



Original Research

In silico assessment of household level closed water cycles: Towards extreme decentralization

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ABSTRACT

Water management in most of the developed world is currently practiced in a highly centralized manner, leading to major infrastructure and energy costs to transport water. To decrease the impacts of water scarcity and climate change, the decentralization of water can increase local robustness. In extremis, decentralization can involve building or house level water supply and treatment. Here, we constructed a MATLAB/Simulink model for two decentralized water management configurations at the household level, assuming the socio-environmental setting of Flanders, Belgium. Independence from the potable water grid and sewer system was pursued through rainwater harvesting, reuse of wastewater streams fit-for-purpose, and discharge via infiltration. The mass balance for water was calculated over the system boundaries showing high potential for independence from the grid with a reasonable treatment train and storage options. Next, the risk of contaminant accumulation within the circular system was assessed, showing a key limitation on decentralized system performance necessitating a system purge. Up to 59% of system rainwater usage was due to the replacement of this purge. Employing treatment units with high (95%) contaminant rejection efficiencies eliminated contaminant accumulation issues. The raw model output was quantitatively assessed by constructing four newly proposed key performance indicators (KPIs), quantifying system independence, circularity, drought tolerance and local water body recharge, which allowed for facilitated system comparison and communication to stakeholders. A sensitivity analysis was performed in which the effect of input parameter variability and uncertainty on system performance was quantified. The sensitivity analysis showed the importance of water recovery and contaminant removal efficiencies of the applied treatment technologies on system performance when contaminant accumulation in the system forms an issue. In systems not severely affected by pollutant accumulation, parameters such as inhabitant number and roof surface had the largest effect. As a whole, this work shows the potential of extreme decentralization of water systems and addresses the obstacle towards implementation formed by the accumulation of contaminants due to system circularity. Additionally, this study provides a framework for operational and technological decision support of decentralized household-scale water systems and, by extension, for future water policy-making.

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1. Introduction

Water management is currently practiced in a highly centralized manner, relying on extensive piping networks for potable water

supply and wastewater collection through sewers [1]. This leads to high costs to transport water and dislocation of water from where it was originally harvested from nature. Moreover, this approach creates limitations on innovation in the water sector, particularly via technology “lock-in” effects [2]. Increasing water scarcity and climate change are pushing the water sector towards alternative

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List of abbreviations

Abbreviation	Model constituent (unit)
Q	Flow rate (m ³ month ⁻¹)
PGW	Purified greywater
PW	Potable water
BW	Blackwater
RW	Rainwater
A _{roof}	Roof surface (m ²)
Rec	Water recovery
MBR	Membrane bioreactor
RO	Reverse osmosis
UV	Ultraviolet light

water management methods, as illustrated by the growing push from policymakers for local reuse and infiltration of rainwater [3,4]. As water distribution in industrialized countries evolved to be supply-driven, leading to sufficient quantities of available high-quality water, the reuse of (municipal) wastewater streams was mostly undervalued [5].

Decentralized water installations are standalone systems used to treat small wastewater flows and local discharge or reuse. Here, collection, treatment, discharge, and potential reuse of wastewater take place near the point of formation [1]. These systems on the scale of a household, building, or district can enable independence from centralized sewer systems or potable water grids and may allow efficient reuse of different water flows [6]. Often-noted advantages of decentralization of water management include a) increasing (local) system resilience next to robustness, b) closing the water loop in the near environment (e.g., local rainwater management and groundwater replenishment), c) increasing water buffer capacity, and d) reducing high-quality water used for applications with a low-quality need [7,8,9,10].

Centralized systems benefit from economies of scale through decreasing treatment costs per unit wastewater as the capacity increases. As a result, decentralized systems are generally only considered when the cost of connection to the sewer or water supply system is too high. Nonetheless, decentralized systems can increasingly compete with centralized systems due to technological advancements, e.g., in membrane technology, and an "economy of numbers". The latter implies the decreasing cost of small-scale treatment systems due to mass production [11,6]. A growing number of ongoing decentralized pilots and full-scale projects are also leading to a more institutional endorsement of the decentralized options [12]. However, it has been often noted that a lack of stakeholder engagement forms an important shortcoming in introducing such new paradigms to the water sector [13].

As the incorporation of decentralized water systems increases water management complexity, the need for comprehensive decision support tools is raised [14]. Over the past few decades, computational models have received increasing interest in addressing water management challenges, allowing for low-cost system evaluation and facilitation of policy development. These models were constructed for various approaches and functioned according to varying temporal and spatial scales [15]. Most research about the modeling of urban water systems has been performed within the predominant centralized paradigm, where initially the focus lay on modeling of separate compartments of the water system (water distribution, water treatment, stormwater drainage), later evolving towards more integrated, holistic approaches [16]. However, modeling of decentralized water systems has most often been performed within this same centralized framework, where complete disconnection from the potable water grid or sewer system is not investigated [14,17] and where water availability is mostly calculated at the system level. Complete disconnection of a water system was previously assessed in simulations performed by

Ref. [18]; though specifically focussing on technological and less on systemic features. This work aims to provide a more integrated look into extreme decentralization.

A potential bottleneck to the implementation of circular water reuse systems is the issue of contaminant accumulation, as incomplete removal of salts, metals, microorganisms, or other contaminants may lead to a build-up to hazardous concentration levels. Although the implications of such accumulation phenomena may have adverse effects on implementing such water reuse systems, the issue has not been addressed and further quantified in the scientific literature to the best of the authors' knowledge.

In this paper, we developed a model to simulate several decentralized water management configurations on a household scale. For two main cases, the potential for extreme on-site decentralization was assessed. Independence from the potable water grid and sewer system was assumed through rainwater harvesting and reusing (waste)water streams generated within the building. As a first step, a water mass-balancing was performed, after which it was coupled to a model for contaminant accumulation within the circular system. Next, the raw model output was quantitatively assessed by constructing key performance indicators (KPIs), which allowed for facilitated comparison between system scenarios and communication to stakeholders. Finally, a sensitivity analysis was carried out to quantify and rank the impact of input parameter variations on system performance. As a whole, the work performed here aimed at providing a framework for the ex ante evaluation of decentralized household-scale water systems. All modeling work was performed in MATLAB/Simulink [19].

2. Methodology

2.1. Two decentralized systems: Scenario construction

Two main configurations for extreme decentralized water management on a household scale were constructed:

- Case A: Household water input consists of harvested rainwater with a high degree of greywater reuse. This allows for disconnection from the potable water grid. Blackwater, i.e., toilet water, is not reused but treated towards discharge standards in the septic or blackwater tank and subsequently discharged.
- Case B: In addition to Case A, blackwater is reused by adding the overflow of the septic pit to the treatment step preceding the purified greywater tank when necessary, i.e., when greywater production is too low. Additionally, a more extensive treatment was assumed to treat the combined grey- and blackwater.

