given by

$$lc_h = \left(\frac{r\left({}^{lp}/_{d} \cdot V_h\right)}{1-(1+r)^{-n}}\right) \cdot n \tag{10}$$

where lp is the price of land in € m^{-2} – € 75000 per hectare (Boerderij.nl, 2021) – and d is the depth of the storage basin.

The maximum storage capacity V_h for each urban area h is determined with a water balance model and daily precipitation data (see Section 2.2).

2.1.3 Constraints: water balance and pipeline capacity

At each vertex the amount of water extracted should be smaller than the amount of water available, which is ensured with

$$\sum_{(i,j)\in E} x_{ij} - \sum_{(j,i)\in E} x_{ji} \leq s_i. \qquad \forall i \in V \tag{11}$$

where x_{ij} are the outgoing flows from vertex s_i and x_{ji} are the incoming flows.

If an edge is not used a flow of 0 is assigned to that edge, but the maximum capacity (u_{ij}) of the edge should not be exceeded, which is ensured by

$$0 \leq x_{ij} \leq u_{ij} \qquad \forall (i,j) \in E \tag{12}$$

For simulations in this study no maximum capacity for the pipelines is defined since the required pipeline capacity is determined by the optimization model. When existing pipelines, with a specific maximum capacity $u_{i,j}$, are re-used this constraint ensures the available capacity is not exceeded.

All vertices in the network can perform the function of a transport hub. This occurs when there is no water available at the vertex ($s_i = 0$) or when the network passes through a vertex but it is not worthwhile to incur the fixed costs to make use of the available water. To make this possible we use

$$\sum_{(i,j)\in E} x_{ij} - \sum_{(j,i)\in E} x_{ji} = 0 \qquad \forall i \in V; s_i = 0 \qquad (13)$$

$$\sum_{(i,j)\in E} x_{ij} - \sum_{(j,i)\in E} x_{ji} \geq 0 \qquad \forall i \in V; s_i > 0 \qquad (14)$$

Equation (13) ensures that the outgoing flow (x_{ij}) is equal to the incoming flow (x_{ji}) for all vertices where no water is available ($s_i = 0$). Equation (14) ensures that a supply site in the middle of the network can function as transport hub.

2.1.4 Complete formulation and model outputs

The complete formulation for the WaterROUTE: Multiple Supply optimization problem is written as

minimize	Objective function: WSNcosts of Equation (1)
subject to	Constraints (11) - (14)

The solution of the optimization problem returns the amount of water flowing over each edge which results in the lowest cost WSN while supplying the required amount of water to the demand sites. Edges which are not used do not contribute to the total WSN costs and are assigned a flow of 0, which is possible due to the piecewise linear formulation in Equation (2), (3), and (7). Each optimization has a maximum runtime of 1200 seconds[2] after which the best feasible solution found up to that point is returned.

2.2 Urban rainwater harvesting

To make rainwater available for industrial use storage basins are needed. Storage basins can convert intermittent precipitation into a constant water availability. The

[2] Run on an Intel® Xeon® W-2133 computer (12 CPUs @ 3.60GHz) with 150 GB of RAM with Python (version: 3.7.9) and the Gurobi solver (version: 9.0.3)

Table 4 - Parameters used in the modified Yield After Spillage algorithm.

Parameter	Description
v_t	Volume in the storage basin at time t (m^3)
q_t	Total roof runoff from an urban area flowing into the storage basing at time t (m^3)
y_t	Yield (the amount of water removed from storage for use in industry) at time t (m^3)
o_t	Overflow from the storage basin at time t (m^3)
d_t	Water demand by the user at time t (m^3)
e_t	Evaporation from the surface of the basin at time t (m^3)
E_t	Potential evaporation from the surface of the basin at time t (m^3)
s	Storage capacity of the storage basin (m^3)

storage capacity of storage basins must be calculated to determine their cost. These costs are used in the optimization model to determine whether rainwater harvesting is preferable to using groundwater. The required storage capacity is calculated by using precipitation data with a daily timestep.

Harvesting rainwater for industry is done at a building scale (buildings with a surface area larger than 50 m^2) in urban areas. Rainwater from all buildings in an urban area is collected and transferred to a storage basin (depth of 3 m) from which the industrial demand site is supplied. Each urban area is considered to have its own storage basin. Sizing of the storage basin is determined based on historical precipitation data with a modified version of the Yield After Spillage (YAS) algorithm (Campisano and Lupia, 2017; D. Jenkins and F. Pearson, 1978; Fewkes and Butler, 2000). The YAS algorithm was used because it yields a conservative estimate for the effectiveness of the rainwater harvesting system irrespective of the time interval used in the model. The parameters used in the modified YAS algorithm are shown in Table 4.

2.2.1 Modified Yield After Spillage algorithm

The water balance in a storage basin is calculated by numerically solving equations (15)–(18) at each timestep. Equations (15)–(18) together form the modified YAS algorithm. The final volume in the storage basin at the end of each timestep is given by

$$v_t = max\begin{cases} v_{t-1} + q_t - y_t - o_t - e_t \\ 0 \end{cases} \tag{15}$$

where the volume is given by the sum of the water remaining from the previous timestep (v_{t-1}) plus the incoming runoff (q_t) minus the water used by the user (y_t), the overflow (o_t), and the evaporation (e_t). If the sum of these terms is smaller than zero, which is physically impossible, the volume of water in the basin is set equal to zero.

The actual amount of water which can be used to cover the industrial demand y_t is given by

$$y_t = min\begin{cases} d_t \\ v_{t-1} \end{cases} \tag{16}$$

where d_t is the potential water demand of the user and v_{t-1} is the amount of water in storage from the previous timestep. If v_{t-1} is smaller than d_t, then only part of the demand can be covered and v_{t-1} is returned. In this study the potential industrial demand is the same for each timestep.

If the storage basin is full it can overflow. The overflow is lost and cannot be used to cover the industrial demand. The overflow o_t at each timestep is calculated with

$$o_t = max\begin{cases} v_{t-1} + q_t - s \\ 0 \end{cases} \tag{17}$$

where v_{t-1} is the volume in storage at the previous timestep, q_t is the runoff towards the storage basin, and s is the maximum storage capacity of the basin. If there is not enough precipitation to fill the basin and to cause overflow the overflow value is set to 0.

Evaporation reduces the amount of water in storage and is calculated for each timestep with

$$e_t = min\begin{cases} v_{t-1} + q_t - o_t \\ E_t \end{cases} \tag{18}$$

where v_{t-1} is the volume in storage at the previous timestep, q_t is the runoff towards the storage, o_t is the overflow, and E_t is the potential evaporation from the basin at timestep t. The potential evaporation depends on the surface area of the storage basin. If the water volume in the basin is smaller than the potential evapotranspiration all the water remaining in the basin is evaporated. The potential evaporation from the surface of the basin is set equal to the daily potential evapotranspiration (Makkink, in mm) retrieved from the closest meteorological station where data is available: Westdorpe (Royal Netherlands Meteorological Institute, 2021a).

For each timestep the difference between the demand d_t and the yield y_t is recorded. If demand and yield are equal then the demand is met, if demand is larger than the yield then there is a water deficit for that timestep.

At the start of each simulation with the YAS algorithm the volume in the storage basin is unknown. To ensure an arbitrarily chosen starting volume does not affect the simulation outputs the precipitation data for each year is used twice. In a first simulation the precipitation data is used to determine the volume in the storage basin at the end of the year. The water volume in the storage basin at the end of the first simulation becomes the starting volume for the second simulation. The second simulation uses the same precipitation data and generates the data used in the WaterROUTE optimization model.

2.2.2 Demand against storage scenarios

The modified YAS algorithm is a simulation model that can be used to accurately determine if a specific demand can be met with a certain storage capacity. The YAS algorithm is not suitable to optimize storage basin capacity directly. To determine the amount of water which can be supplied by each city in the study area the modified YAS algorithm was run for several scenarios. Each scenario pairs a specific water demand with a specific storage capacity. For each scenario the sum of the deficits, $\sum(d_t - y_t)$, is recorded as a data point. For each urban area the storage capacity (V_h) required for different daily demand d_t values is determined from these data points (Figure 3). There is a maximum water demand for each city which cannot be increased by increasing the capacity of the storage basin. Increasing the storage capacity beyond this maximum reduces the water availability because evaporation increases due to the larger surface area of the basin. Subsequently a linear regression from the recorded demand/storage combinations (see Supplementary Information 2 for a graphical representation) is used for the objective function of the WaterROUTE optimization model.

3 WaterROUTE optimization inputs

The WaterROUTE model is demonstrated by creating water supply networks using harvested rainwater and groundwater to supply a single industrial site in Zeeuws-Vlaanderen, the Netherlands. The simulation requires three inputs: the rainwater availability from urban areas (see Section 3.1 and Supplementary Information 3 for details), the groundwater availability in the region (see Section 3.2 for details)

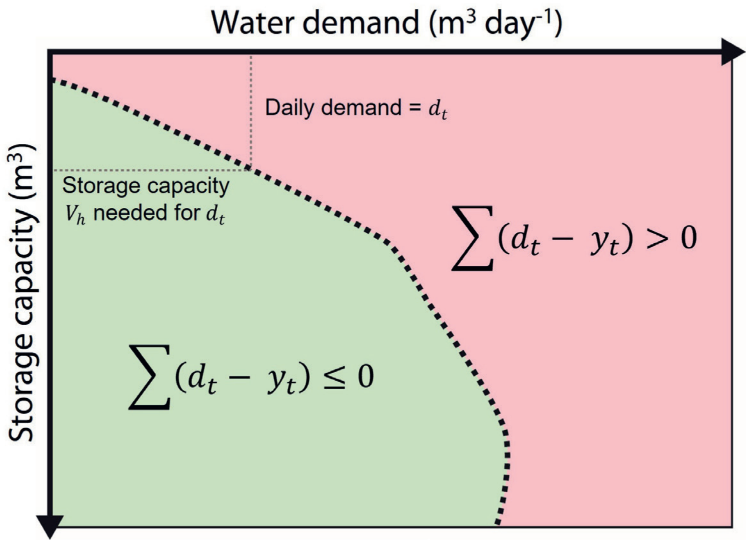


Figure 3 - Visual representation of the scenario outputs of the modified Yield After Spillage model.

and the preliminary network from which the lowest cost network is selected (see Section 3.3 for details).

There are 74 urban areas and 25 groundwater locations in the region (Figure 4). From the urban areas a total of 6.7 Mm^3 $year^{-1}$ of rainwater can be harvested in the wet year (2012) and 4.6 Mm^3 $year^{-1}$ in the dry year (2018). Harvesting the maximum amount of water requires a storage capacity of 1.03 Mm^3 for the precipitation in 2012 and 0.99 Mm^3 for the precipitation in 2018. The total amount of groundwater available is 6.119 Mm^3 $year^{-1}$. The preliminary network in this study connects the 25 groundwater supply locations, the 74 urban locations, and the single demand locations and consists of 2030 potential pipeline segments. From these 2030 pipeline segments the WaterROUTE optimization model selects the set of pipelines which results in the lowest cost water supply network.

3.1 Rainwater availability

The rainwater availability is based on the precipitation on roof surfaces that becomes runoff. The roof runoff (q_t) is calculated based on historical daily precipitation data and a runoff coefficient (RC) of 0.85. Typical runoff coefficients are between 0.7 and 0.9 (Farreny et al., 2011b). Daily precipitation data for two years, one wet (2012) and one dry (2018), were retrieved from the Royal

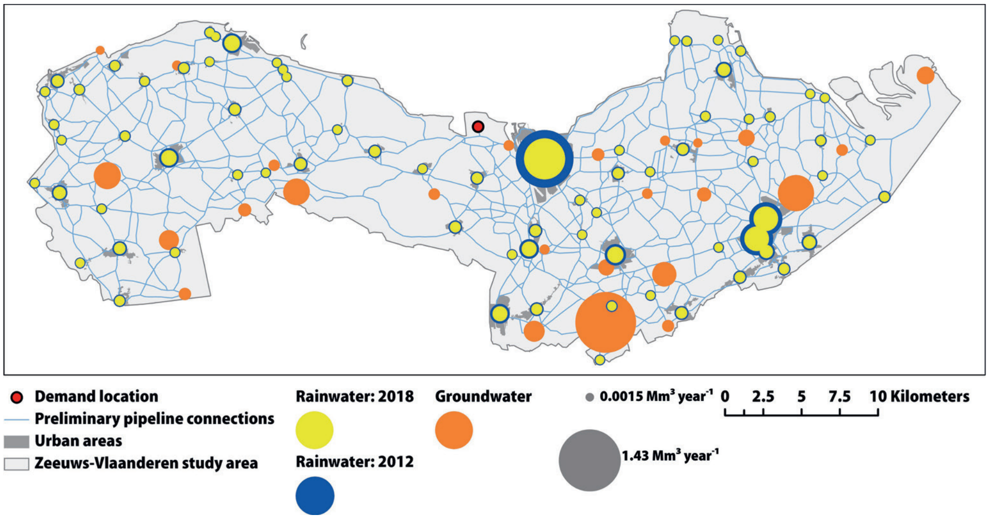


Figure 4 - Water supply locations and preliminary pipeline connections for the Zeeuws-Vlaanderen simulation. The size of the circles represents the amount of water available. The largest circle represents an availability of 1.43 Mm^3 year^{-1}, and the smallest 0.0015 Mm^3 year^{-1}. The rainwater availability of 2018 is displayed on top of the rainwater availability of 2012.

Netherlands Meteorological Institute (Royal Netherlands Meteorological Institute, 2021b). The precipitation data from the meteorological stations in Zeeland was interpolated using a Kriging algorithm with a Power semivariogram model in ArcGIS Pro[3]. For every building with a surface area above 50 m^2 in each urban area in Zeeuws-Vlaanderen we determine the daily precipitation (in mm) through a spatial overlay with the interpolated rainfall data. The location and surface area of each building in the study area was retrieved from a publicly available dataset (Kadaster.nl, 2021). The total runoff from an urban area on a specific day is calculated with

$$q_{h,t} = \sum_{i=1}^{|R_h|} A_{i,h} \cdot P_{i,t} \cdot RC_i \tag{19}$$

where $q_{h,t}$ is the rainwater runoff (m^3) from urban area h on day t, $|R_h|$ is the set of roofs in urban area h, A_i is the area (m^2) of roof i in urban area h, $P_{i,t}$ is the precipitation (mm) over roof i on day t, RC_i is the runoff coefficient of roof i (set to 0.85 for all roofs).

