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# TOWARDS A ROBUST AND FLEXIBLE NUMERICAL FRAMEWORK FOR INTEGRATED URBAN WATER SYSTEM MODELING

Clara Chauvet<sup>1,2,3\*</sup>, Jean-Raynald de Dreuzy<sup>2</sup>, Zahra Thomas<sup>1</sup>, Gwenaëlle Carfantan<sup>3</sup>,  
Hervé Andrieu<sup>4</sup>

<sup>1</sup>*Agrocampus Ouest, Sol Agro et Hydrosystème Spatialisation, 35000 Rennes, France*

<sup>2</sup>*Geosciences Rennes, UMR CNRS 6118, University of Rennes 1, 35042 Rennes Cedex, France*

<sup>3</sup>*SETUR, 35176 Chartres de Bretagne, France*

<sup>4</sup>*LUNAM Univ, IRSTV FR CNRS 2488, Nantes, France*

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## Abstract

Urban water system modeling offers an integrated approach to propose adapted solutions to the multiple issues faced by evolving urban water systems including hydrological variability, climate change and socio-economic factors. We design a generic and flexible numerical framework based on the integration of elementary infrastructure tools in a graph-based network. Additionally to centralized units, we consider decentralized elementary infrastructure tools such as Low Impact Development (LID) systems, local treatment units and temporary storage of harvested precipitations and grey water reusable for undrinkable uses. Infrastructure tools are represented by a hierarchy of classes in an object oriented language to integrate both common and more specifically designed systems. The integration of several instances of such objects in a connected network should eventually optimize urban and environmental planning, thanks to adaptation capacities through the infrastructure tools diversity. We propose an automatic derivation of equations from the elementary systems and their interconnection. We show how well-chosen system behaviors lead to robust and reliable differential algebraic equations, which can be integrated with advanced numerical schemes. As an illustration of our approach, we show how temporary storage may efficiently complement grey water and harvested precipitations through a connected and smart urban water network.

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\* Corresponding author. Tel.: +33-644-802-527;  
E-mail address: [clara.chauvet@univ-rennes1.fr](mailto:clara.chauvet@univ-rennes1.fr)

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## 1. INTRODUCTION

Integrated Urban Water System Models (IUWSMs) and Integrated Urban Water Cycle Models (IUWCMs) concepts are based on the integration in an interconnected network of one to several infrastructure tools considered as elementary components of the urban water network [1]. They contribute to determine the beneficial effect of diversifying decentralized water resources [2, 3], of urban planning with integration of different spatial scales [4], and of energy savings [5]. They address emerging issues in urban planning accounting for socio economic changes and environmental adaptation. IUWSMs and IUWCMs should additionally ensure spatial integration of the sustainable urban water cycle, as well as uncertainties on water uses and economics.

We set the basis of a new robust and flexible numerical framework designed to comply with those different constraints in a modular way. The framework further called “Blue Urban System” is designed to integrate a large range of infrastructure tools represented in a generic way through a numerical framework based on Object Oriented Programming. Each element of the network can generate a complete set of equations modeling its behavior in quantitative terms. Their combination in a network leads to a set of Differential Algebraic Equations (DAEs) that can be solved using state of art numerical methods.

Our Blue Urban System framework decomposes the complexity of integrated urban water models in three levels, which are namely (1) the description of the elementary infrastructure tools, (2) the description of their interconnection through classical graph theory and (3) the automatic derivation of a set of differential algebraic equations and their integration with adapted numerical methods. Our framework is aimed at separating the different sources of complexity (urban design, algorithmic implementation, numerical integration) and should contribute to propose adaptation strategies to environmental and societal changes through the use of a wide diversity of infrastructure tools.

## 2. METHODS

We first describe the combined centralized and decentralized urban water cycle on which we further illustrate our 3 step generic methodology to model the dynamical behavior of a network of diverse infrastructure tools.

### 2.1. ILLUSTRATIVE CENTRALIZED AND DECENTRALIZED WATER CYCLE

The centralized and decentralized urban water cycle is made up of interconnected infrastructure tools. It is modelled as a set of infrastructure tools also called nodes hereafter. The system should adapt to some extent to the water demand, the water reuse capacity and to climate stochasticity through the use of a temporary storage tank (ST) (Fig. 1).