Choices made were based on assumptions within the context of an average household in the Flanders region in Belgium and within the boundaries of a single free-standing house (see Table 1). The following water flows are distinguished: Greywater (GW), purified greywater (PGW), rainwater (RW), potable water (PW), and blackwater (BW). Purified or treated greywater is defined as water applicable for direct non-potable reuse. Potable water originating from rainwater is considered suitable for human consumption. Moreover, blackwater, or toilet wastewater, is presumed to flow into a septic tank (blackwater tank) which either overflows into the environment (Case A), cf. onsite sewage facilities, or is reused along with greywater with a more extensive treatment (Case B). Four storage tanks are considered in the system: A potable water tank, a rainwater tank, a purified greywater tank, and a blackwater tank. The tanks are assumed to have realistic dimensions. Between the storage tanks, different water flows take place (see Figs. 1 and 2). The following treatment trains are considered: a) treatment of rainwater through reverse osmosis (RO), followed by subsequent

Table 1

General scenario parameters adapted within the context of an individual household in Flanders. i.e. = inhabitant equivalent. *Not considering losses through leakage and consumption of bottled water.

Model constituent	Value	Reference
Roof surface	106 m ²	[20]
Inhabitants	2.3 i.e.	Federaal [21]
Average water use*	3.3 m ³ i.e. ⁻¹ month ⁻¹	Vlaamse [22]
Rainfall 2012–2017	See reference	[23]; Waterinfo.be, n.d.
Rainfall harvest correction factor	0.81	Vlaamse [24]
Volume rainwater tank	10 m ³	–
Volume potable water tank	1 m ³	–
Volume purified greywater tank	1 m ³	–
Volume blackwater tank	10 m ³	–
MBR recovery	90%	[25]
RO recovery	80%	[26]

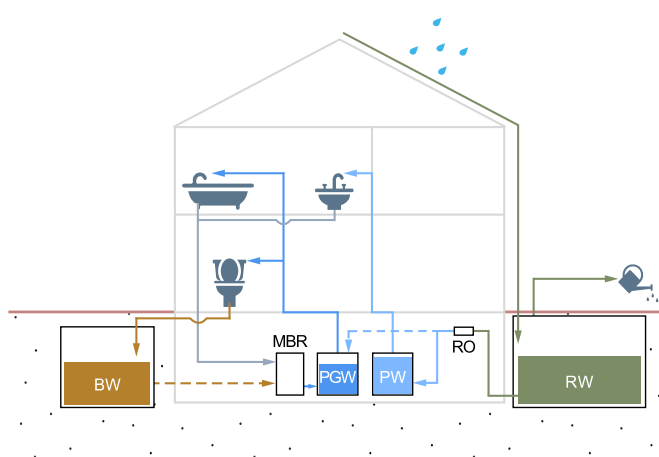


Fig. 1. Simplified representation of the assumed system configuration. Not all household water applications are shown. The dotted lines indicate configuration-dependent flows.

ultraviolet light (UV) disinfection and remineralization, b) greywater treatment with an ultrafiltration membrane bioreactor (MBR) followed by UV disinfection (Case A), and c) combined greywater and blackwater treatment (Case B) through a more extensive MBR-RO treatment step followed by UV disinfection and remineralization. Treatment technologies were chosen because of the small footprint and the long establishment. The previous applications of these technologies for similar purposes in the past are also taken into account. All forms of water consumption are assumed to take place uniformly over the year, excluding water used for plants and gardens, as this use would not be evenly distributed throughout the year in a temperate climate. Instead, a normal distribution is chosen balanced around the warmest month, July ($X \sim N(7, 1)$, July being the 7th month), which the authors consider to be more characteristic than uniformity.

Every scenario was conducted in a continuous manner, with every flow considered to happen evenly distributed across the month (a month defined as 1/12th of a year). This way, daily fluctuations could be neglected. Scenarios were simulated over five years.

Potable and purified greywater tanks always remain filled to guarantee water availability in the household. The rainwater tank offsets any decline of water level in these tanks. Therefore, the only tank possibly running dry over time is the rainwater tank. An empty rainwater tank, which has depleted below a certain water level, is immediately refilled (see further).

Average monthly precipitation data is used from the period 2012–2017, containing the relatively wet year 2012 (983.1 mm) and the relatively dry year 2015 (700.85 mm), when compared to the average Flemish yearly rainfall of 858 mm [23]; Waterinfo.be, n.d.). Rainwater is harvested on the entire roof surface with a projected horizontal surface A_{roof} . Several correction factors are included in calculating the total amount of harvested rainwater from the roof ($Q_{\text{RW,Harvested}}$) based on the assumed prefiltering step (downpipe or self-cleaning filter, a correction factor of 0.9) and assuming a symmetrical sloping roof (also a correction factor of 0.9) (eq. (2.1)) (Vlaamse Milieumaatschappij, 2000). Considering that the roof is used in its entirety and oriented symmetrically in opposite wind directions, any further effects of the slope and orientation of the roof are neglected.

All wastewater production in the household, except for toilet wastewater, is defined as greywater. No losses of water occur when a household application is used. This means the amount of inflow equals the outflow of an application. Cleaning and gardening both form an exception to this rule, as they entail no return stream to the system. Greywater was collected in an unaerated buffer tank, followed by treatment in an MBR to purified greywater. It is subsequently stored in a 1 m³ purified greywater tank.

Treated rainwater is assumed to be safe for potable reuse and stored in the potable water (PW) tank. PW is considered to be recirculated over a UV disinfection unit to avoid regrowth of bacterial contamination. The water recovery in this treatment step is 80%, which is relatively high but justifiable [26].