[3] ArcGIS Pro build number: 2.4.19948

3.2 Groundwater availability

In this research 25 well clusters are considered as potential groundwater extraction locations. The well clusters were identified based on the interface between the fresh and salt groundwater and the transmissivity of the groundwater system in a previous study (Willet et al., 2020; Willet et al., 2021). The groundwater system of Zeeuws-Vlaanderen is characterized by the presence of fresh groundwater on top of more saline groundwater resources, as shown by extensive monitoring, mapping, and modelling (Delsman et al., 2018). Extraction rates are maximized to a rate which leads to a maximum drawdown of 50 mm per well cluster to prevent abrupt upconing of the saline groundwater below the fresh groundwater towards the well screen. Within well clusters individual wells are placed 100 m from each other in a grid pattern to avoid drawdown superposition. The total number of wells over the 25 well clusters is 2079 (see Supplementary Information 4 for well cluster specific data).

3.3 Preliminary pipeline network for optimization

To determine the optimal network configuration using both groundwater and harvested urban water as alternative water resources a preliminary set of possible pipeline connections between all supply and demand locations is needed. The optimization model selects the subset which covers the demand of the user at the lowest cost from the preliminary set of connections. In this study the preliminary network represents a water supply network in the planning phase and where no pipelines have been placed yet. GIS software is used to generate the complete set of possible connections based on the best route between them according to the methodology presented in Willet et al. (2020). The main steps of the procedure are:

(1) Determine the relative weights for pipeline placement in different land-use types in consultation with water supply experts. The weights represent the relative costs to place pipeline infrastructure in one type of land-use compared to another.
(2) Create a cost of passage surface (Douglas, 1994) for pipeline placement in the region based on the weights for the different land-use types. Land-use types were retrieved from a publicly available dataset (Centraal Bureau voor de Statistiek, 2012).
(3) Determine the route with the lowest cost for each possible pair of demand-supply and supply-supply locations using the previously generated cost of

passage surface. We also include connections between supply locations (supply to supply) because this makes it possible for supply locations to simultaneously serve as transport hubs in the network.

Determining the relative weights of different land use types is important because these local spatial characteristics can significantly affect the price of placing infrastructure (Feldman et al., 1995). Infrastructure planning based on lowest cost route methods is an effective way to incorporate spatial data in planning processes (Atkinson et al., 2005; Collischonn and Pilar, 2000; Douglas, 1994).

4 Results

The WaterROUTE model is used to create water supply networks for the Zeeuws-Vlaanderen study area based on the water demand of a single industrial demand location. Groundwater and harvested rainwater from urban areas are the potential water sources. Precipitation data from a wet year (2012) and a dry year (2018) is used to investigate the effect of drought on water supply network design.

We investigate three scenarios:

- Rainwater harvesting and groundwater in a wet year (2012)
- Rainwater harvesting and groundwater in a dry year (2018)
- Only groundwater (referred to as the No Rainwater – NR – scenario)

For each scenario the WaterROUTE model is run multiple times with increments of 0.1 Mm^{-3} $year^{-1}$ for a water demand between 2 Mm^{-3} $year^{-1}$ and the maximum amount of water available.

4.1 Network configurations for a demand of 2 Mm^3 $year^{-1}$

The best solution to supply a demand of 2 Mm^3 $year^{-1}$ is with a network of 18.5 km in 2012, 18.1 km in 2018, and 22.8 km for the NR scenario (Figure 5). In 2012 almost all water (97%) is rainwater which comes from four cities, and the rest (3%) comes from a single groundwater well cluster. In 2018 the water is more evenly distributed between rainwater (44%) and groundwater (56%). Supplying 2 Mm^3 $year^{-1}$ in the NR scenario requires four groundwater supply locations to cover the demand.

Compared to the 2012 network the costs for the 2018 network are 30% higher and 52% higher for the NR scenario. Even though the network for 2018 is shorter than for 2012 the costs are higher because a pipeline with a larger diameter is

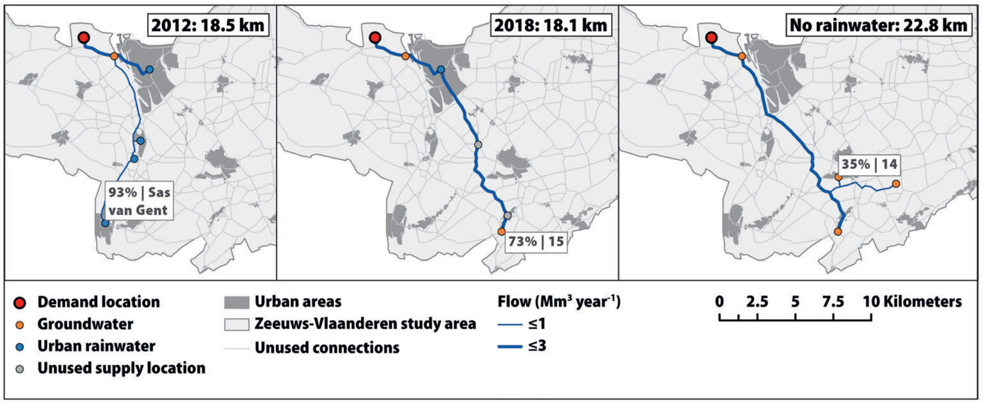


Figure 5 - Water supply network configurations for a demand of 2 Mm^3 year^{-1} for 2012, 2018 and without harvesting rainwater from urban areas. Labels show which percentage of the maximum water availability is used from specific locations. Supply locations without a label are operated at 100% capacity. The format of the label is (operation rate | Well cluster number or urban area).

needed for most of the network. In 2018 the whole network is composed of a pipeline with a $k = 4$ (see Table 2) cost function. For 2012 most of the pipelines have a $k = 2$ cost function. These results show the potential cost savings when rainwater is more abundantly available.

The 2018 network passes through two urban areas where rainwater is not harvested. At these urban areas there is not enough rainwater available to justify placing a storage basin. This result shows how WaterROUTE can be used to determine where the implementation of water technologies is worth the required investment costs. This property of WaterROUTE can be extended to other technologies – such as desalination – besides storage basins or well placement costs. The water supply network still passes through these urban areas because this results in the shortest pipeline network. In subsequent detailed design stages the pipeline route should avoid these urban areas to reduce costs.

4.2 Network configurations for a demand of 6.12 Mm^3 year^{-1}

The maximum amount of water which can be supplied with only groundwater is 6.119 Mm^3 year^{-1}. Supplying the same amount of water when rainwater is also harvested leads to a significantly shorter WSNs with lower costs (Figure 6). Using rainwater from urban areas reduces the length of the WSN by 60% in 2012 and 53% in 2018 compared to using only groundwater. By using rainwater the costs are reduced by 43% in 2012 and 32% in 2018 compared to using only groundwater. The number of supply locations when using rainwater is reduced to

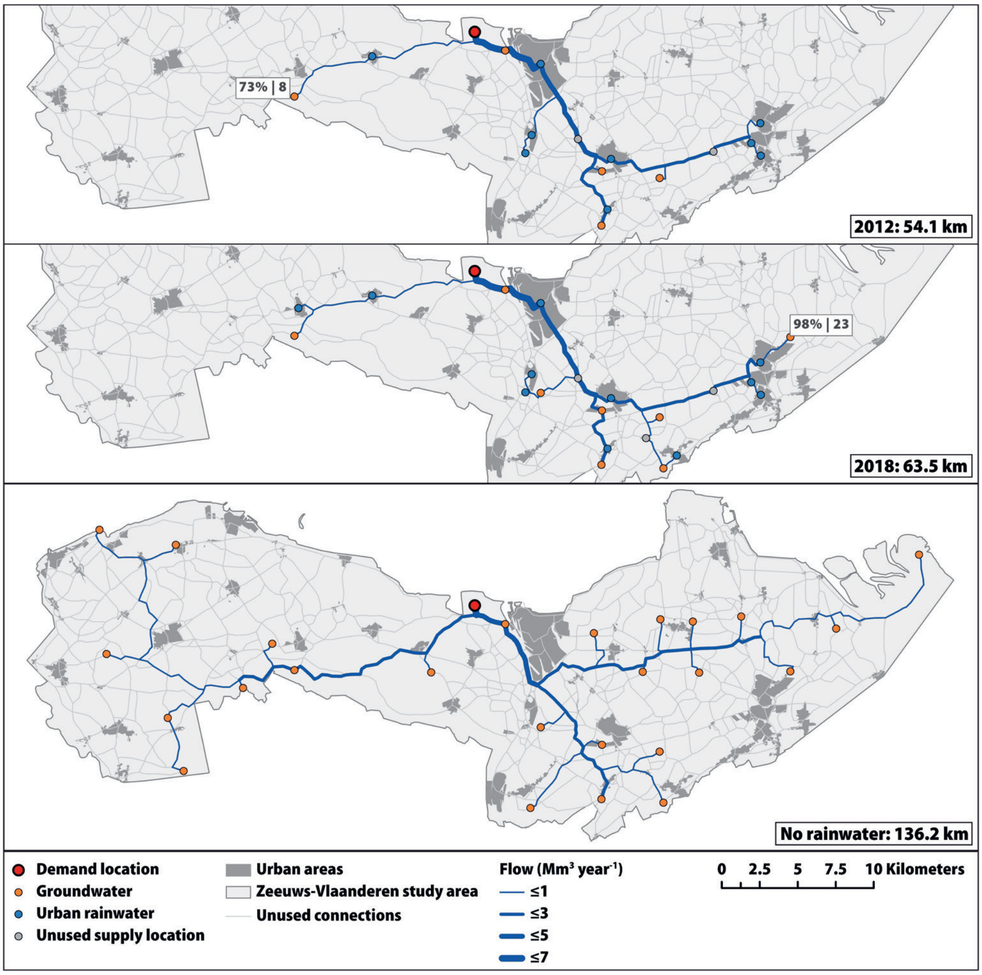


Figure 6 - Water supply network configurations for a demand of 6.119 Mm^3 $year^{-1}$ for 2012, 2018 and without harvesting rainwater from urban areas. Labels show which percentage of the maximum water availability is used from specific locations. Supply locations without a label are operated at 100% capacity. The format of the labels is (operation rate | Well cluster number or urban area).

19 for 2018 and to 14 for 2012 instead of using all 25 groundwater well clusters. The main branches of the WSN share the same layout when rainwater is included. When rainwater is not included the eastern supply locations are reached with a separate branch.

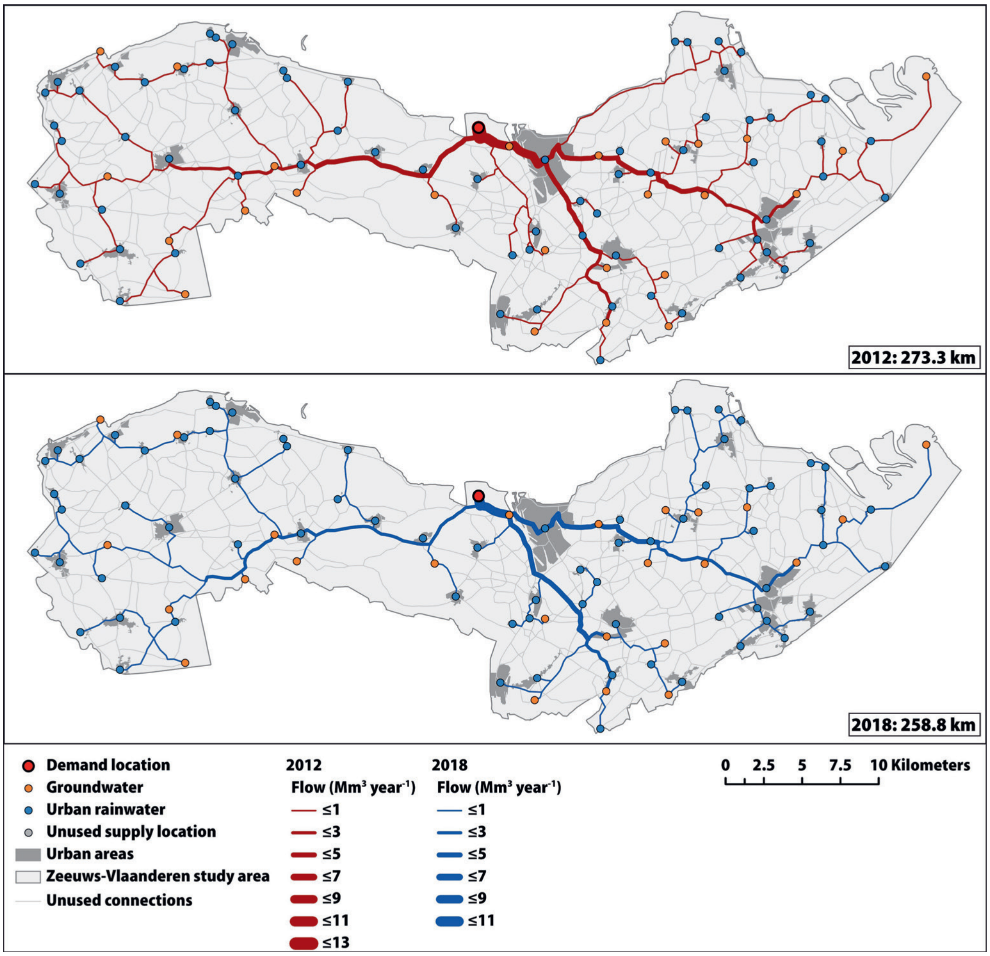


Figure 7 - Water supply network configurations for the maximum possible demand in 2012 and 2018.

4.3 Network configurations for the maximum demand in 2012 and 2018

The maximum supply is 12.83 Mm^3 $year^{-1}$ in 2012 and 10.75 Mm^3 $year^{-1}$ in 2018 when using all groundwater and rainwater resources. The networks for 2012 and 2018 are not identical even though the same supply locations are included (Figure 7). The non-linear cost function representing the costs for pipelines is the underlying reason for this outcome. The 2012 WSN is 5.6% longer than the 2018 WSN and is also 5.6% more expensive. While the relative difference in length and costs are identical the total amount of water delivered to the demand location in 2012 is 19.4% more – a 3.5% more water per percentage point increase in costs.

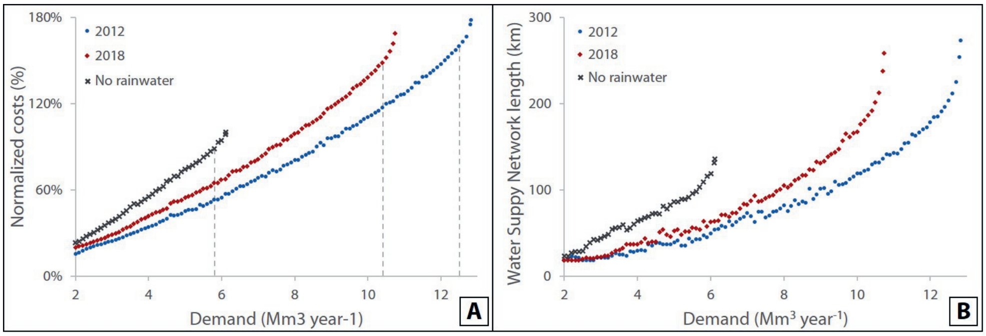


Figure 8 - Normalized WSN costs in relation to the demand of the water user (A). The costs are normalized based on the NR scenario that supplies 6.119 Mm^3 year^{-1} to the demand site. The vertical dashed lines indicate the transition towards an exponential increase in costs. WSN length in relation to the demand of the water user (B).