Water demand is partitioned between Drinkable Water (DW) and Undrinkable Water (UW) depending on uses. The waste water coming out (C1) is separated in black water (toilets exclusively) and grey water (bathing, laundry and kitchen sink). While black water is driven towards the waste water Treatment Plant (TP) outside of the city, grey waters are treated locally through local Treatment Units (TU) and collected together with harvested rainwaters into a temporary storage tank, which preferentially supplies the undrinkable water demand. Undrinkable water is supplied by grey water and harvested precipitations as long as fluxes to the tank and water in the tank can meet the demand. When the tank is empty and the incoming flux cannot supply all the demand, an additional supply from centralized drinkable water network is required. In the tank, water “overflows” when the volume of water is higher than the storage capacity of the tank. The overflowing flux (spill) is discharged to a biodiversity area. The urban water cycle considered here includes connections with Low Impact Development (LID) infrastructure tools like vegetated roofs, infiltration and biodiversity zones such as defined by Fletcher et al. [6]. Water fluxes sent to the water treatment plant, LID and natural environment are quantified in order to improve water management strategies.

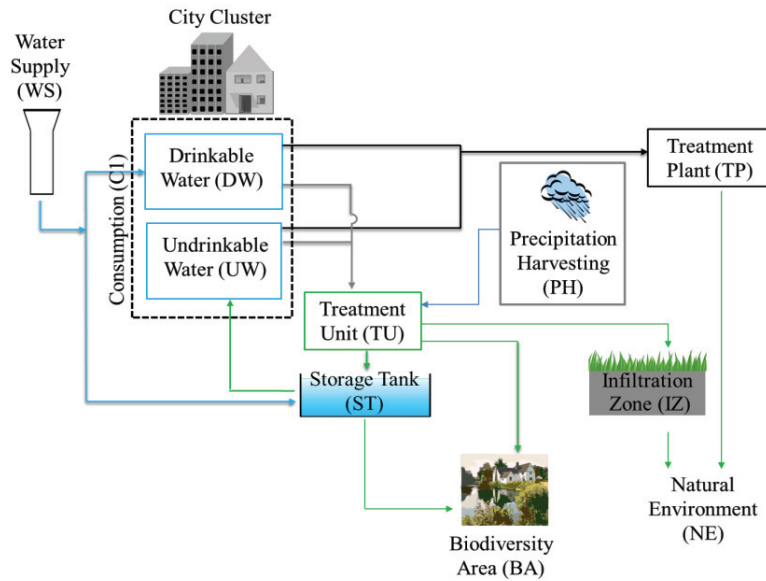


Fig. 1 The illustrative centralized and decentralized urban water network

## 2.2. ELEMENTARY INFRASTRUCTURE TOOLS

Elementary infrastructure tools are defined with common and specific properties following the hierarchy of objects found in Object Oriented Programming. Infrastructure tools have one to several input and output fluxes. They are described by a limited number of state variables which behavior can be fully modelled by a set of differential and algebraic equations. State variables and input/output fluxes can be related in some advanced ways as long as they can be expressed in functional terms. While elementary tools share common properties, they can be made highly specific to adapt to specific requirements within the urban water system. Specialization of otherwise common infrastructure tools is achieved through inheritance in the object oriented framework.

From the example of Fig. 1, we define five elementary infrastructure types (Table 1). Input and Output nodes are inlet or outlet of defined input and output fluxes. For example, the water supply system has a forced flux, generically noted  $f$ , which could also be adapted to match real water demand [4, 7]. As opposed to forced fluxes, the variable fluxes will be noted  $\phi$ . The example of Fig. 1 has four forcing fluxes, including the drinkable and undrinkable water demands, the global water consumption, and the precipitations.

Adapter and partitioner nodes have one input and two output fluxes. The adapter has one output forced flux adapting the relation between the other output and input fluxes. The partitioner has two output and one input computed fluxes. Fluxes are partitioned according to a ratio noted  $p$ . A local treatment unit is represented by a partitioner where the input grey water flux is divided into a treated grey water part driven to the temporary storage tank and the remaining untreated water directly disposed to the biodiversity area. The ratio  $p$  represents the treatment efficiency. The drinkable water distribution unit is represented by an adapter. It adapts the undrinkable needs to required drinkable water.