A potentially large obstacle to implementing small-scale closed-loop water systems is the accumulation of contaminants within the circular system. In the assumed configuration, the PGW tank is specifically vulnerable to such accumulation (as illustrated in Fig. 2). Here, pollutants are able to accumulate through the incomplete removal of pollutants by the treatment step. Therefore, in parallel with simulating the water flows within the system configuration, the accumulation of contaminants within the PGW tank was simulated. In order to assess concentration accumulation holistically the concept of a limiting contaminant was introduced. Here, a limiting contaminant is defined as a contaminant, which is particularly challenging to remove from water streams and thus susceptible to accumulation in circular water systems. Sufficient data on the presence of the contaminant ought to be available. Simulation of limiting contaminant accumulation in system compartments thus leads to knowledge on the vulnerability of certain compartments for contaminant accumulation. This knowledge does not inform us about the overall quality of treated water. In this paper, chloride is chosen as a limiting contaminant as the associated removal efficiencies for membrane treatment are

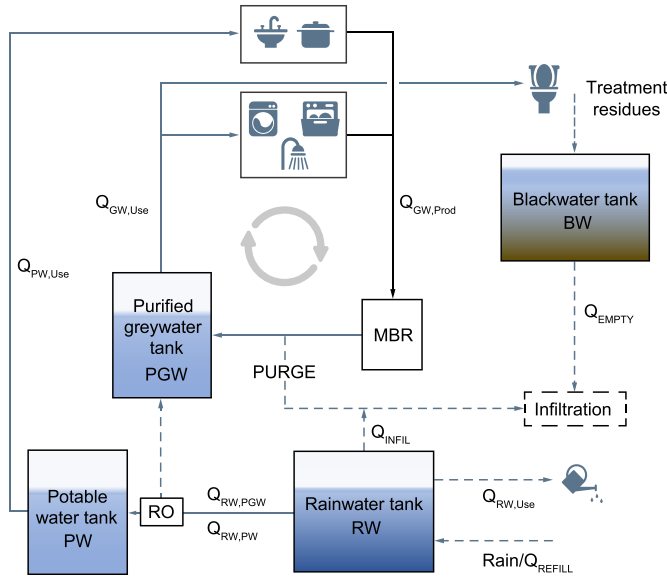


Fig. 2. Schematic representation of system configuration and flows (Case A). The grey circling arrows illustrate the circularity within the decentralized system (where the system is most vulnerable to contaminant accumulation).

relatively low, and chloride present relatively high in the wastewater flows. Chloride concentrations are attributed to the different wastewater flows per application [27,28] and rainwater [29,30]. Chloride removal efficiencies are set at 0% for MBR treatment and 95% for RO treatment, conservative assumptions based on expert knowledge. Furthermore, a 5% removal efficiency is assumed for the septic pit as chloride marginally accumulates in the sludge [27]. A purge of contaminated water is implemented in the system by introducing an outgoing flow from the PGW tank and replacing it with potable water (Case A) or extensively treated blackwater (Case B). As such, salts are removed from the PGW tank, preventing excessive accumulation. The outgoing water flow is infiltrated as the water in the purified greywater tank should be of sufficient quality for non-potable reuse and thus infiltration. As locally harvested rainwater is expected to be the only influx in the system, no more than a natural deposition of water would need infiltration. No effects of system maintenance are considered in this work, for more context on this matter, see Ref. [2]. The cost savings associated with piped networks, for both potable water and wastewater, are highly case-specific and will not be discussed in detail here.

2.2. Model structure

2.2.1. Mass-balance equations

$$Q_{RW,Harvested} \left(\frac{m^3}{month} \right) = \dots Rainfall \left(\frac{l}{m^2 \cdot month} \right) 0.9 \cdot 0.9 \cdot A_{roof} (m^2) \cdot 0.001 \left(\frac{m^3}{l} \right) \quad (2.1)$$

Table 2

Water flows defined according to the application (VMM, 2018). Q indicates the presence of a water flow. These flows apply both as an input to or as an output (waste flow) of the application.

Application	Variable	Flow (m ³ month ⁻¹)
Bath & Shower	Q _{BTSH}	2.02
Bathroom sink	Q _{BS}	0.66
Washing machine & Handwash clothes	Q _{WM}	1.16
Dishwasher	Q _{DW}	0.16
Kitchen sink	Q _{KS}	1.20
Toilet	Q _{TL}	1.49
Cleaning	Q _{CL}	0.18

$$Q_{PW,Use} = Q_{BS} + Q_{KS} \quad (2.2)$$

$$Q_{RW,Use} = Q_{RW, Garden} \quad (2.3)$$

All water flows are defined in m³ month⁻¹. A schematic representation of all water flows is given in Fig. 2. Table 2 shows the flows entering in and originating from (as no losses are assumed to occur) household applications.

Potable water use (Q_{PW,Use}) is limited to the kitchen and bathroom sink (eq. 2.2). Direct rainwater use (Q_{RW,Use}), only for garden applications (Q_{RW,Garden}), was defined by equation 2.3.

The total greywater production (Q_{GW,Prod}) by household applications is given by equation (2.4). The amount of greywater reused in household applications (Q_{GW,Use}) is defined by equation (2.5).

$$Q_{GW,Prod} = Q_{BT} + Q_{SH} + Q_{BS} + Q_{WM} + Q_{DW} + Q_{KS} \quad (2.4)$$

$$Q_{GW,Use} = Q_{BT} + Q_{SH} + Q_{WM} + Q_{DW} + Q_{TL} + Q_{CL} \quad (2.5)$$

When the RW tank runs below a minimal available volume (RW_{fail}), a refill occurs (Q_{REFILL}). RW_{fail} was set at 0.5 m³. Alternatively, when the rainwater tank overflows, this water is sent towards the PGW tank through the same treatment steps as Q_{RW,PGW} to add cleaner water for reuse. As stated earlier, the PGW tank is purged regularly to avoid the accumulation of contaminants.

Furthermore, the BW tank continuously leads blackwater towards infiltration (Case A and B) or additionally sends blackwater towards treatment for reuse in the PGW tank (Case B).

The water mass balance for the 4 tanks (the potable water (PW) tank, the rainwater (RW) tank, the purified greywater (PGW) tank, and the blackwater (BW) tank) can thus be described as follows:

$$\frac{dPW}{dt} = RO_{rec} \cdot Q_{RW,PW} - Q_{PW,Use} \quad (2.6)$$

$$\begin{aligned} \frac{dRW}{dt} = & Q_{RW,Harvested} - Q_{RW,Use} - Q_{RW,PW} - Q_{RW,PGW} \\ & + \dots Q_{REFILL} - Q_{INFIL} \end{aligned} \quad (2.7)$$

Case A and Case B differ in the applied calculation of the volume of water in the purified greywater tank and the blackwater tank (equations (2.8) and (2.9)). Here, emptying of the blackwater tank is expressed by Q_{EMPTY} . The recovery of the treatment unit is defined by equation (2.10), with the feed and the permeate, to and from the treatment unit represented by Q_{Feed} and $Q_{Permeate}$, respectively.