These results show the value of an optimization tool such as WaterROUTE to reduce network costs, even when the supply locations have been defined beforehand.

4.4 Network costs and length in relation to demand

The relative differences in WSN costs depend on the amount of water available and become larger as the demand which needs to be supplied increases (Figure 8-A). WaterROUTE can be used to identify the demand quantity where network costs start to increase exponentially. For the Zeeuws-Vlaanderen simulations this occurs when the final ~4% of water must be added to the network. Performing the same analysis in another study area can reveal if this value can be used as a rule of thumb for decentralized water supply network design or if it is specific to each study area. Due to the limited runtime of the optimization model subsequent demand values sometimes show a decrease instead of an increase in costs (see Supplementary Information 6 for the optimality gap of each simulation).

The length of the networks shows a more erratic behavior than the costs as demand increases (Figure 8-B). This indicates that minimizing network length is not necessarily the best strategy to minimize costs. In the lower demand ranges (up to around 3.3 Mm^3 year^{-1}) the length of the WSN remains stable at around 20 km for both 2012 and 2018 while the total WSN costs steadily increase. This behavior indicates the importance of the costs associated with infrastructure other than pipelines.

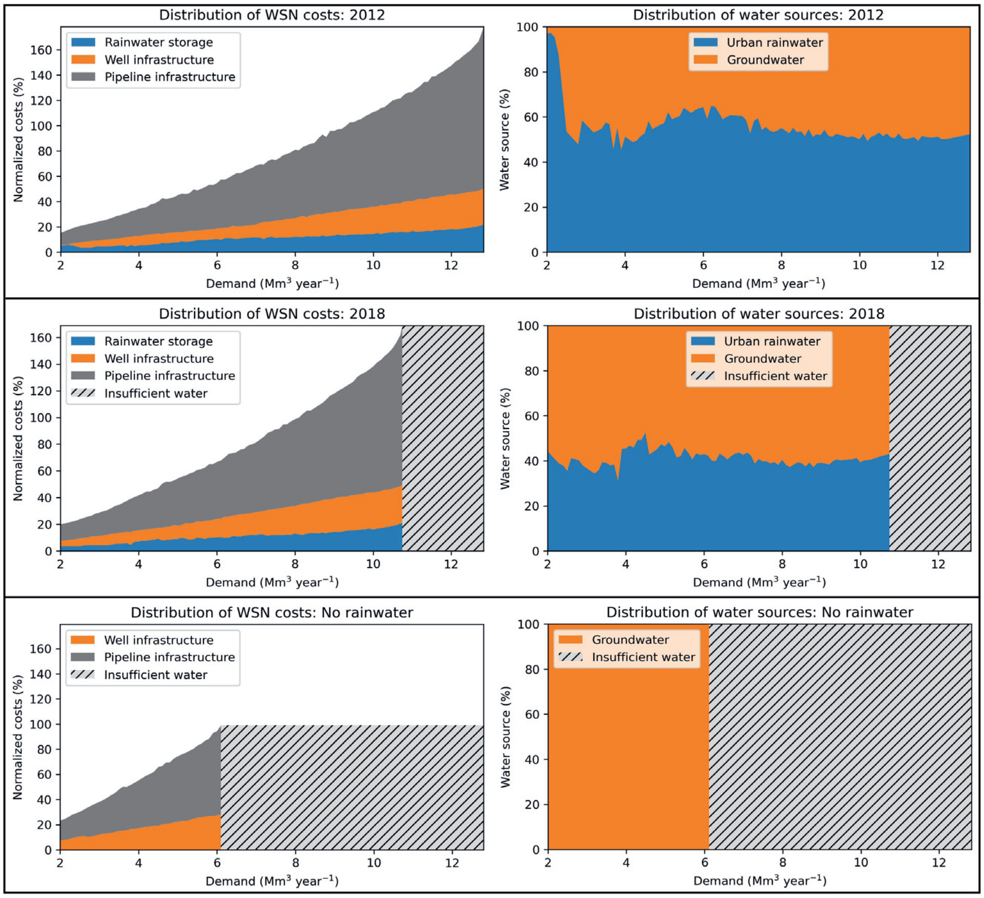


Figure 9 - The distribution of normalized costs within water supply networks for an increasing demand (left) and the distribution of water by source for an increasing demand (right). The costs are normalized based on the NR scenario that supplies 6.119 Mm^3 year^{-1} to the demand site.

4.5 Distribution of water sources and costs for different levels of demand

The largest share of the costs comes from the pipelines that are required to construct the water supply networks (Figure 9). The average share of pipeline costs is 66.1% in 2012, 64.6% in 2018, and 69.1% in the NR scenario. In all scenarios the share of pipeline costs first decreases between 2.0 Mm^3 year^{-1} and 3 Mm^3 year^{-1} and then steadily increases up to the maximum demand. The initial decrease in the share of pipeline costs is caused by the presence of large water sources (the city of Terneuzen and well cluster 15) close to the demand location. Once these large water sources are used at maximum capacity many smaller

Chapter 5

supply locations must be connected to the network. In the 2018 the range in the share of pipeline costs is the largest. For a demand of 2.8 Mm^3 $year^{-1}$ in 2018 pipelines contribute 59.3% of the total costs, while this amount increases to 70.7% for a demand of 10.75 Mm^3 $year^{-1}$.

The share of water coming from different types of supply sources becomes less erratic as demand increases (Figure 9). Across all simulations for 2012 the largest amount of water comes from harvested rainwater (55.9%) and the remainder from groundwater (44.1%). In 2018 this distribution is reversed and the largest amount of water comes from groundwater (58.8%) instead of harvested urban rainwater (41.2%). The fact that the distribution of water sources stabilizes as demand increases indicates that rainwater and groundwater are competitive in terms of costs, also in dry years. The amount of rainwater or groundwater used in the WSN depends on the water availability at each source combined with their vicinity to the demand location. This is illustrated by the large share (up to 97.2%) of water that comes from rainwater when the demand is below 2.4 Mm^3 $year^{-1}$ in 2012. The presence of urban areas in the vicinity of the demand location makes the use of faraway groundwater sources ineffective. Once demand increases to 2.5 Mm^3 $year^{-1}$ it becomes more cost effective to use well cluster 15 instead of some of the smaller nearby urban areas.

5 Discussion

5.1 WaterROUTE functionality

The modelling tools developed in this study add additional functionality to the previously developed WSN and WaterROUTE models (Willet et al., 2020; Willet et al., 2021). The main contribution of this study is the methodology through which different types of supply locations can be incorporated into regional water supply networks. This is achieved by representing water supply locations as two-vertex elements and by introducing an automated procedure to assign location specific cost functions for each of the water supply locations in the optimization model. In this study we test WaterROUTE with groundwater and harvested rainwater from urban areas as potential water supply locations. From this starting point other water supply sources, such as treated industrial or domestic wastewater, can be added to create regional circular water supply networks.

The new WaterROUTE functionality evaluates the benefits of adding alternative water sources in decentralized water supply networks. Making use of more regionally available water resources does not only increase the total availability of water in a region but also significantly reduces the costs of (decentralized) water supply networks. By including harvested rainwater as a potential water supply source WSN costs can be reduced by 31% on average when compared to a baseline in which rainwater is not harvested. This average increases to 38% based on the precipitation in a wet year and drops to 25% in a dry year. Changing precipitation patterns due to climate change (Dore, 2005; Kitoh and Endo, 2016) can not only affect the total amount of water available but consequently will also influence the design of regional water supply networks. WaterROUTE provides decision makers with a link between models of future precipitation patterns (KNMI, 2015) and long-term regional planning.

The WaterROUTE model developed in this study can also be used to create WSNs with more than one demand location. The current formulation of the optimization model in WaterROUTE creates water supply networks that supply all users at the lowest cost. If users are spread out over the study area and the total water demand is low compared to the water availability this can result in several smaller network. If demand locations are close together and the total demand approached the regional water availability a large and connected network is more likely. Adding additional demand locations should be accompanied by the addition of more water supply sources to ensure there is a feasible solution for the optimization problem.

5.2 Storage for intermittent water sources

Storage of intermittent (rain)water becomes more cost effective the more water is available and the smaller the differences between wet and dry periods. The total amount of water harvestable from rainwater is 46% more for 2012 compared to 2018 but the total amount of storage required increases by only 4%. Further reduction of storage costs can be achieved by increasing flexibility at the demand site. Increasing storage basin size shows diminishing marginal benefits (Campisan et al., 2017; Melville-Shreeve et al., 2016; Palla et al., 2011), meaning that the first cubic meter of storage is significantly more cost effective than the last. The current implementation of WaterROUTE considers 100% water supply security from harvested rainwater over the simulation period. Reducing this value to 80% for the city of Terneuzen (the largest urban area in the study area) reduces the required storage capacity by 39%. Designing flexible industrial processes that are less dependent on a single steady water supply can therefore lead to significant reductions in WSN costs.

In this study the storage basins for rainwater are located close to the urban areas where the water is harvested. Another possibility is to use a single large storage basin at the demand location where rainwater is stored after it is transported. Using a single large storage basin reduces infrastructure costs because the fixed costs for construction are minimized. Developing an effective method to optimize WSNs with a single centralized storage facility is suggested for future research. A possible drawback of using a single storage basin is that it may inhibit the possibility to use the local storage basins to buffer peak precipitation events.

5.3 Competing purposes for limited water resources

The use of harvested rainwater from urban areas should not conflict with the possibility to use the same rainwater directly within cities. The possibilities for direct reuse of rainwater in households is limited (Agudelo-Vera et al., 2012b) but the optimal allocation of water for industrial purposes instead of domestic purposes should be further investigated. Besides covering domestic or industrial water demands urban rainwater can also be used to restore the heavily modified water balance of urban areas (Claire Welty, 2009).

WaterROUTE can be used to evaluate the possible symbiosis between industrial and urban areas after local water requirements for ecosystems within cities have been satisfied. Connecting industrial areas with urban areas for the exchange of resources can alleviate the pressure of industrial areas on ecosystems. This is especially the case when the water use intensity, in terms of water use per surface area, of industrial areas surpasses the water use intensity of urban areas. Evaluating the potential symbiosis between industry and urban areas in terms of carbon dioxide (Fang et al., 2017) is already on the research agenda. WaterROUTE provides part of the modelling tools required to expand the field of urban industrial symbiosis to water resources.

5.4 Rainwater harvesting

The harvesting of rainwater is limited to roof surfaces in this study. Including runoff from other sealed surfaces increases the potential amount of water available but also causes variability in the contaminations present. Depending on the type of surface from which rainwater is harvested the concentration of contaminants may vary (Farreny et al., 2011a; H.J. Liefting et al., 2020). Depending on the water quality requirements of the demand site additional treatment may be needed. Mixing of water with different qualities to deliver fit for purpose water (Bauer et al., 2019) is an alternative to water treatment. Mixing of water in decentralized water supply networks is demonstrated in Willet et al., 2021 for a single contaminant (salt) in a network with fewer pipeline connections. Adding quality parameters to rainwater and groundwater in WaterROUTE requires simplification of the preliminary network to make optimization computationally feasible. Several methods and algorithms to simplify water supply networks exist (Huang et al., 2019; Lina Perelman et al., 2008; Martínez-Solano et al., 2017). The proposed two-vertex representation of water supply sites is also suitable to incorporate treatment costs into the objective function of the optimization model. Alternatively, negative costs can be assigned for incorporating wastewater streams with a low quality into the water supply network, stimulating cascading/reuse of water.

The infrastructure required within cities to harvest rainwater was not included in this study. There are several potential benefits to the implementation of water systems which collect rainwater separately (J.G. Langeveld, 2019; Wang et al., 2013). Decision makers in urban areas can use WaterROUTE to investigate the potential benefits of a transition towards a separating sewer system. WaterROUTE can be used for this purpose by generating regional scenarios which can be evaluated by relevant stakeholders.

6 Conclusions

We show that the use of multiple types of water supply sources, groundwater and harvested urban rainwater, not only increases the amount of water available for the water user but also significantly reduces the costs of a decentralized water supply network (WSN). When rainwater harvested from urban areas is included as a potential alternative water supply source in the study area of Zeeuws-Vlaanderen WSN costs are reduced by up to 42% compared to only using groundwater. On average 67% of the WSN costs come from the pipeline network and 33% from the costs to place and operate groundwater well infrastructure or storage basins for harvested rainwater in the simulated scenarios. Rainwater harvesting and groundwater are competitive in terms of costs. The usage of a rainwater source or a groundwater source depends on their location in relation to the demand location and the amount of water available. Expanding the number of potential water sources – for example with treated wastewater – is expected to further reduce costs while increasing water availability of demand locations. The share of the costs for the pipelines increases as the water demand at the demand location increases and the WSN becomes more extensive as a consequence. With

WaterROUTE the implications – both financial and in terms of configuration – of a reduced water availability on decentralized water supply networks can be investigated and visualized. The scenarios produced with WaterROUTE can be used by decision makers for long-term regional planning. Especially in areas where water scarcity is expected to increase this information is valuable to make timely changes to the regional water supply system.

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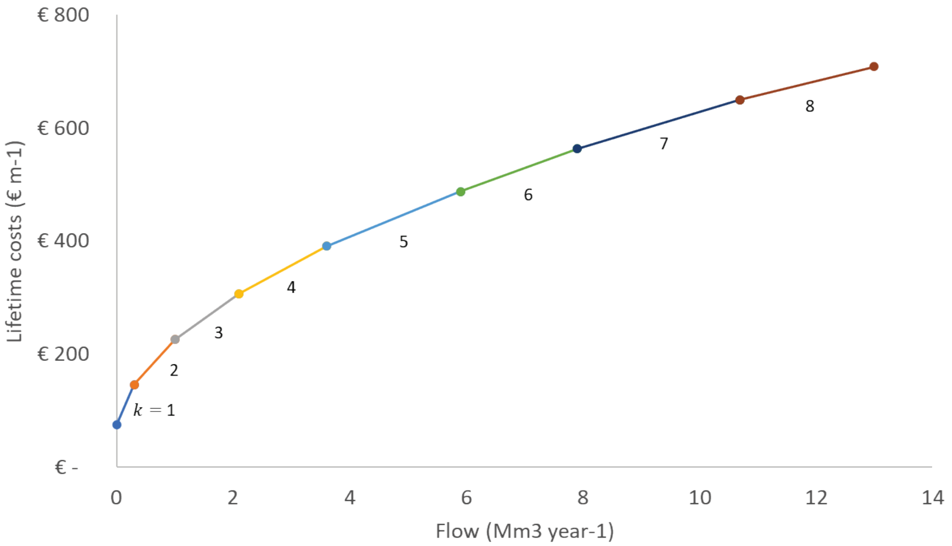
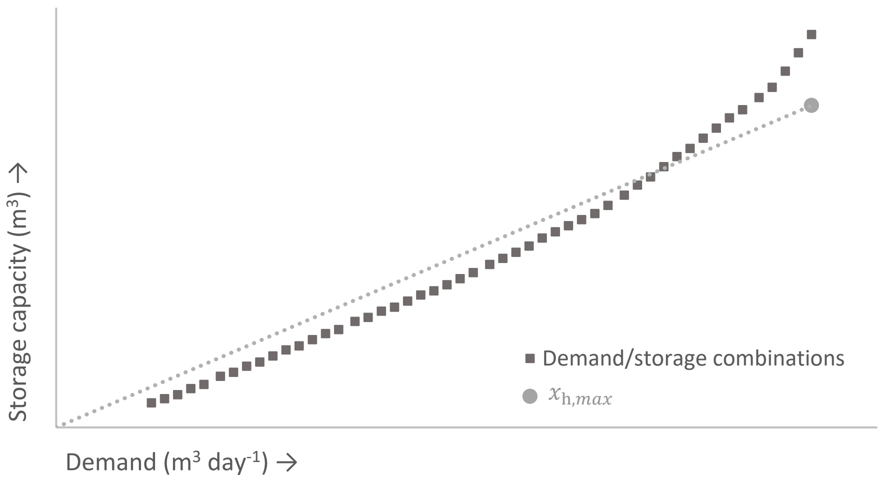
Supplementary Information

Supplementary Information 1 - Piecewise linear approximation of lifetime investment and operational costs for water distribution pipelines.



Supplementary Information 2 - Example of the linear regression approximation for the storage capacity required based on the daily water demand from an urban area. The demand/storage combinations are generated with the modified Yield After Spillage model by running 30000 scenarios for each urban area.



Supplementary Information 3 - Harvestable rainwater (in m^3 day^{-1}) for each urban area based on the modified YAS model. The total amount of rainwater available is 6.7 Mm^3 $year^{-1}$ in 2012 and 4.6 Mm^3 $year^{-1}$ in 2018.

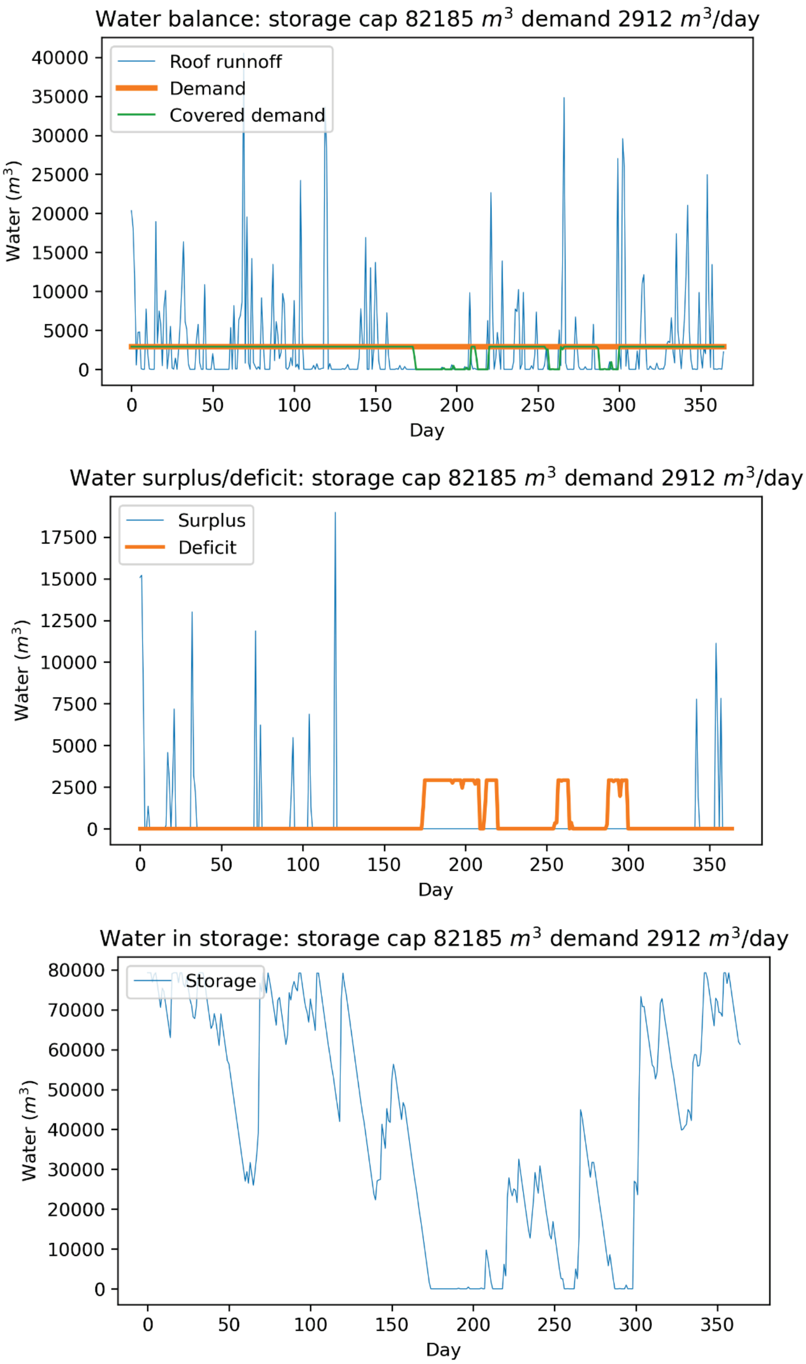
Urban area	2012	2018	Urban area	2012	2018
Aardenburg	315	230	**Nummer Eén**	0	0
Absdale	19	13	**Oostburg**	726	523
Axel	862	579	**Ossenisse**	40	27
Biervliet	230	164	**Overslag**	20	14
Boerenhol	16	12	**Paal**	14	9
Braakman	35	24	**Philippine**	238	161
Breskens	726	533	**Retranchement**	52	39
Cadzand	107	81	**Reuzenhoek**	24	16
Cadzand-Bad	274	206	**Sas van Gent**	718	492
Clinge	427	293	**Sasput**	7	5
Draaibrug	25	18	**Schapenbout**	8	5
Driewegen	17	12	**Schoneveld**	73	54
Eede	135	99	**Schoondijke**	222	159
Emmadorp	30	20	**Sint Anna ter Muiden**	19	14
Graauw	103	70	**Sint Jansteen**	517	363
Groede	153	113	**Sint Kruis**	41	30
Heikant	226	156	**Slijkplaat**	8	5
Heille	33	24	**Sluis**	395	291
Hengstdijk	46	31	**Sluiskil**	259	174
Het Heem	23	17	**Spui**	38	26
Hoek	230	159	**Terhofstede**	9	6
Hoofdplaat	107	76	**Terhole**	39	26
Hulst	1757	1205	**Terneuzen**	3671	2434
IJzendijke	282	198	**Turkeye**	4	0
Kapellebrug	186	129	**Vogelwaarde**	246	167
Kloosterzande	444	301	**Walsoorden**	65	43
Koewacht	287	198	**Waterlandkerkje**	40	28
Kruispolderhaven	9	6	**Westdorpe**	266	179
Kuitaart	26	17	**Zaamslag**	250	169
Lamswaarde	69	46	**Zaamslagveer**	23	15
Magrette	28	19	**Zandberg**	19	13
Nieuw Namen	137	95	**Zandstraat**	36	24
Nieuwe Molen	32	21	**Zeedorp**	6	4
Nieuwvliet	67	50	**Zomerdorp Het Zwin**	41	31
Nieuwvliet-Bad	107	79	**Zuiddorpe**	99	66
Noordstraat	13	9	**Zuidzande**	76	56

Chapter 5

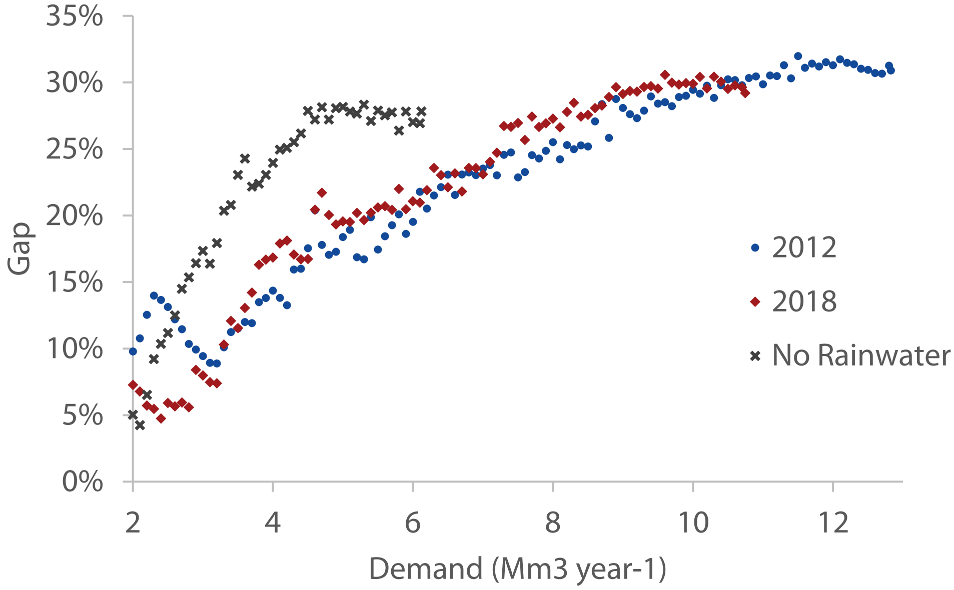
Supplementary Information 4 - Well cluster data.

Cluster number	Maximum extraction (Mm^3 $year^{-1}$)	Number of wells
1	0.508	164
2	0.010	10
3	0.046	47
4	0.079	53
5	0.315	157
6	0.107	22
7	0.130	39
8	0.498	92
9	0.088	49
10	0.059	28
11	0.117	101
12	0.343	196
13	0.046	14
14	0.206	83
15	1.432	331
16	0.436	109
17	0.099	18
18	0.060	34
19	0.154	54
20	0.046	31
21	0.024	11
22	0.220	79
23	0.757	296
24	0.086	23
25	0.253	38

Supplementary Information 5 - Example of the water balance data from the Yield After Spillage model. The displayed data is for Terneuzen in 2018.



Supplementary Information 6 - Optimality gap of the WaterROUTE simulations for the Zeeuws-Vlaanderen study area.



Chapter 6
Discussion

Table 1 - Overview of findings in this thesis.

Chapter	***Objective***	***Method***	***Main findings***	***Conclusions***
Chapter 2 Review of methods to assess sustainability of industrial water use	To identify methods to evaluate the sustainability of water use and determine whether they are applied in industry	Systematic literature review	- Only 26% of the reviewed papers use methods which can adequately evaluate water use - The 'mixed' industrial sector is most consistent in the use of adequate evaluation methods	Improving and increasing data availability for existing methods is more beneficial than developing new methods
Chapter 3 Water supply network model for sustainable industrial resource use	To create a modelling framework which can optimize decentralized water supply network layout based on local land use conditions	- Geographic Information Systems modelling - Hydrological modelling - Mathematical programming	Decentralized water supply network costs increase with a stepwise pattern as the demand for water at the demand location increases	Spatial data and mathematical optimization can effectively be combined to design regional decentralized water supply networks
Chapter 4 WaterROUTE: a model for cost optimization of industrial water supply networks when using water resources with varying salinity	To extend the modelling approach presented in *Chapter 3* to deliver 'fit-for-purpose' water to the demand location based on the salinity of groundwater in a region	- Geographic Information Systems modelling - Hydrological modelling - Mathematical programming	Small changes in water quality at the demand location have a significant effect on decentralized water supply network design in terms of configuration and costs	WaterROUTE can assist decision makers when making regional water supply scenarios based on the anticipated changes in (groundwater) quality
Chapter 5 Decentralized water supply network optimization using harvested rainwater and groundwater as alternative water sources	To extend the modelling approach presented in *Chapters 3 and 4* to create water supply networks which can make use of multiple sources of water	- Geographic Information Systems modelling - Water balance simulations - Mathematical programming	Harvested urban rainwater and groundwater resources can be complementary when designing regional decentralized water supply networks	Using multiple sources of water in decentralized water supply networks significantly reduces costs and makes it possible to optimally use all renewable water sources in a region

1 Introduction

This research was motivated by the expectation that water resource availability for industry in the Netherlands cannot be guaranteed in the future unless adequate measures are taken. Over the course of the project this expectation has become apparent on multiple occasions. In the timespan of this research extreme drought has been followed up by extreme precipitation and flooding. The Netherlands is becoming a country which is more and more exposed to water extremes, both too wet and too dry.

The year 2018 will go down in the history books as the second driest (recorded) year in Dutch history. The precipitation deficit in 2018 peaked at 309 mm on the 8th of August during the second heat wave of that year (R. Sluijter et al., 2018). Some industries were asked to reduce production because surface water temperatures had become too high to accept further discharge of cooling waters. Nonetheless, the industrial sector remained relatively unscathed with damages of only a few million euros. Agriculture suffered the hardest losses with an estimated damage between 820 million and 1400 million euro (Ilse van de Velde et al., 2019). Not only humans were impacted by this drought. Several animal and plant species in vulnerable water dependent ecosystems were negatively affected (Natuurmonumenten, 2019). Climate models predict more severe droughts to occur in the future for the northern hemisphere and recent droughts and severe heatwaves in North America, Siberia, and the Eastern Mediterranean region show this is already becoming a reality.

The year 2021 paints a totally different picture for Western Europe. Extreme weather events in the south of the Netherlands, Belgium, Germany, Luxemburg, and Switzerland led to extensive flooding and several casualties. On the 13th and 14th of July more than 150 mm of precipitation was recorded in some parts of Limburg, in the south of the Netherlands. This is more than twice the average amount of precipitation for the whole month of July (KNMI, 2021). Occurrence of such extreme weather events has increased over the past 100 years and is expected to increase in the future (Adri Buishand et al., 2011). Extreme precipitation is also result of climate change since air with a higher air temperature can store more water, leading to more rainfall (G. Lenderink et al., 2011; KNMI, 2021). The annual precipitation in the Netherlands has increased by 16% between 1951 and 2009 (Buishand et al., 2013). This absolute increase in precipitation does not directly reduce the occurrence of drought. Precipitation increasingly occurs during the winter or in heavy rainfall events in the summer (Buishand et al., 2013). Without adequate retention or infiltration, precipitation becomes runoff and is lost. Coupled with increased evapotranspiration due to higher temperatures the increase in yearly precipitation does not directly translate to a reduction in the occurrence of drought.