$$\frac{dPGW}{dt} = RO_{rec}Q_{RW,PGW} + MBR_{rec}Q_{GW,Prod} - Q_{GW,Use} - Purge \text{ (Case A)} \quad (2.8)$$

$$\frac{dPGW}{dt} = RO_{rec}(Q_{GW,Prod} + Q_{BW,PGW} + Q_{RW,PGW}) - Q_{GW,Use} - Purge \text{ (Case B)}$$

$$\frac{dBW}{dt} = Q_{TL} + (1 - RO_{rec}) \cdot (Q_{RW,PW} + Q_{INFIL}) - Q_{EMPTY} + \dots(1 - RO_{rec})Q_{RW,PGW} + (1 - MBR_{rec})Q_{GW,Prod} \text{ (Case A)} \quad (2.9)$$

$$\frac{dBW}{dt} = Q_{TL} + (1 - RO_{rec})(Q_{RW,PW} + Q_{INFIL}) - Q_{BW,PGW} + \dots(1 - RO_{rec})(Q_{GW,Prod} + Q_{BW,PGW}) \text{ (Case B)}$$

$$\text{Recovery} = \frac{Q_{Permeate}}{Q_{Feed}} \quad (2.10)$$

2.2.2. Control strategies

To optimally use the available rainwater, both the purified grey water tank and the potable water tank are kept full as much as possible. This is accomplished through on/off controllers with deadband (implemented using MATLAB/Simulink Relay functions). When the volume of the respective tank drops below a minimum threshold (PW_{min} and PGW_{min} – defined as 95% of the resp. total volume), the controller is switched on, and the tank is refilled with treated rainwater at a flow rate of $36.5 \text{ m}^3 \text{ month}^{-1}$ (equal to 50 L h^{-1}). Once the volume in the resp. tank reaches its maximum value, the controller is switched off again. In Case B, the purified greywater tank is refilled with treated blackwater instead of treated rainwater.

The purge quantity exiting PGW, with a flow rate equal to the other control flows, depends on the amount of purge necessary to avoid excessive accumulation of chloride. Here, as the purified greywater is reused in applications not requiring potable water quality, the point of excessive chloride accumulation is set at 350 mg L^{-1} [31]. Once this threshold is reached, the on/off controller regulating the purge is switched on. The control action switches off at 95% of the limit of excessive accumulation.

2.3. Reference configurations

Four reference water reuse configurations on a household level were constructed based on existing systems. This allows for a comparison between the scenarios in which extreme decentralization is pursued and reuse scenarios already implemented in practice. The reference configurations are 1) rainwater used for toilet flushing and in the washing machine and gardening applications, 2) rainwater used for the same applications as (1) but with a larger household size (4 instead of 2.3), 3) a greywater treatment system (GTS) with characteristics similar to the commercial Hydraloop® installed, which allows for collection and treatment of greywater from the washing machine, shower, and bath and reuse

as a feed for toilet and washing machine use, and 4) a GTS and a rainwater treatment system (RTS) with characteristics similar to the commercial Drop2Drink® installed, the latter allowing potable water production from rainwater (here used as the feed for the kitchen sink). All configurations entail connection to the potable water grid and sewer system.

2.4. Key performance indicators

In order to characterize the performance of the different reuse configurations, key performance indicators (KPIs) were defined. This allowed for a quantitative comparison between the performance of the decentralized treatment systems. The KPIs aim to create a more straightforward view into the predicted performance of the system than an analysis of the model output time series would provide, while the data is still available. The following four KPIs were constructed:

- 1) The independence factor (IF) is defined as a measure of the autonomy of the system in terms of water input and output. This KPI consists of an import component, which is divided into local import (harvested in close vicinity to the water system, e.g., rainwater harvesting) and external import (e.g., connection to the potable water grid or refill of storage tanks by truck), and an export component, which in its turn is divided between local export (e.g., infiltration of rainwater and/or treated blackwater) and external export (e.g., connected to a sewer system or emptying the blackwater tank by vacuum truck). Both independence of input and output are weighted equally.

$$\text{IF} = 0,5 * \frac{\text{Local water import} \left(\frac{\text{m}^3}{\text{month}} \right)}{\text{Total water import} \left(\frac{\text{m}^3}{\text{month}} \right)} + 0,5 * \frac{\text{Local water export} \left(\frac{\text{m}^3}{\text{month}} \right)}{\text{Total water export} \left(\frac{\text{m}^3}{\text{month}} \right)} \quad (2.11)$$

- 2) Circularity factor (CF). This KPI shows the fraction of wastewater, produced in the system, reused in household applications. It can also be seen as a measure for the vulnerability of the decentralized system for contaminant accumulation, although treatment efficiencies would also need to be considered here.

$$CF = \frac{\text{Purified wastewater reused} \left(\frac{\text{m}^3}{\text{month}} \right)}{\text{Wastewater produced} \left(\frac{\text{m}^3}{\text{month}} \right)} \quad (2.12)$$

- 3) Recharge Factor (RCF) measures the amount of water remaining in the near environment. It is defined as the fraction of water imported into the system from the local environment (e.g., through rainwater harvesting) and the water flow returning to the local environment (e.g., through infiltration or garden use).

$$RCF = \frac{\text{Local export} \left(\frac{\text{m}^3}{\text{month}} \right)}{\text{Local import} \left(\frac{\text{m}^3}{\text{month}} \right)} \quad (2.13)$$

- 4) Drought Tolerance Factor (DTF) indicates how effective the system is in overcoming a heavy drought (no rainwater input) with peak monthly rainwater use. The reference period for the drought is a 10-year drought in Flanders counting 29 days [32], and peak monthly rainwater use is defined as the highest monthly outflow out of the rainwater tank (including direct rainwater use and rainwater conversion for other water applications) over the five year simulation period.

$$DTF = \frac{\left(\frac{\text{Volume rainwater tank} (\text{m}^3)}{\text{Peak monthly rainwater use} \left(\frac{\text{m}^3}{\text{month}} \right)} \right)}{10 \text{ years drought duration (month)}} \quad (2.14)$$

2.5. Global sensitivity analysis

In order to assess the relative influence of individual system properties on the KPIs for Case A (configuration without blackwater reuse), a global sensitivity analysis was performed. Here, the effects of variations in the model parameters on the output values are evaluated. The parameters are quantitatively ranked according to their relative influence on the output through a set of sensitivity indices (or "importance measures") [33,34]. Performing a global sensitivity analysis (GSA) was preferred as it enables varying parameters across the entire parameter space, contrary to a local sensitivity analysis (LSA) where the input parameters are only varied around a reference or nominal value. More specifically, a variance-based sensitivity analysis, the Sobol method with Sobol quasi-random sampling, was applied to obtain both first-order and total effect sensitivity indices [35,36]. The MATLAB code for this analysis was adapted from Ref. [37]. The first-order sensitivity index is defined as the relative influence of each parameter on the model output, while the total effect sensitivity index also includes

Table 3
Chosen parameters and range for the sensitivity analysis.