The Dutch water infrastructure is largely based on the historical need to get rid of water as fast as possible. As water availability changes, this paradigm needs to shift to ensure water availability year-round. Water must not only be discharged efficiently during peak precipitation events but also retained for periods of reduced water availability. The direction proposed in this thesis is to consider decentralized instead of centralized systems, using alternative water resources, as a part of the adaptations needed to ensure sustained water provision for industry. Centralized water supply infrastructures lack flexibility and are becoming increasingly expensive to maintain (Pahl-Wostl et al., 2011). Decentralized systems can deliver 'fit-for-purpose' water from alternative water resources which can reduce costs and demands from freshwater reserves (Capodaglio, 2021). By reducing industrial demands on freshwater the water availability for agriculture and ecosystems increases. Centralized infrastructures in many western societies have been built in the period of 1950 to 1980 and are approaching the end of their useful lifetime. There is now a window of opportunity to accelerate the transition towards decentralized systems or a hybrid between centralized and decentralized systems. However, the design of decentralized systems is complex because temporal and spatial aspects of demand and supply must be considered in detail. The objective of this research was to develop modelling tools to assist in the design of decentralized water supply systems for industry using alternative water resources. The WaterROUTE model was developed to achieve this objective.

In this thesis the concept of environmental compatibility is introduced and set as a boundary condition for the use of alternative water resources and water supply network design. Environmental compatibility means that water use by humans should be tailored to the local water system where it takes place. For example, water extractions should be compatible with the water needs of local ecosystems, the risk for salinization, or effects on land subsidence.

Table 1 provides a general overview of this thesis. In the rest of this chapter the contributions of this thesis are discussed. First, WaterROUTE is discussed in the context of the research fields it contributes to. Then, a reflection on the spatial and temporal challenges for decentralized water supply network design and the extent to which these have been effectively incorporated in WaterROUTE is given. Subsequently, an example for further integration of WaterROUTE with regional water resource management is elaborated. Lastly, a reflection on the transition towards environmentally compatible water supply networks is given.

2 WaterROUTE connecting research fields

WaterROUTE is a modelling framework that can be used to connect the urban metabolism and industrial ecology fields, specifically concerning water resources. The urban metabolism field considers cities as living organisms requiring energy, water, and other resources to function (Abel Wolman, 1965). Cities depend on their hinterlands to supply these resources and to assimilate the waste they produce (Kennedy et al., 2007; Xuemei Bai, 2007). Industrial ecology takes the same approach towards resource flows within industrial systems (Xuemei Bai, 2007).

Industrialization and urbanization are closely linked in the development of an area. Cities arise due to industrialization and industries in turn are located close to cities. Industries and cities are linked through their resource flows. Resources often first pass through an industrial process before ending up in the cities where they are used. The linkages and interdependencies between industries and cities is an argument to bring the industrial ecology and urban metabolism fields closer together. Methodologically the two fields already show similarities. The spatial and functional linkages between the fields is an additional argument for further integration (Xuemei Bai, 2007). The interconnections and relationships between industries, cities, agriculture, and the environment are depicted in Figure 1.

Within urban metabolism several methods have been developed to evaluate and categorize resource flows within cities (Li and Kwan, 2018; Zhang, 2013). The methods used in urban metabolism studies first focused on the analysis of processes but have evolved to also include the optimization and regulation of resource flows (Figure 2). As urban metabolism methods evolved over time and computational restrictions diminished, it has been argued that a network analysis approach should be applied to better understand the internal and external connections between industry, agriculture,

the domestic sector, and the environment (Zhang et al., 2009; Zhang, 2013). Such a network approach is also needed to better understand where interventions

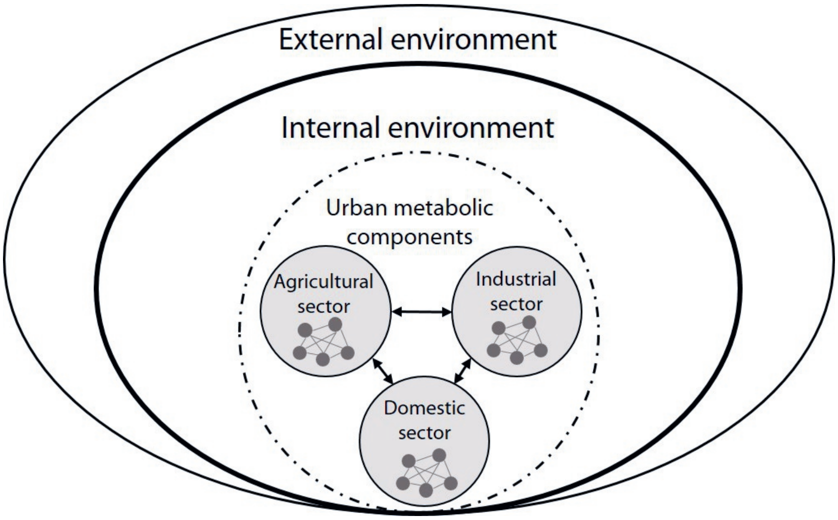


Figure 1 - Depiction of the urban metabolic system and its interconnections. Adapted from Zhang et al., 2009.

can be most effective in the endeavor to shift from a linear to a circular urban/industrial metabolism.

The Urban Harvest Approach (UHA) was developed as an urban metabolism tool in 2012 (Agudelo Vera, 2012). The UHA focuses on changing the metabolic flows in a city by changing resource use starting at the smallest scale (one house) and then expanding to larger scales (housing blocks, neighborhoods, cities, and peri-urban areas). The UHA is a tool to understand resource flows within cities and to investigate potential improvements to resource flows by generating scenarios in which three strategies are applied. The UHA uses three strategies to improve the urban metabolism: demand minimization, output minimalization, and multi-sourcing. The generation and evaluation of scenarios is valuable to understand the impact of interventions but can only partially be considered as an optimization method. The WaterROUTE model developed in this thesis connects the UHA methodology developed in the urban metabolism field with industrial ecology in terms of water resources management (Figure 2).

WaterROUTE is connected to the UHA through the multi-sourcing step of the UHA and is designed as an optimization methodology which uses simulation model results as inputs. Multi-sourcing entails supplying the remaining demand for resources with locally available renewable resources. Multi-sourcing should only

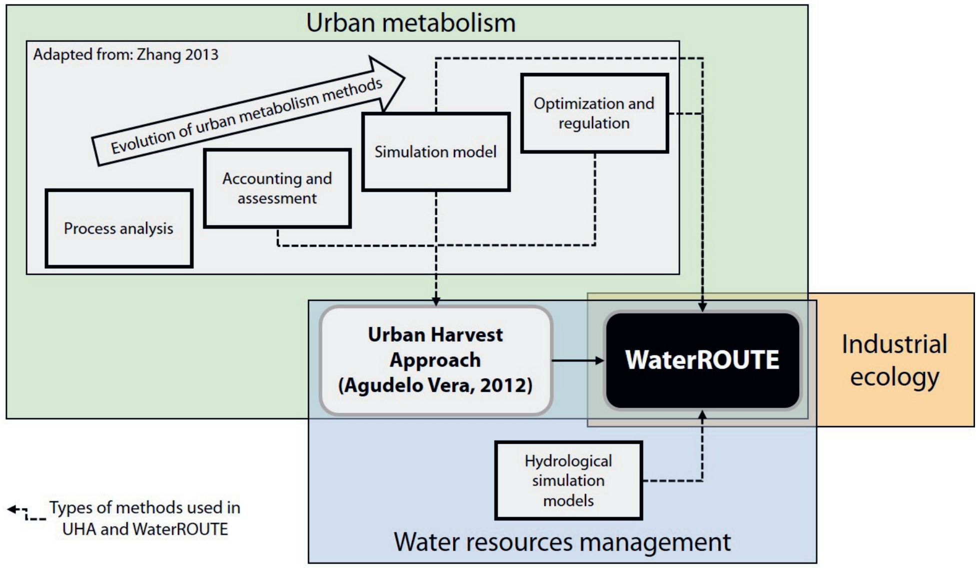


Figure 2 - WaterROUTE in relation to other urban metabolism methods and the overlap with industrial ecology and water resources management. The content of the grey box was adapted from Zhang, 2013.

be considered after the demand and output of resources has been minimized. Implementing the proposed UHA interventions at the smallest scale was shown to potentially lead to a surplus of water resources at a city scale (Agudelo Vera, 2012). These surpluses could then be exported to be used elsewhere. WaterROUTE aids in the design of decentralized water supply networks which make use of these renewable surplus water resources. Such water resource networks make multi-sourcing possible on larger geographical scales.

WaterROUTE has three main components which are combined to design water supply networks (Figure 3). First, simulation models are used to determine the regional water availability with environmental compatibility as a boundary condition. This first step is comparable with the identification of local renewable resources in the multi-sourcing step of the UHA. Determining the sustainability and allocation of (multi-sourced) water resources is where WaterROUTE overlaps with the (sustainable) water resources management field (Loucks, 2000). Second, the spatial characteristics of the region are processed to determine the possible pathways to connect demand with supply. Third, optimization is used to reduce the near infinite number of possible water supply network configurations to a manageable set for decision makers. While WaterROUTE can be used within the

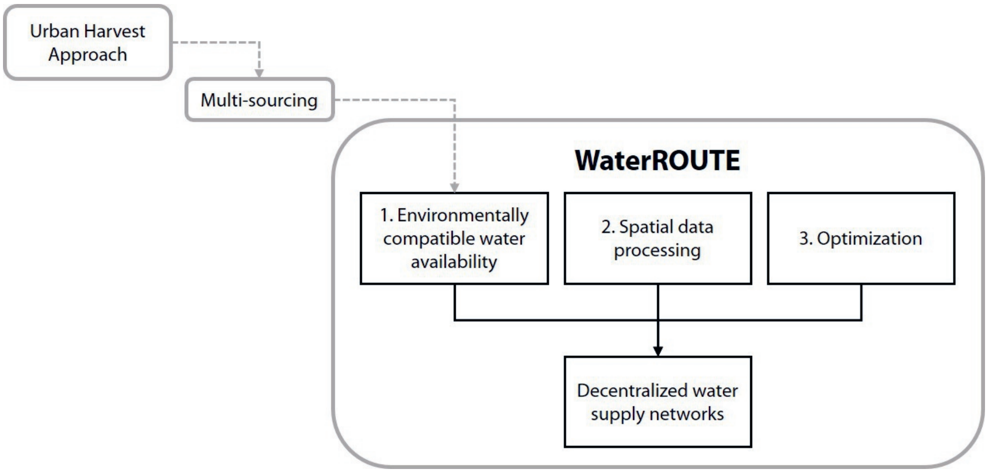


Figure 3 - Components and output of WaterROUTE.

urban metabolism field, its applicability and contributions extend beyond cities. In this thesis it is applied to optimize the water resource flows between industry, the regional environment, and urban areas. Industries and cities can be seen as components of a water ecosystem and tools such as WaterROUTE enable the connection between their demand and supply for water resources. The main contribution of this thesis to the urban metabolism, industrial ecology, and water resources management fields is the development of modelling and design tools that connect the demand and supply of resources in space, quantity, quality, and time.

3 Water demand and supply: space, quantity, quality, and time

Improving regional resource management requires high resolution spatial and temporal data on resource supply and demand (Agudelo Vera, 2012; Metson et al., 2018; Voskamp et al., 2018; Wielemaker, 2019). In this thesis it is argued that besides high resolution data on demand and supply one needs to include transport and storage, since these will remain necessary to match supply and demand. To determine if and how resources should be stored and/or transported between demand locations and supply locations, modelling tools are needed which can process spatial and temporal data for decision making. Spatial and temporal variations are reflected in the quantity and quality of water demand and supply and in the possibility to transport water from one location to another. In this thesis, a stepwise approach to incorporate spatial, temporal, water quantity, and water quality aspects of resource allocation was taken. This approach was used to make the resource allocation problem manageable. In this section it is discussed how these aspects were included in the design of decentralized water supply networks with WaterROUTE and possible future steps are highlighted.

3.1 Space

In **Chapter 3**, the foundations for WaterROUTE are laid by setting up the modelling framework to design decentralized water supply networks based on local spatial data. The novelty of the approach presented in **Chapter 3** is that spatial data is used to assess the possibility to transport water between supply and demand locations.

3.1.1 Pipeline routing

The construction of water transport infrastructure is expensive and time consuming, especially in a densely populated and highly regulated country as the Netherlands. Determining the most cost-effective decentralized water supply network not only depends on the total kilometers of pipeline but also on the areas where pipelines pass through. Traditional approaches to pipeline routing are very labor intensive (Durmaz et al., 2019) and are being replaced by geo-information science (GIS) tools using spatial multicriteria decision making (S-MCDM) methods. Spatial data on land use and subsoil characteristics is used extensively in the oil and gas industry to determine the optimal route for pipelines (Durmaz et al., 2019; Feldman et al., 1995; Yildirim et al., 2017). The use of these methods can reduce economic, environmental, social, and temporal costs significantly (Yildirim et al., 2017) and their use is growing in the environmental sciences field (Huang et al., 2011).

WaterROUTE makes use of a simplified (S-MCDM) method based on expert knowledge about the effects of land use on pipeline placement costs. This expert knowledge it converted to weights for every of land use. WaterROUTE focuses on combining the knowledge of experts with spatial data to create a water supply network which can be optimized. Using more sophisticated and formalized methods such as simple additive weighting (SAW) (Coutinho-Rodrigues et al., 2011), the analytic hierarchy process (AHP) (Chen et al., 2010), elimination and choice expressing reality (ELECTRE) (Figueira et al., 2016), or the technique for order preference by similarity to ideal solution (TOPSIS) (Coutinho-Rodrigues et al., 2011) is suggested to further enhance pipeline routing within WaterROUTE.

By using these methods additional criteria besides the costs to place pipeline infrastructure can be included. Non-technical and engineering criteria, such as right of way (ROW) costs, is one of such criteria which can be added to WaterROUTE using spatial data.

WaterROUTE currently overlooks social acceptance of water transport projects and how this can affect the ROW. ROW costs are highly variable depending on the location where a pipeline project takes place (Rui et al., 2011). In WaterROUTE spatial aspects affecting pipeline construction costs are translated into shorter or longer pipeline sections. The length of pipeline sections in turn affects the costs of pipeline placement. Incorporating ROW can be done during the creation of the preliminary network by assigning a high cost to areas where ROW is expected to be costly. Another option is to incorporate ROW within the optimization procedure. Incorporating ROW within the optimization procedure entails changing the cost function of specific pipeline segments based on their spatial location and the social acceptance in that area.

Irrespective of the number of spatial criteria included in WaterROUTE the resolution of the input data needs to be suitable. The resolution of the spatial data influences the accuracy of pipeline routing when using GIS methods. Using low resolution data at the initial design stage can lead to costly route changes once detailed planning of the project starts (Tiffany and Devine, 2017). Such route changes can occur because crucial landscape features affecting route selection are excluded from the analysis when data resolution is too low. Increasing data resolution from a 100 m digital elevation model to a 30 m digital elevation model was shown to result in a cost reduction of 35% for a 150 km pipeline (Durmaz et al., 2019). More sophisticated S-MCDM methods and higher resolution spatial data will improve pipeline routing within WaterROUTE but will not resolve optimal junction placement.

3.1.2 Junction placement

The optimization model in WaterROUTE uses a preliminary network in which all supply and all demand locations are connected directly and with an interconnecting network (Figure 4-A). Running an optimization model without all possible connections can lead to water supply networks that are unnecessarily long and expensive. For example, the interconnecting network configuration in Figure 4 leads to excessive costs when only one water supply location is needed (Figure 4-B). Alternatively, using only direct connections leads to excessive costs

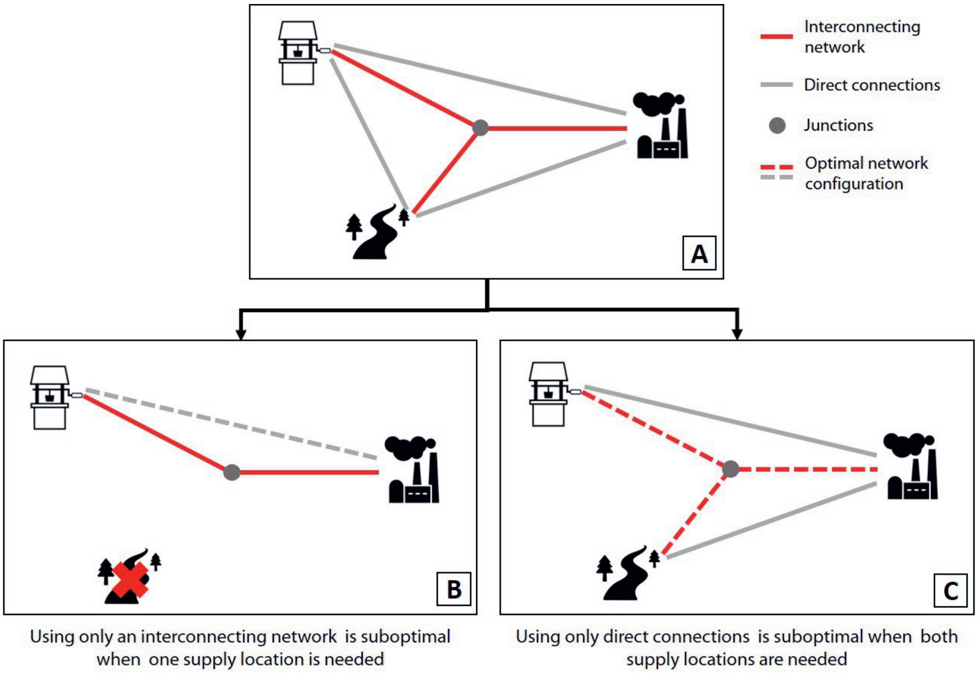


Figure 4 - Representation of the possible connections between water supply and water demand locations (A). Not using all possible connections in a preliminary network can lead to a suboptimal water supply network (B-C).

when both supply locations are needed (Figure 4-C). Generating a preliminary network based on direct connections is possible with current GIS software. Creating the most efficient interconnecting network requires optimizing the placement of pipeline junctions.

Optimal placement of pipeline junctions, a more fundamental spatial/mathematical problem, has not been addressed in WaterROUTE and is posed as a challenge for mathematicians. When connecting N nodes in the Euclidean plane the shortest network to connect all nodes is achieved with at most $N-2$ junctions J where pipelines intersect at an angle of 120 degrees (Figure 5) (F.K. Hwang, 1991). The number of junctions needed, and their location, can only be determined once the locations of the nodes are known. In WaterROUTE the optimal placement of junctions in a preliminary network is complicated because: (1) the costs for pipeline placement are not uniform in all directions and (2) the number and location of the supply sites needed (the nodes) is not known beforehand.

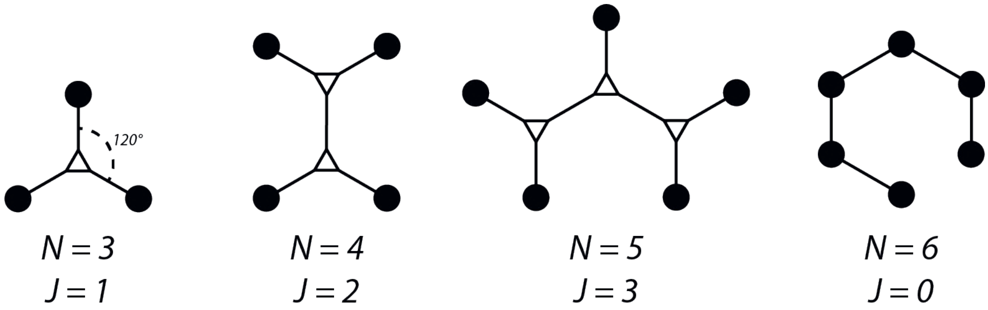


Figure 5 - Shortest interconnecting networks connecting N nodes (circles) by placing at most N-2 junctions J (triangles).

Least cost route methods for pipeline placement have shown that connecting supply and demand locations with a straight line leads to higher costs (Durmaz et al., 2019; Feldman et al., 1995; Yildirim et al., 2017). The reason for this is that the cost surface for pipeline placement does not resemble a flat Euclidean surface but can have peaks and troughs depending on local spatial characteristics (Figure 6). For the creation of pipeline networks this means that the placement of junctions does not necessarily occur at a 120-degree angle.

Depending on the water requirements at the demand location the number of supply locations that must be used changes. For the optimal placement of junctions, the number of supply locations needs to be known beforehand. The computational requirements to solve the junction placement problem in the Euclidean plane are already considerable. Therefore, it is expected that connecting the WaterROUTE optimization procedure in an iterative way with the junction placement problem is expected to be computationally infeasible.

The first step for optimal junction placement in decentralized water supply networks is to determine the extent to which the total water supply network costs can be reduced. This can be done by estimating optimal junction placement manually based on the water supply locations identified in one of the WaterROUTE outputs. After manual junction placement the total network costs can be compared. If there is a significant reduction in costs the second step is the development of methods to automate junction placement on a non-Euclidean cost surface. A possible way to approach this problem is to mimic the way nature has solved network design problems. Examples can be found in the networks fungi

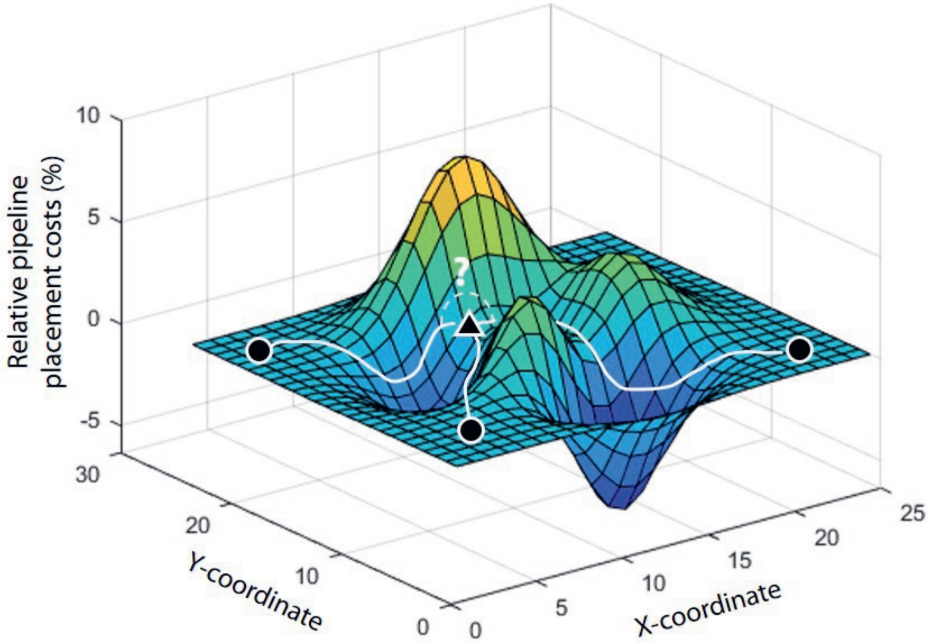


Figure 6 - 3D visualization of a cost surface for pipeline placement with three nodes connected by a network with a single junction. The location of the junction, and the angle between pipelines, cannot be determined in the same way as in a Euclidean plane. (The surface plot visualization was adapted from https://www.mathworks.com.)

create to transport nutrients (Bebber et al., 2007; Tero et al., 2010) or network creation in the field of ecology (Dale and Fortin, 2010). Both steps are suggested for future research.

3.2 Space and quantity

The optimal configuration of a water supply network depends on the spatial distribution of water resources in relation to the location where there is a water demand.

3.2.1 Supply locations

In **Chapter 3**, hydrological simulation models are used to determine the location and available water quantity of groundwater resources in the study area. The spatial differences of the hydraulic properties in the subsoil are used to identify possible groundwater well locations and analytical methods are used to establish the maximum extraction per well cluster. Environmental compatibility of the overall water supply network is ensured by limiting the maximum extraction rate

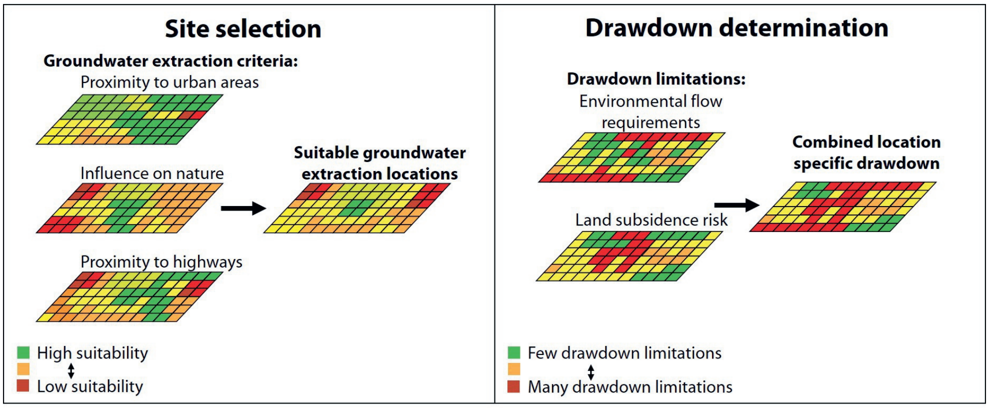


Figure 7 - Visualization of the way spatial multicriteria decision-making can be applied to the selection of groundwater extraction locations or to determine local drawdown limits.

at each well cluster to avoid excessive drawdown of the groundwater level or upcoming of saline water from below. The above approach provides a good starting point to determine suitable locations for groundwater extraction based on environmental compatibility and can be extended with additional criteria. Additional spatial data can be used to further refine the selection of potential extraction locations by adding constraints based on these criteria.

Spatial data can be used for the selection of suitable water supply locations in relation to existing infrastructure, urban areas, or protected nature. Spatial multicriteria decision making is a suitable method when the location of an action can influence a decision (S. Chakhar and V. Mousseau, 2008a, 2008b). For example, the S-MDCM method for site selection of an industrial facility (Rikalovic et al., 2014) can be adapted to select suitable groundwater extraction locations. The current extraction rates used in **Chapter 3** are based on a single drawdown value for the entire study area. Specifying location specific drawdown values based on the local conditions at a high resolution is an additional way to make water availability spatially dependent. Location specific drawdown values can be made dependent on local environmental flow requirements (the amount of water required to maintain ecosystems (Pastor et al., 2014)) or areas where ground subsidence needs to be avoided. The way additional spatial aspects can be used to determine environmentally compatible water availability in a region is shown in Figure 7. Figure 7 shows how spatial data and different criteria can be combined to select suitable sites for groundwater extraction or to determine acceptable drawdown levels.

In **Chapter 5** additional potential water supply locations are identified based on the location of urban areas and the yearly precipitation at each of them. High resolution spatial data on roof surface area in combination with location specific precipitation data makes it possible to calculate the amount of runoff for each city. Additional spatial data on different types of roof surface – which affects the runoff coefficient – can further enhance the accuracy of the runoff calculations (Farreny et al., 2011).

3.2.2 Demand locations

In this thesis water supply network design for a single, known, industrial demand location was investigated. Spatial data is valuable to determine additional water demand locations and to estimate their water demand patterns (House-Peters and Chang, 2011). Additional demand locations in a region can be agricultural fields, cities, ecosystems, or other industrial areas. Increasing the number of demand locations in WaterROUTE is currently possible if water quality is not included. Using multiple demand locations in WaterROUTE reveals the optimal configuration to supply each location based on their specific water demand. Figure 8 shows how WaterROUTE can be used to design a water supply network for multiple demand sites. Depending on the water demand (quantity and quality), the location of the demand locations, and the water availability in the region, the result can be multiple small networks for each demand site (Figure 8-A), or a larger connected network between multiple demand locations (Figure 8-B). This functionality can be used to investigate scenarios in which there are multiple demand locations competing for the same scarce water resources.

3.3 Space, quantity, and quality

In **Chapter 4**, the model developed in **Chapter 3** is renamed to WaterROUTE and is expanded to include water quality in the optimization of water supply networks. The inclusion of water quality makes the delivery of fit-for-purpose water possible. Delivering fit-for-purpose water is considered one of the main benefits of decentralization in the urban water cycle (Capodaglio, 2021). Fit-for-purpose means that water is delivered to the demand location at the specific water quality that is required, which is made possible by technological innovations (Capodaglio, 2021). In the area of fit-for-purpose water reuse, decentralization shows great potential for cost and environmental

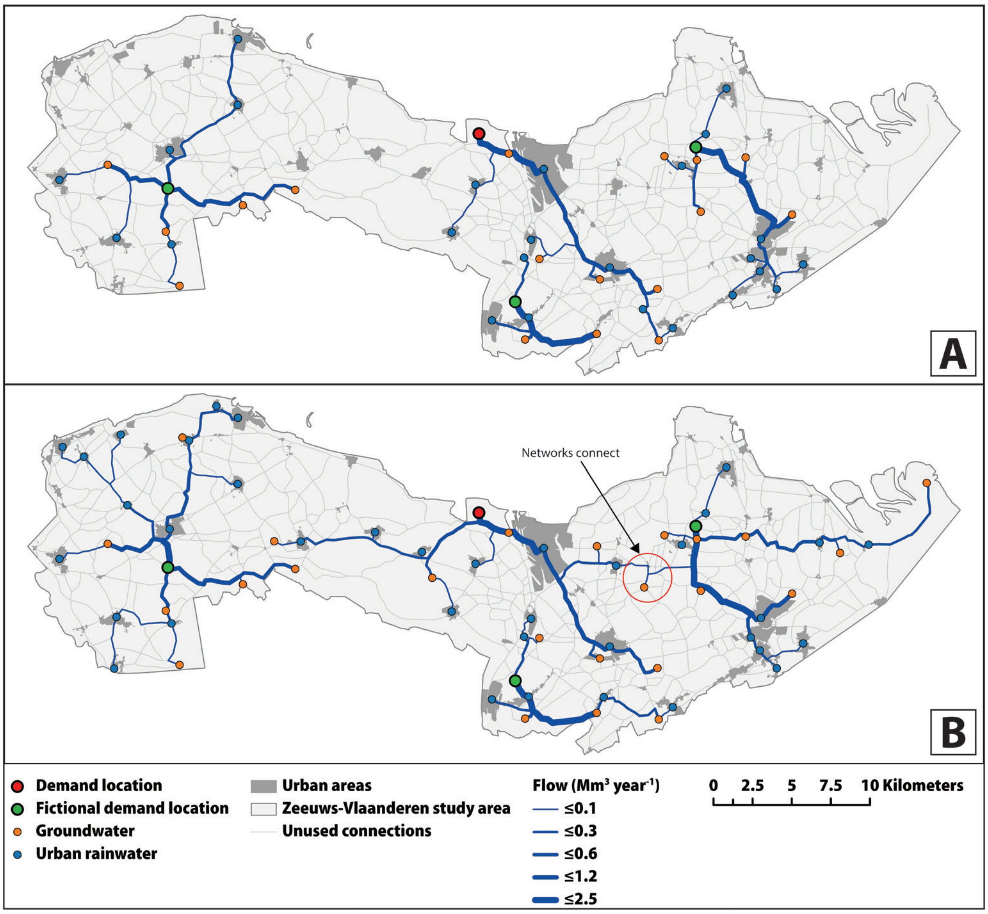


Figure 8 - WaterROUTE for water supply network design involving multiple water demand locations. Each demand location has a demand of 2.2 Mm^3 year^{-1} (A) or 2.5 Mm^3 year^{-1} (B). Urban rainwater availability is based on the precipitation data of 2018 used in ***Chapter 5****. The red circle indicates the location where smaller networks connect as the demand grows.*

savings (Brown et al., 2010; Capodaglio, 2017; Libralato et al., 2012; U.S. Environmental Protection Agency (USEPA), 2012). Current fit-for-purpose water research mainly examines the potential to reuse wastewater close to where it is produced. WaterROUTE makes it possible to evaluate fit-for-purpose water supply at larger spatial scales, which is not limited to wastewater reuse. In **Chapter 4** fit-for-purpose water supply network design is tested with saline groundwater instead of wastewater.