Input parameter (unit)	Range
Roof surface (m ²)	79.5–132.5
Inhabitants (i.e.)	1.725–2.875
Volume rainwater tank (m ³)	7.5–12.5
MBR recovery (%)	60–95
RO recovery (%)	60–95
MBR chloride removal (%)	0–20
RO chloride removal (%)	80–100

The sensitivity analysis was performed with the four KPIs (IF, CF, RCF, DTF) as target output values. More than 20,000 samples of the parameter values were taken within the specified range per sampling round.

interactions between parameters [38]. The chosen parameters and their ranges are given in Table 3. Ranges for treatment removal efficiencies are based on literature [39] and expert experience, other ranges are chosen within a 25% range from the considered average values given previously.

3. Results

3.1. Water mass-balance for both decentralized configurations

Both configurations for extreme decentralization (with and without reuse of blackwater) were simulated, and the resulting time series outputs are shown in Fig. 3 for available rainwater (RW) in the rainwater tank and accumulated chloride in the purified greywater (PGW) tank. Both simulated configurations show relatively high potential for independence from the grid (as quantified further on). Case A, which represents the configuration without blackwater reuse and with a high level of greywater reuse through membrane bioreactor treatment, shows large fluctuations in rainwater availability in the rainwater tank. This is a result of the relatively large volume of rainwater necessary to replenish the PGW tank to avoid excessive accumulation of chloride, the limiting contaminant. Input water into the rainwater tank, and thus the system, consists of 94.8% of harvested rainwater (352.7 m³) and 5.2% of imported water during two RW tank refills (19.1 m³) over the five-year period. This need for imported water can already be compensated by a slightly larger roof surface of 125 m², instead of the assumed 106 m², or by an additional 7 m³ rainwater tank volume. By then, the storage volumes become very substantial.

The largest rainwater use is for replenishment of the PGW tank (59%, 220.1 m³), including excess rainwater automatically being sent towards the PGW tank, followed by refill of the potable (PW) water tank (37%, 139 m³) and rainwater for garden use (4%, 13.5 m³). Case B shows fewer fluctuations in available rainwater due to blackwater being reused in the PGW tank instead of rainwater. No refills of the RW tank were necessary. A large fraction of the effluent of the rainwater tank is still sent towards the PGW tank as excess rainwater, which would otherwise be infiltrated (57%, 200.2 m³). Furthermore, 39% of rainwater is used for potable water production, and 4% is used for garden applications. Case B shows little issues with limiting contaminant accumulation as the combined greywater and blackwater treatment is more extensive (chloride removal efficiency of 95%). Due to the extensive reuse of available water flows entailing relatively little outtake of rainwater from the rainwater tank, the RW tank must, theoretically, only be 2 m³ (instead of 10 m³) in volume to avoid necessary refills over the simulation period.

During the five-year period, a total volume of 338.5 m³ of water was infiltrated in Case A and 328.7 m³ in Case B. This water consists of treated greywater and blackwater streams not being reused. The difference in infiltration volume between both cases lies in the refills of the rainwater tank and the initial filling of the blackwater tank for Case A.

3.2. Accumulation of limiting contaminants

In both decentralized configurations, a relatively large purge volume was necessary. Defined as a flow of cleaner water replacing water with accumulated non-degradable contaminants, this purge was successfully avoided the excessive accumulation of chloride (defined as the limiting contaminant). The purge consists of a true purge, applied if excessive contaminant accumulation is measured, and a preventive purge with excessive treated rainwater that would otherwise be infiltrated. Over the five-year simulation period, 62 m³ of true purge and 94.1 m³ of otherwise infiltrated rainwater

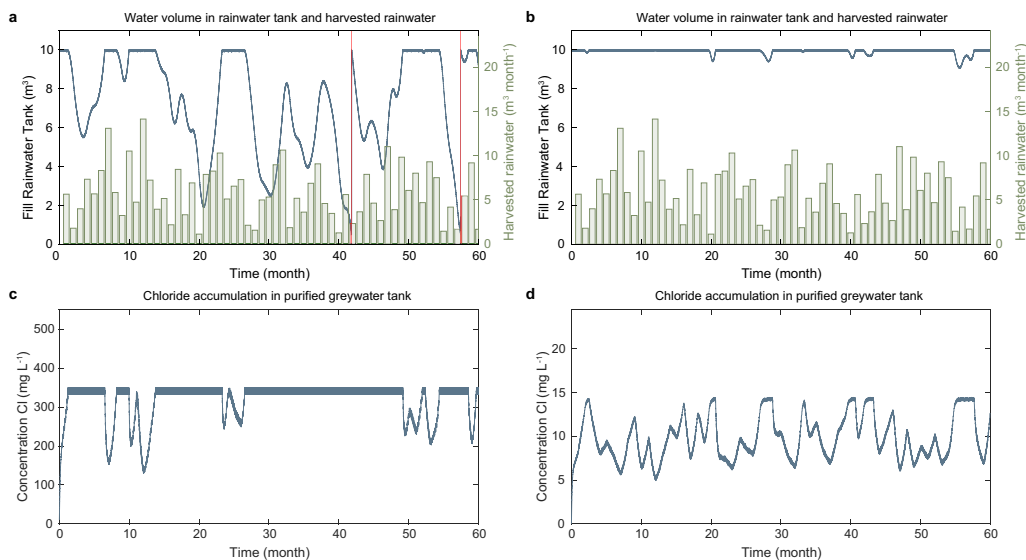


Fig. 3. Simulation results over the five-year period with (a) + (c) no reuse of blackwater, (b) + (d) with reuse of blackwater. The red vertical line indicates a refill of the rainwater tank.

entered the PGW tank for Case A. In this scenario, chloride concentration levels did not exceed 350 mg L^{-1} . For Case B, no true purge was necessary as accumulation levels remained low (16.7 mg L^{-1}), and 160.2 m^3 of treated rainwater was added to the purified greywater tank. The absence of excessive contaminant accumulation in Case B is a combined effect of the higher treatment efficiency of RO vs. MBR and the reuse of blackwater which leaves more rainwater available for a preventive purge of the PGW tank.

3.3. Performance assessment of decentralized configurations and comparison to reference configurations

Key performance indicators (KPIs) were developed to assess system performance for both decentralized configurations as the time series output does not allow for a clear-cut performance assessment. Furthermore, comparison between system scenarios is facilitated. Fig. 4 shows the resulting key performance indicators for both systems applying extreme decentralization and comparing reference configurations already available in practice. It can be seen that both systems with extreme decentralization entail slight differences in their performance assessment output. Case B is more independent from the grid (IF; Case A: 97.4, Case B: 100) and more circular (CF; A: 69.9, B: 74.9) due to the added blackwater reuse, which avoids the need for a refill of the rainwater tank. Net infiltration is also higher for Case A, thus it has a slightly higher recharge factor (RCF; A: 99.8, B: 97). Both configurations are capable of surviving a 29 days' drought period with no rain input and peak rainwater use (DTF; A: 100, B: 100).

The KPIs were constructed to allow for a quantitative comparison with reuse scenarios not encompassing complete disconnection from the grid. Independence factors for these scenarios are relatively low due to disposal of unused wastewater flows in the sewer system and a large quantity of imported potable water from the grid (IF; Reference 1: 20.3, R2: 19.7, R3: 2.1, R4: 2.7). System circularity increased in the configurations where greywater is reused in the greywater treatment system (GTS) (CF; R1: 0, R2: 0, R3: 42.8, R4: 42.8), and local recharge increased with decreased rainwater use (RCF; R1: 54.9, R2: 25.5, R3: 100, R4: 74.6). Finally, system drought tolerance decreased with increasing reliance on

rainwater from the rainwater tank (DTF; R1: 82.5, R2: 51.1, R3: 100, R4: 100).

3.4. Sensitivity analysis

A global sensitivity analysis was performed on both reuse configurations to assess the impact of different system parameters on the key performance indicators. First-order and total effect sensitivity indices for the chosen parameters in relation to the output key performance indicators were established. First-order sensitivity indices show the direct influence of variations in the input parameters on the output performance indicators. The total effect sensitivity indices serve as an indicator for the total contribution of each parameter on output variability, which includes interaction between parameters as a result of nonlinearity. The difference between total and first-order effect sensitivity indices is thus a measure of the indirect influence of parameters on the key performance indicators. First-order sensitivity indices can be expressed in percentage, with an index of 1 describing 100% of the variance attribution on output parameters. A threshold of two orders of magnitude (10^{-2} or 1%) was chosen to define a significant impact.

First, a sensitivity analysis was performed on Case A, the configuration for extreme decentralization without blackwater reuse (Fig. 5). The recovery of the greywater treatment (MBR) unit is shown to be the only parameter that significantly affects the circularity factor (CF), with 100% of the CF's variability explained by variations in this parameter. This throws light on the importance of the greywater treatment unit in avoiding the excessive accumulation of contaminants in the reuse system. The Independence Factor (IF) and the Recharge Factor (RCF) are both strongly influenced by multiple input parameters: The number of inhabitants (for IF: 14%, RCF: 19%), the size of the roof surface (IF: 16%, RCF: 14%), the pollutant removal efficiency of the greywater treatment unit (IF: 7%, RCF: 9%) and the recovery of the rainwater treatment unit (IF: 16%, RCF: 9%). In terms of system drought tolerance (DTF), performance variance was found to be due to changes in the rainwater tank volume (31%), the recovery of the greywater and rainwater treatment (RO) unit (both 14%), and the pollutant removal

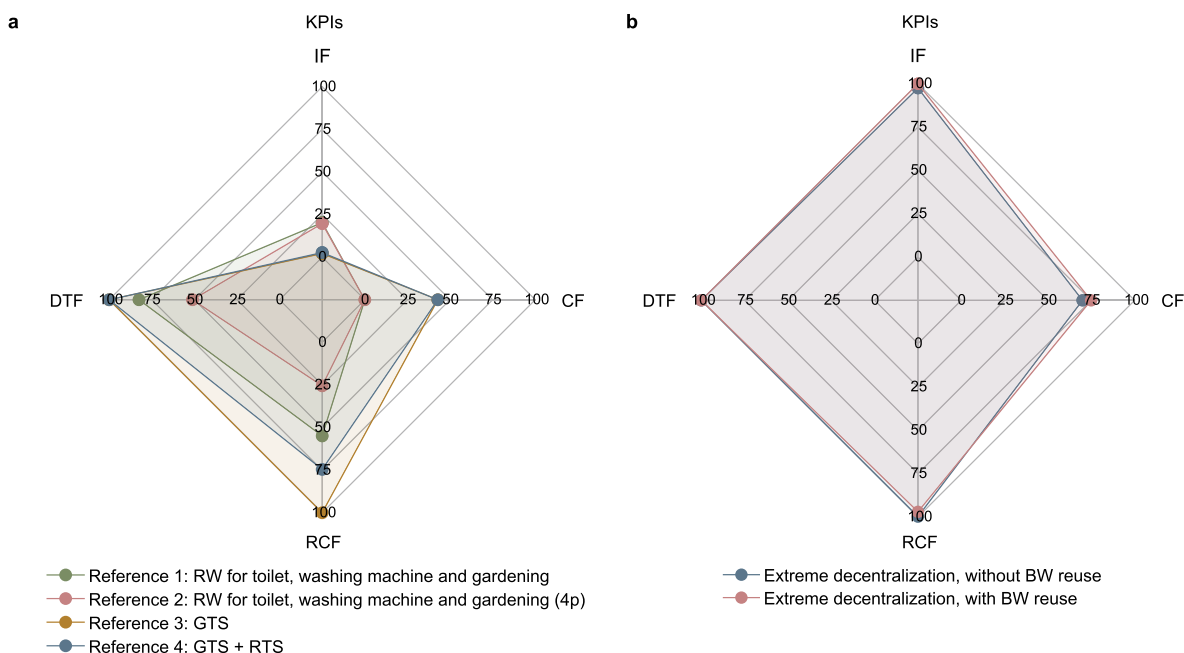


Fig. 4. Comparison of system performance indicators (a) between the reference configurations, (b) between both configurations for extreme decentralization. GTS = Greywater treatment system, RTS = Rainwater treatment system, IF = Independence Factor, CF = Circularity Factor, RCF = Recharge Factor, DTF = Drought Tolerance Factor.