In WaterROUTE an effective way to include the spatial differences in water quality of alternative water resources is achieved for a single demand location. Water quality is added to the optimization problem through a mass balance for the salt (expressed in terms of chloride, Cl^-) which is present in the brackish groundwater. The total amount of chloride extracted from the groundwater well clusters must be accounted for at the demand location (Figure 9-A). This methodology makes it possible to evaluate the spatial location of water sources together with water quality and quantity simultaneously. WaterROUTE makes it possible to determine if a faraway water source with a good water quality should be considered instead of a closer by water source with a lower quality. A possible future application of WaterROUTE is to investigate other contaminants than salt or multiple contaminants. The mass balance approach of contaminants in WaterROUTE makes it possible to use any other substance to design fit-for-purpose water supply networks.

Integrating additional water users such as agriculture in decentralized water supply networks can increase the optimal use of regionally available alternative water resources. WaterROUTE must be expanded with additional non-linear constraints to make fit-for-purpose water supply networks with multiple users possible (Figure 9-B).

Further development of WaterROUTE in terms of water quality entails the incorporation of treatment technologies directly within the optimization model. The possibility to use treatment technologies to reach the desired water quality not only yields the optimal network configuration, but also the optimal placement of treatment facilities. A possible way to implement water treatment in the optimization model is by using/modifying the two-node representation of storage facilities presented in **Chapter 5**. The possibility to implement decentralized treatment at specific locations in the network further enhances the possibility to deliver fit-for-purpose water.

3.4 Space, quantity, and time

In **Chapter 5**, the WaterROUTE model is upgraded a final time to make design of decentralized water supply networks with additional alternative water sources possible. In **Chapter 3** and **Chapter 4** only groundwater was used. In **Chapter 5** the structure of WaterROUTE is adjusted so that harvested rainwater can be used as an alternative water resource. The intermittent nature of rainwater availability requires a method to bridge the temporal mismatch between supply and demand. However, bridging this temporal mismatch should not compromise the possibility to account for the spatial mismatch as was done in **Chapter 3** and **Chapter 4**. The approach taken in **Chapter 5** is to convert the intermittent

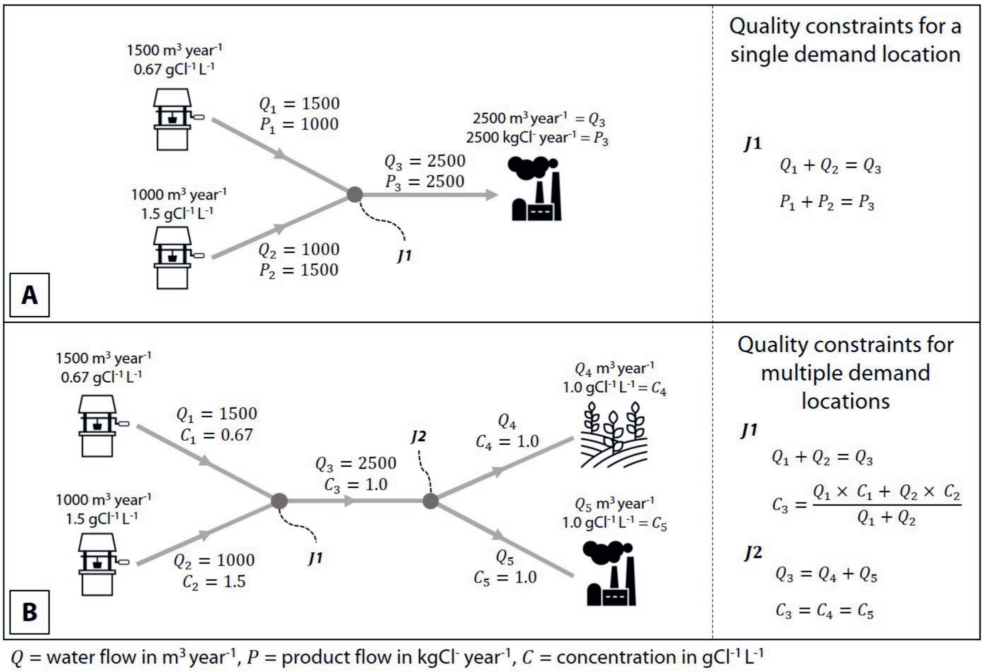


Figure 9 - Water supply network model including water quality for a single demand location in the current WaterROUTE model (A). Extending WaterROUTE with water quality to include multiple users is possible if water quality is correctly tracked through the network (B). Tracking water quality over every pipeline requires additional non-linear constraints.

availability of rainwater into a constant supply by using storage infrastructure. Considering that water availability is expected to become more intermittent in the future due to changes in precipitation patterns makes WaterROUTE a valuable tool to explore alternative water supply solutions.

In WaterROUTE the design of storage infrastructure is based on a time series of real precipitation data in combination with a water balance model. The optimization problem involving storage design and network layout simultaneously is solved by representing water supply sources as two-node elements and by converting precipitation data into a linear function relating demand to the costs for storage infrastructure. The consequence of this procedure is that the optimization of storage basins is separated from the optimization of the water supply network. Ideally these two optimization problems are solved simultaneously.

Further research on decentralized water supply networks with storage facilities requires the development of new optimization problem formulations for multireservoir systems. The urban areas from which rainwater is harvested can be seen as a multireservoir system. The optimization and design of multireservoir systems is computationally demanding due to the large number of potential configurations (Nagy et al., 2002). Mathematical optimization approaches for single reservoir design considering both quantity and quality are well developed (Chaves et al., 2003; Xu et al., 2020). This is also the case for the design of reservoir networks (Travis and Mays, 2008) and the optimization of water distribution network *operation* with storage facilities (Chang et al., 2018). The optimization problem presented in **Chapter 5** differs from the above examples because reservoir size and network configuration need to be considered and optimized simultaneously.

4 Wastewater as alternative water source - WaterROUTE applied to WWTP effluents

Besides the groundwater and rainwater resources investigated in **Chapters 3, 4, and 5** other alternative water resources can also be analyzed with WaterROUTE. One of the possible alternative sources is municipal wastewater treatment plant (WWTP) effluent. Only 2.4% of the wastewater treated in Europe is reused. North America performs slightly better with 3.8% (van Rensburg, 2016). One of the main barriers for wastewater reuse for direct human consumption is public perception/social acceptance (Duong and Saphores, 2015), often described as the 'yuck' factor (M. Po et al., 2003). WaterROUTE provides a way to circumvent the 'yuck' factor by delivering 'fit-for-purpose' treated wastewater to industry. Water reuse in industry is more easily accepted because direct human contact is limited or non-existent (Capodaglio, 2021).

The exchange of water between urban areas and industry is feasible and can generate environmental benefits (Lu et al., 2020). The difficulties in setting up resource exchange networks between industries can be avoided by using municipal WWTP effluent. Resource exchange between industries creates mutual dependencies which are sometimes considered as a barrier to implementation (Neves et al., 2019). For example, dependence on the 'waste' flows of another company is seen as a barrier to resource exchange due to the increased attention to waste reduction measures (Wolf et al., 2005). The exchange of water resources with urban areas can reduce this uncertainty since urban water consumption, and consequently the amount of wastewater produced, is relatively stable.

From an infrastructural perspective one of the main advantages of using domestic WWTP effluent in decentralized water supply networks is that additional infrastructure is needed to a limited extent. Harvesting urban rainwater requires large storage basins to convert intermittent precipitation into a constant water supply. Extraction of groundwater resources requires drilling of wells and constructing pumping infrastructure. Collection of WWTP effluent is relatively simple because sewerage and wastewater treatment infrastructure is already present for 95.5% of Dutch households (Partners 4 Urban Water en Deltares, 2020). Incorporating WWTP effluent in decentralized water supply networks changes the function of sewers from *waste collection* to *resource collection*.

In the area of Zeeuws-Vlaanderen part of the industrial demand of DOW Terneuzen is currently already covered by WWTP effluent from the city of Terneuzen. WaterROUTE can be used to evaluate the exchange of such flows and to determine when one water source should be preferred over another. In the following sections the potential synergy of using WWTP effluent together with other alternative water resources is highlighted and discussed. This is done based on a simple example simulation where treated wastewater is one of the alternative water sources in WaterROUTE.

4.1 WWTP effluent as alternative water source in Zeeuws-Vlaanderen

The population of Zeeuws-Vlaanderen produces around 4.17 Mm^3 of wastewater per year based on a per capita water use of 118 L day^{-1} (Nibud - Nationaal Instituut voor Budgetvoorlichting, 2021). This water is treated and most of it is discharged to surface waters and to the sea. WaterROUTE can be used to determine the optimal network configuration when WWTP effluent is used as an alternative water source in decentralized water supply networks. A preliminary analysis of a situation where WWTP effluent, groundwater, and urban rainwater are all used as alternative water sources for water supply, in terms of water quantity, is given below.

Running WaterROUTE for a demand of 10 Mm^3 $year^{-1}$ at DOW Terneuzen with urban rainwater, groundwater, and WWTP effluent shows that urban areas are valuable sources of water (Figure 10). This example assumes that WWTP effluent is available at every urban area in the study region and that the additional infrastructure costs for WWTPE effluent are negligible. In most cities rainwater harvesting and the use of WWTP effluent are combined. Using rainwater and WWTP effluent at the same location is very cost effective in terms of pipeline

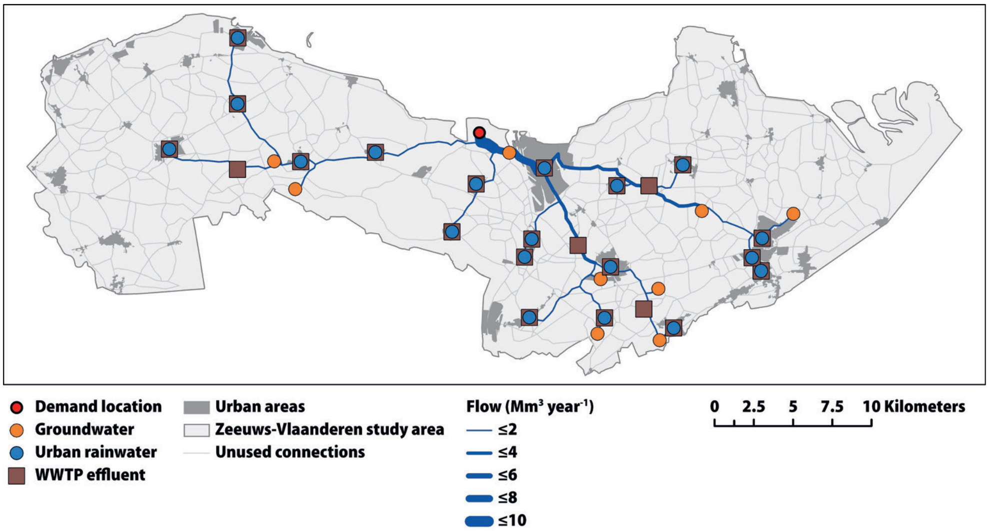


Figure 10 - Water supply network configuration for a demand of 10 Mm^3 year^{-1} using groundwater, urban rainwater, and wastewater treatment plant effluent (WWTP effluent) as alternative water resources. Urban rainwater availability is based on the precipitation data of 2018 used in ***Chapter 5****.*

placement. Nonetheless, at several urban areas only WWTP effluent is used (shown by locations with only a brown square in Figure 10). This shows that in some situations using WWTP effluent is cost effective, but rainwater harvesting is not. The reason for this is that for some urban areas the costs for rainwater storage infrastructure are too high in relation to the amount of water provided by rainwater harvesting. Using WWTP effluent on the other hand requires almost no additional infrastructure, which makes it an interesting water source whenever new pipeline infrastructure is placed in the vicinity. This example shows how WaterROUTE can be used to decide between co-located alternative water resources.

Figure 11 shows that all alternative water resources are used simultaneously as the demand increases. This indicates that the configuration of the network is mostly determined by the costs for the pipeline infrastructure instead of the costs for rainwater harvesting or groundwater exploitation. If the costs for pipeline infrastructure were lower this would result in most water being supplied with WWTP effluent for a demand up 4.17 Mm^3 year^{-1}, which corresponds to the maximum amount of WWTP effluent available. Up to a demand of around 3 Mm^3 year^{-1} most water is supplied by the large urban area close to the demand location.