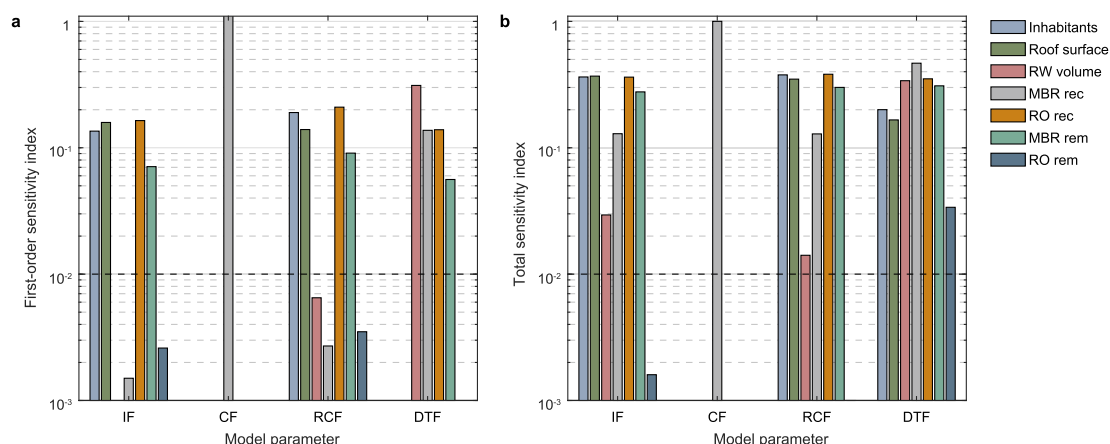


Fig. 5. (a) First-order and (b) total effect sensitivity indices resulting from the global sensitivity analysis for Case A for the chosen model parameters in relation to the output key performance indicators. **Output:** IF = Independence Factor, CF = Circularity Factor, RCF = Recharge Factor, DTF = Drought Tolerance Factor. **Input:** RW = Rainwater tank, MBR = Membrane bioreactor, RO = Reverse osmosis unit, rec = recovery, rem = removal (of chloride). The dotted line indicates the threshold of two orders of magnitude.

efficiency of the MBR (6%). Chloride removal efficiencies by the rainwater treatment unit show no significant direct impact on any output parameter variations within the selected efficiency range. All the foregoing notions of relative influence exclude measures of indirect parameter influences due to interaction. The latter are included within the total sensitivity indices. For the circularity outcome of this scenario, no interactions between parameters play a significant role. However, 62%, 55%, and 62% of the variance of the Independence Factor, Recharge Factor, and Drought Tolerance Factor, respectively, is due to interactions between parameters. It can be seen that the volume of the rainwater tank and the MBR recovery have a significant indirect effect on the Independence Factor and the Recharge Factor, whereas the Drought Tolerance Factor is indirectly influenced by the roof surface, the number of inhabitants, and the RO removal capacity. In general, it can be concluded that the MBR recovery has the largest overall influence on the key

performance indicators. The influence of other technology-related parameters such as RO recovery and MBR removal capacity is in the same order of magnitude as non-technological parameters such as the number of inhabitants and the roof surface. This indicates that the an important gain in the key performance indicators is still possible through improvements in the efficiency of the chosen technologies.

For Case B, the system configuration with blackwater reuse, some differences in the resulting sensitivity analysis can be noted (Fig. 6). First, the sensitivity analysis for the Independence Factor (IF) is not shown as no functional results were generated here. This is due to IF remaining 100% throughout all scenarios with varying input values, as the extensive reuse of waste streams at no time leads to any necessary import of potable water. As such, the variation of IF through variations of input parameters could not be assessed. Second, as the configuration does not apply the

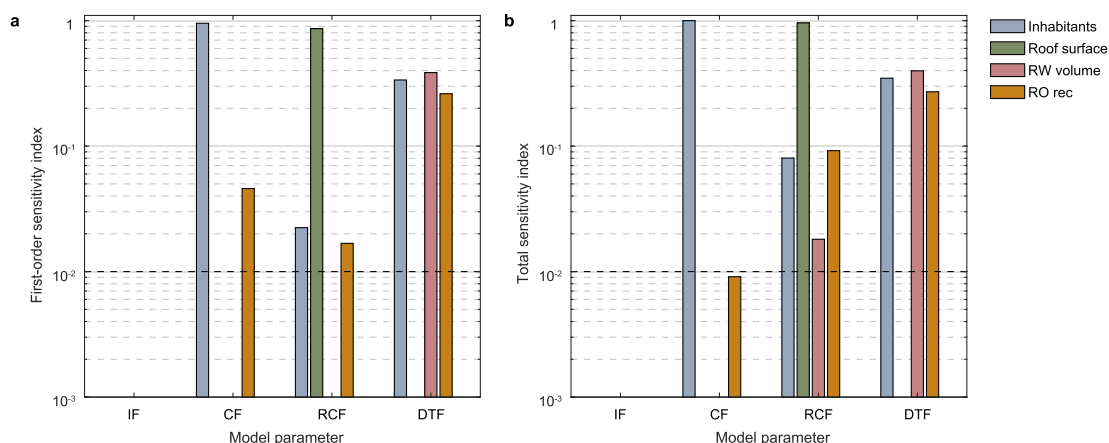


Fig. 6. (a) First-order and (b) total effect sensitivity indices resulting from the global sensitivity analysis for Case B for the chosen model parameters in relation to the output key performance indicators. **Output:** IF = Independence Factor, CF = Circularity Factor, RCF = Recharge Factor, DTF = Drought Tolerance Factor. **Input:** RW = Rainwater tank, RO = Reverse osmosis unit, rec = recovery, rem = removal (of chloride). The dotted line indicates the threshold of two orders of magnitude.

previously described MBR treatment steps, the associated input parameters (MBR recovery and MBR limiting pollutant removal) are not included in the sensitivity analysis.

In Case B, excluding interactions between parameters, the variance in system drought tolerance (DTF) can be attributed to the number of inhabitants (34%), the volume of the rainwater tank (39%), and the recovery of the treatment units (26%). The Circularity Factor (CF) and, to a certain extent, the Recharge Factor (RCF) are both significantly influenced by the number of inhabitants (CF: 95%, RCF: 2%) and the water recovery of the treatment units (CF: 5%, RCF: 2%). The RCF is most strongly influenced (for 86%) by variations in the roof surface. For CF, RCF, and DTF, 5%, 11%, and 3% of the variance, respectively, are due to interactions between parameters. Chloride removal efficiencies by the (MBR-)RO units show no significant impact on any output parameter variations within the selected efficiency range. Hence, when comparing both scenarios, it can be concluded that for scenario B, the key performance indicators are much less dependent on the parameters related to the treatment technologies. The largest influence can be attributed to non-technical parameters such as the number of inhabitants and the roof surface. Hence, only very limited performance improvement can be obtained through technological modifications within the scope of the key performance indicators defined here.

4. Discussion

The primary objectives of the performed simulations in this study were to assess the potential for extreme decentralization of water management on a household scale in terms of water management and construct a number of indices that can quantify the system performance from different viewpoints. Complete independence from the grid was considered for two reuse configurations. Here, the fundamental water system constructed was based on rainwater as system input and infiltration of untreated rainwater, treated greywater, and treated blackwater as system outputs. The constructed model proved to be easily tailored to varying system circumstances, all ranging within the context of a household system with these fundamental water type attributions. Therefore, this model could be used to assess decentralized system functioning in other environmental and social circumstances and with other technological features. Furthermore, coupling this model to environmental impact indicators and economical assessment methods could allow for a thorough comparison between the centralized water management paradigm and the case of

extreme decentralization [40,6]. To the best of the authors' knowledge, the only instance of an application of extreme decentralization in a residential context is a pilot installation designed and demonstrated by the team of James D. Englehardt, referred to as a net-zero water (NZW) concept. Here, wastewater from a 4-person dorm room is reused alongside 10–20% rainwater make-up. The researchers apply a treatment train consisting of active carbon filtration, MBR, iron-mediated aeration, another ultrafiltration step, and advanced oxidation [41].