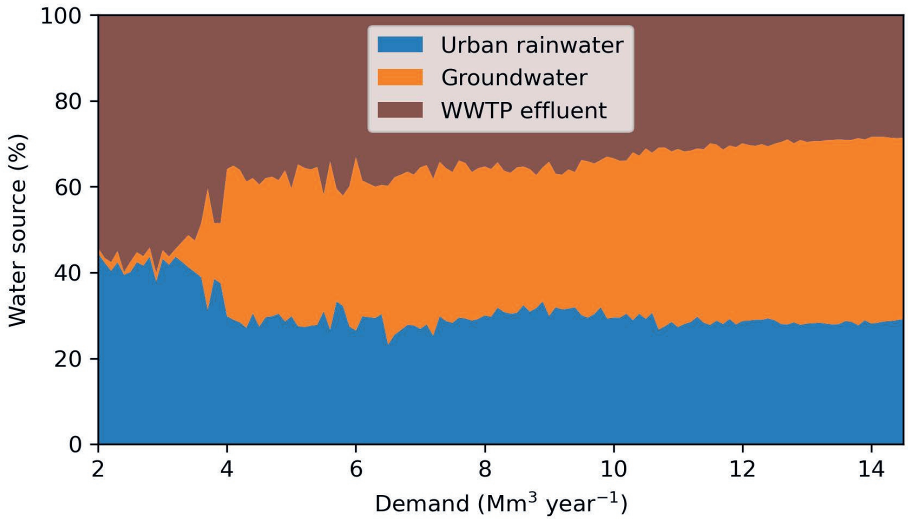


Figure 11 - Distribution of water by source for an increasing demand when using urban rainwater, groundwater, and wastewater treatment plant effluent (WWTP effluent) as alternative water resources.

4.2 Identifying additional benefits with WaterROUTE

In the previous section the use of WWTP effluent is seen as an additional constant water supply source which can increase the total availability of water in the region. An alternative approach is to use WWTP effluent mainly during the summer when there is a reduced availability of rainwater. With such an approach the storage capacity required for rainwater can be reduced while increasing reliability of supply for the demand site. Such an approach can be investigated with WaterROUTE by running different scenarios for summer and winter periods to identify how much WWTP effluent is needed to supplement rainwater in the summer.

Incorporating WWTP effluent in decentralized water supply networks can also have benefits for municipal wastewater treatment plants. By delivering fit-for-purpose water with a decentralized water supply network it becomes possible to re-evaluate the level of treatment required at the municipal treatment plant. Depending on the purpose for which industry uses the water less stringent effluent requirements are acceptable, which in turn reduces treatment costs at the municipal WWTP. Delivering fit-for-purpose water is also possible with decentralized treatment technologies. A shift from centralized municipal wastewater treatment technologies towards decentralized treatment can result in lower economic and environmental costs (Garrido-Baserba et al., 2018). These potential cost savings can be included in WaterROUTE in the future by assigning negative costs for specific water resources in the objective function. This can reveal the value of fit-for-purpose treatment and stimulate the research and implementation of new treatment technologies.

Another benefit that can be investigated and quantified with WaterROUTE is the possibility to avoid curtailment. By using WWTP effluent industry is guaranteed a base flow of water during droughts. During droughts water for industry is curtailed before drinking water (Rijkswaterstaat, 2020). This curtailment can be (partially) avoided by making use of WWTP effluent.

5 Outlook

The availability of modelling tools such as WaterROUTE is essential for regional scale planning and water resource exchange between different water sources and users. Enhancing and optimizing resource flows between industry, urban areas, agricultural and the local environment as shown in Figure 1 is needed to make water use environmentally compatible. As the number of potential supply and demand locations increases modelling tools such as WaterROUTE are needed to create an initial set of feasible solutions which can be used for further evaluation.

The work in this thesis shows that optimization of resource flows across spatial and temporal scales in the context of urban metabolism/industrial ecology is possible. WaterROUTE provides a good starting point to design decentralized water supply networks. The WaterROUTE modelling framework is flexible and can be extended in many ways.

5.1 Space, quantity, quality, and including time

The individual elements to include spatial and temporal aspects in the design of decentralized water supply networks have been developed and tested in this thesis. These individual elements can be combined in new and different ways depending on the requirements of new study areas. One area which has not yet been investigated in this thesis are temporal variations in water quality. WaterROUTE can be extended to deal with temporal variations in water quality by combining the modelling approaches presented in **Chapter 4** and **Chapter 5**. The methods presented in **Chapter 4** are suitable to handle water quality in decentralized water supply networks. The methods presented in **Chapter 5** can be used to include treatment technologies in the optimization model. The growing body of literature on (waste)water treatment technologies and their costs

(Gallego-Valero et al., 2021) can be used to generate location specific cost functions for water treatment. The result of such an analysis can reveal whether storage, treatment, or transport is the most effective.

5.2 Optimizing for different or multiple objectives

WaterROUTE focuses on the economic costs of a water supply networks. Optimization based on other objectives is also possible and suggested for future research. A few options are discussed below:

Minimizing CO_2 emissions: greenhouse gas emissions from the water sector are significant on a global scale (Rothausen and Conway, 2011). The construction and operation of new water supply networks can be expressed in terms of CO_2 equivalents instead of economic costs. The construction of new water supply networks requires several materials. The production of construction materials lead to CO_2 emissions, the embodied carbon emissions of materials (Nishimura et al., 1997). The differences in the embodied CO_2 of construction materials inevitably makes the use of some water resources more CO_2 intensive than others. For example, the materials needed for drilling groundwater wells can be completely different from the materials needed for water storage basins. There are also CO_2 emissions associated to the operation of water supply networks, mostly because of the energy required for pumping (Rothausen and Conway, 2011). WaterROUTE can be used to design water supply networks which minimize CO_2 emissions by expressing the construction and operation of a water supply network in terms of CO_2 equivalents (kg CO_2-eq m^{-3}). The current formulation of the objective function in WaterROUTE can be used for this purpose with minor modifications if data is available for the embodied CO_2 of the different components.

Multiple objectives: the current version of WaterROUTE is based on minimizing a single objective, the economic costs of a water supply network. Decisions concerning water resources generally involve several stakeholders with potentially conflicting interests (Silva et al., 2010). WaterROUTE can be combined with other models to evaluate the suitability of alternatives based on differing interests. An example of such an application is determining whether desalination is preferable over water transport with Data Envelopment Analysis (Belmondo Bianchi et al., 2020). Such analyses can be further expanded within WaterROUTE and in combination with other models. Another option is to reformulate the optimization problem in WaterROUTE as a multi-objective optimization problem.

5.3 Optimizing with height differences

WaterROUTE has been applied and tested in a country with minimal height differences, the Netherlands. The inclusion of height differences adds an additional dimension to the spatial aspects that influence water supply network design. Adding height differences in the WaterROUTE model can be done within the optimization problem and in the creation of the preliminary network.

The height differences in the study area of Zeeuws-Vlaanderen are so small that the added pumping costs to overcome them is neglectable in comparison to the normal infrastructure and operational costs. For example, the added pumping costs to overcome height differences would be less than 0.5% for the network supplying 12.83 Mm^3 $year^{-1}$ with groundwater and rainwater in **Chapter 5**. In areas where height differences are considerable the added pumping costs should be added to the optimization problem. This can be achieved by adding height data for each vertex to the preliminary network. The height difference between the starting vertex and end vertex of every potential pipeline connection – the edges – can then be calculated. These height differences can then be used to calculate pumping costs based on the flow over a pipeline and can be added as an additional term to the objective function of the optimization problem.

Height differences can also be used as a criterion for the creation of the cost surface which is used to create the preliminary pipeline network. Areas with a steep slope are less accessible for machinery, resulting in higher costs for pipeline infrastructure. At the same time ridges are less affected by erosion, which makes them suitable for pipeline placement (Durmaz et al., 2019).

6 Realizing environmentally compatible water use

As shown in **Chapter 2** the way industrial water use is currently evaluated usually does not coincide with the requirements for environmentally compatible water use. In most cases industry evaluates water use based on the question: how much water is being used? Instead of asking the question: how much water <u>should</u> be used? Asking, answering, and acting on this second question must happen at every location where the natural water system is altered to create an environmentally compatible water supply system. Luckily, the development of evaluation methods has continued and there is an abundance of tools ready to assist decision makers in answering this question. However, it is up to society to demand regulatory changes that enforce the use of adequate evaluation methods.

Only by using adequate evaluation methods it becomes possible to set boundary conditions on water use that are compatible with the local environment.

The idea that cities and industrial systems function like living organisms in an ecosystem – as advocated by the urban metabolism (Koenraad Danneels, 2018) and industrial ecology fields (Xuemei Bai, 2007) – implies that they are subject to some form of natural selection. Natural selection causes populations of organisms to evolve towards a (local) optimum in the adaptive/fitness landscape (Kaplan, 2008; S. Wright, 1932). Continuous changes in nature result in a dynamic adaptive landscape to which organisms can adapt (Laughlin and Messier, 2015). For example, a certain trait may provide a competitive advantage in a specific environment but can become less useful at the environment changes.

The current linear resource use and environmentally degrading practices of cities and industries can be seen as beneficial traits to reach a (local) optimum in the adaptive landscape where they operate. The current adaptive landscape for industry favors economic profitability over sustainability. Regulatory changes are needed to alter this adaptive landscape and to make environmental compatibility a competitive advantage instead of a burden. The European Green Deal (European Commission, 2019) and the Green New Deal in the United States (U.S. Government Information, 2019) are evidence that the adaptive landscape is changing. Tools such as WaterROUTE are available for the journey towards a new optimum in this new adaptive landscape.

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Summary

Humanity is dependent on the natural water cycle and ecosystems for its freshwater resources. As the global demand for water grows – due to population growth and increased levels of consumption – the pressure on water systems increases, jeopardizing ecosystem health and the provision of water for human consumption. Redesigning water supply systems to make effective use of decentralized alternative water resources can contribute to long-term water security; this is investigated in this thesis.

Using alternative water resources such as rainwater, (brackish) groundwater, or treated wastewater can be facilitated by delivering 'fit-for-purpose' water with a decentralized water supply network (WSN). 'Fit-for-purpose' entails delivering water with the quality required by the user instead of enforcing a single water quality in the complete water supply system. Especially in the industrial sector, where different processes require specific water qualities, delivering fit-for-purpose water can reduce this sector's demand on scarce freshwater resources. Decentralization of water supply systems makes a transition to fit-for-purpose delivery possible and economically interesting. The challenges that must be overcome for such a transition involve the spatial and temporal mismatch between the supply and demand for water resources.

The objective of this thesis is to develop modelling tools for the design of water supply networks using alternative regional water resources. The boundary condition for these water supply networks is that they should be environmentally compatible, meaning that the environmental impacts of water use are quantified and used for the design of a WSN at every location where the natural water system is altered. To reach this objective two research questions were formulated:

1. *Which methods are available to effectively evaluate the sustainability of industrial water use and to what extent are these methods currently used?*
2. *What is an effective modelling framework to optimize environmentally compatible water supply networks based on the spatial and temporal variability of water supply and demand in terms of both water quantity and water quality?*

The first research question is used to better understand the industrial water system and to set the boundary conditions for environmentally compatible water use. The second research question is used to guide the development of new modelling tools.

After a general introduction in **Chapter 1**, in **Chapter 2** a systematic literature review on the evaluation methods currently used to assess industrial water use is presented. The projected increase of industrial water demands makes effective evaluations of industrial water use essential to reach sustainability goals. An existing assessment framework is used to evaluate the effectiveness of the methods used in industry to determine if water use exceeds the thresholds of natural systems in terms of water quantity and quality. A total of 82 different assessment methods were identified in 340 papers. Out of all reviewed papers only a minority (26%) were considered to use methods that are suitable to evaluate the sustainability of water use on a system level. Examples of good practices are highlighted to aid researchers and practitioners when selecting evaluation methods and to provide a starting point for future methodological development. The findings of this chapter are used to define the boundary conditions for the design of water supply networks in the following chapters.

Chapter 3 shifts to the development of modelling tools to match the regional water supply and demand with decentralized water supply networks (WSNs). The construction of WSNs requires new pipeline infrastructure. In this chapter special attention is paid to the importance of the local conditions that affect the costs of pipeline infrastructure. For example, placing a new pipeline in an urban area is significantly more expensive than placing the same pipeline along a country road. In this chapter we present a modelling approach that takes these local conditions as inputs to create WSN configurations that are optimized in terms of the investment costs of pipeline infrastructure. The model determines the optimal pipeline route, the amount of water flowing over each pipeline segment, and reveals if a small increase in demand causes a relatively large increase in WSN costs.

In **Chapter 4** the modelling approaches developed in **Chapter 3** are further developed to include the fit-for-purpose water concept in the design of decentralized WSNs. By mixing water with different salinities originating from several groundwater well clusters fit-for-purpose water can be delivered to the demand location. Hydrological modelling is used to simulate changes in groundwater salinity up to 2110 which increases over the complete study area. We investigate three scenarios – 2030, 2045, and 2110 – to show the effect of increasing groundwater salinity on the costs of delivering fit-for-purpose water with a decentralized WSN. The results show that small changes in the maximum salinity at the demand location coupled with salinization of groundwater have significant effects on the optimal configuration of a WSN and therefore on long-term regional planning. In this chapter the configuration of the WSN is also optimized based on the economic costs for infrastructure investments.

Chapter 5 further develops the modelling tools for WSN design. The focus of this chapter is on WSN design where some water sources are constantly available (e.g., groundwater) while some are intermittent (e.g., harvested rainwater). To use groundwater and rainwater simultaneously the location specific infrastructure costs for each water supply location must be used in the optimization model. The infrastructure needed for rainwater harvesting is a storage basin, while the exploitation of groundwater requires drilling wells and pumping infrastructure. By changing the representation of water supply sources in the optimization model it becomes possible to include the effects of these differences in the design of WSNs. The results show that rainwater and groundwater are competitive in terms of costs, even when the availability of rainwater is limited. In this chapter the optimization of WSNs occurs based on both the operational and investment costs for water infrastructure.

This thesis ends with a synthesis and discussion of the results in **Chapter 6**. This chapter starts with the contributions of this thesis to different research fields: urban ecology and industrial ecology. It is argued that the modelling tools developed in this thesis can be used to connect these fields and to model/evaluate water resource networks between industry, agriculture, and urban areas. The temporal and spatial challenges associated with WSN design are discussed and research directions for future model development are presented. A brief showcase demonstrates how the developed modelling tools can be used with additional alternative water resources (treated wastewater) and with multiple demand sites. The chapter ends with a reflection on the necessary conditions to initiate a transition towards environmentally compatible water supply systems. It is argued that such a transition starts by increasing the use of effective water assessment methods, as elaborated in **Chapter 2**.

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Joeri Willet was born on the 28th of January of 1991 in the city of Cuenca, Ecuador. He spent his childhood in Peru, Bolivia and the Netherlands. After graduating from high school in Bolivia he moved to Wageningen to study Environmental Sciences in 2009. In 2015 he obtained a MSc degree in Urban Environmental Management with a specialization in Urban Systems Engineering. In 2016 Joeri started the research in this dissertation at the Environmental Technology Department. As a PhD candidate Joeri supervised several MSc students and was involved with teaching of several courses. Joeri will continue working at the Environmental Technology department, where he teaches and performs research.

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- *Water supply network model for sustainable industrial resource use*. Environmental Technology for impact, 4 June 2020, Wageningen, The Netherlands

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