Comparison between decentralized systems and subsequent decision-making and communication to stakeholders is facilitated by using key performance indicators (KPIs), of which four were defined in this paper. It must be noted that the aim is to allow for a comparison between decentralized systems entailing different levels of disconnection from the grid, for example, including both the case of complete disconnection from the grid and a system implementing rainwater reuse for toilet flushing. In this way, the KPIs are not optimized to solely compare cases of extreme decentralization, as can be illustrated by the assessment of drought tolerance, for which the studied configurations entailing extreme decentralization all obtain a maximal score. The KPIs should also not be used to calculate a surface in the radar charts, as the KPIs have no numerical relationship weighing their importance at present. Very likely, this weighing will be very locally driven, with drought tolerance being critical in areas with prolonged drought periods relative to infiltration being key in areas with limited water buffering in the area. Most of the KPIs are constructed to promote keeping water flows local (e.g., local infiltration of water outflows). Previous use of performance indicators to assess decentralized systems put more focus on the impacts of the system on the existing (centralized) infrastructure [14,42].

This work assessed the potential issue of accumulating contaminants within small-scale circular systems due to incomplete contaminant removal throughout the treatment units. Chloride was chosen as the limiting pollutant as it is a) present in wastewater in relatively high concentrations, and b) the system showed to be highly susceptible to chloride and (more general) salt accumulation issues. Nutrient and other contaminant balances, which were not considered as the assumed removal efficiencies, were sufficiently high to avoid accumulation within the system. This is in line with research by Ref. [18]; in which the problem was first recognized and in which treated wastewater discharge and rainwater make-up were recommended. This study found that implementing a purge (diversion of treated water towards infiltration) as a solution to

excessive contaminant accumulation plays a crucial role in the resulting water mass balance, as large quantities of freshwater are necessary for purge compensation, putting stress on the available water buffers. Smart control of the system with preventive purges of excess rainwater is an important feature for optimal use of available water resources and increased independence. The application of more efficient treatment steps within the decentralized system could further reduce or eliminate the issues arising through this accumulation of contaminants. In this paper, maintenance considerations were not addressed as maintenance could be expected to occur when necessary, offered by, for instance, the supplying company, with control and monitoring by relevant utilities or trusted entities, applying maintenance contracts (cfr. boilers and heat pumps). The effect of performance loss by the treatment units was assessed in the sensitivity analysis, showing that a variation in performance (a change in the recovery or removal efficiencies of treatment units) would have significantly impact system performance. Future simulations of contaminant behavior in decentralized systems could apply more detailed technological assumptions and control and monitoring strategies to obtain more insight into the potential hazards of contaminant accumulation in such small-scale, circular systems. In this sense, a basis can be formed for HACCP (Hazard Analysis and Critical Control Points)-type analyses to start developing adequate monitoring approaches.

As of yet, the tangible applicability of this work is limited to new developments and extensive building retrofitting. Also, this model was constructed on many case-specific assumptions, simplifying the uncertain socio-environmental context in which decentralized systems function. This would likely require modifications in order to apply for future research objectives. The case for extreme decentralization cannot be made in every context, but no one-fits-all water management solution is sought after in our research. For instance, the chosen water input in the system here, assumed to be rainwater harvested on the roof, was shown to have a large impact on system functioning with long dry periods leading to the necessity of external water refills. Rainwater was preferred as an external water source over local water sources such as rivers, lakes, and groundwater as it entails no direct extraction from the environment and has relatively predictable quality characteristics. Also, the potential of rainwater as a source was studied here since it has the additional challenge of variable supply. The large precipitation quantity and uniformity in time, being free of strong seasonal fluctuations, for the Flanders region of Belgium showed a relatively reliable rainwater source. Therefore, adoption of other climatic circumstances would have a high impact on the resulting system performance and the value attributed to the KPIs. In other locations globally, the case would look different, e.g., in arid regions, the input towards the system may need to be desalinated water, but principally the model framework and stepwise analysis that was developed here could be upheld for cases with diverse inputs and parameter sets. Furthermore, implementation of precipitation data on an hourly or daily basis instead of the current monthly time-frame would allow for a more in-depth look into the effects of first-flush diversion (in which the first, most contaminated fraction of a precipitation event is not collected in the rainwater tank), precipitation pattern changes due to climate change and including temporal variations in water use by consumers.

The performed simulations shed light on the significance of greywater management in optimizing the exploitation of available water quantities in the context of a household, in a similar manner to urine control as a critical factor in nutrient management. Also, a high level of internal water reuse within the studied system configurations showed to limit water storage needs. This could have positive implications on the feasibility of households adopting such systems as free space in and around homes might form an important

bottleneck. Ultimately, we need to consider aspects holistically – the more capabilities a house has for internal recycling (thus, the higher our four KPIs), the less water needs to be supplied to the house at high energy investment. The choice is then made based on energy for a water treatment system relative to energy embedded in the imported water. Here, a key to creating a full environmental picture of novel water management strategies is also to include energy inputs for the different treatment steps, besides materials investments.

5. Conclusion

A model was constructed for two decentralized water management configurations on a household scale to assess the potential for extreme on-site decentralization. Independence from the potable water grid and sewer system was assumed through rainwater harvesting and reuse of wastewater streams. Water mass balances were simulated and coupled to a model for contamination accumulation within the circular system. The magnitude of this contaminant accumulation led to a large purge of treated water streams towards infiltration being necessary, significantly impacting water management. To our knowledge, this study was the first to quantify and holistically address this obstacle to the implementation of small-scale circular water systems. Next, the raw model output is quantitatively assessed through the construction of Key Performance Indicators (KPIs), which allowed for a comprehensible comparison between water management scenarios and would facilitate communication to stakeholders. Finally, a sensitivity analysis was performed. This showed the importance of water recovery and contaminant removal efficiencies of the applied treatment technologies on system performance when contaminant accumulation in the system forms an issue. In systems not severely affected by pollutant accumulation, parameters such as inhabitant number and roof surface had the largest effect. Extreme decentralization based on rainwater as a water source was shown to be feasible considering typical rainfall patterns in Flanders and a minimum rainwater storage of 10 m³. Future research could expand on the case-specific assumptions such as climatic conditions and their implementation and include more detailed technological assumptions. As a whole, the work performed here provided a framework for the ex ante evaluation of decentralized household-scale water systems.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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