The fourth type of node is the collector. Collectors have two input and one output fluxes. For example the system that collects both harvested precipitations and treated grey water to drive them towards the temporary storage tank is a collector node.

Table 1 Infrastructure type symbols and input/output fluxes (left column) with the associated equations describing their behavior (right column)

General functioning	General equations
	$f_{In} \text{ OR } \varphi_{In}$ $f_{Out} \text{ OR } \varphi_{Out}$
	$\varphi_{In} = f_{Out} + \varphi_{Out2}$
	$\varphi_{Out1} = p \varphi_{In}$ $\varphi_{Out2} = (1 - p) \varphi_{In}$

General functioning	General equations
	$\varphi_{Out} = \varphi_{In1} + \varphi_{In2}$
	$\dot{V} = s (\varphi_O + \varphi_{IN} - f_{sup})$ $\varphi_S = (1 - s) (\varphi_O + \varphi_{IN} - f_{sup})$ $0 = \varphi_O - i f_{sup}$

The last type of node is the temporary storage tank. It is aimed at adapting the variability in the water availability (grey water, harvested precipitations) to fluctuations of water consumptions. It should ensure that the demand is met whatever the water level in the reservoir (empty, filled, intermediary). It should be periodically emptied to preserve water quality. The evolution of the water volume derives from the flux balance equation given in Table 1. It is complemented by two additional algebraic equations that modify the flux balance when the reservoir is full or empty. When the tank is full, the required undrinkable water  $f_{sup}$  comes directly from the available water  $\varphi_{IN}$ , the rest of it ( $\varphi_S$ ) being disposed without going into the tank. When the tank is empty, the demand ( $f_{sup}$ ) is met by adding an optional flux  $\varphi_O$ . To avoid too much discontinuity in the fluxes, the shift between the different regimes is controlled by two smooth functions  $s$  and  $i$ . The function  $s$  smoothly controls the spillage of the reservoir when it attains its maximal capacity ( $v_{max}$ ):

$$s_{v_C, v_{max}} = \delta(\varphi_{IN} + \varphi_O - f_{sup} > 0) g_{v_C, v_{max}}(v) + \delta(\varphi_{IN} + \varphi_O - f_{sup} \leq 0) \tag{1}$$

with  $\delta$  the classically defined Dirac functions. The function  $i$  controls the optional flux when the volume is emptying:

$$i_{0, v_{min}} = g_{0, v_{min}}(v). \tag{2}$$

$i$  is generally 0 and becomes positive when an optional water flux is needed, i.e. when the volume  $v$  becomes lower than the threshold  $v_{min}$ . The function  $s$  is generally 1 and becomes smaller than 1 when the volume becomes larger than a threshold  $v_C$  close to  $v_{max}$ . The function  $g$  is the polynomial of degree 3 of continuous values and derivative expressed as:

$$\begin{cases} v < v_1 & g(v) = 0 \\ v_1 < v < v_2 & g(v) = \frac{(v - v_1)}{(v_2 - v_1)} \left[ 1 + (v - v_2) \left( \frac{-2v + v_2 + v_1}{(v_2 - v_1)^2} \right) \right] \\ v > v_2 & g(v) = 1 \end{cases} \tag{3}$$

**2.3. GRAPH BASED NETWORK REPRESENTATION**

The network of elementary system is modelled by a graph with edges linking the different nodes. The graph representation is conceptually general and attractive because of the ample knowledge available on graph properties [8]. The centralized/decentralized example of section 2.1 can be represented in a corresponding graph by introducing adapted nodes for collecting and dividing water fluxes (Fig. 2). Using the convention previously defined, fixed and computed fluxes are generically denoted  $f$  and  $\varphi$ , respectively. We labelled the fluxes by their origin and target nodes as indices.

In Fig. 2, the drinkable water flux coming from the Water Supply station  $\varphi_{WS\_AD}$  is divided through the adapter node

AD into the drinkable water need  $f_{AD\_C1}$  and the additional flux  $\varphi_{AD\_ST}$  required when harvested precipitations and grey water are not sufficient to meet undrinkable needs. The waste water coming out of the C1 consumption node is divided through the divisor PA into a black water flux  $\varphi_{PA\_TP}$  driven to the water Treatment Plant node TP and a grey water flux  $\varphi_{PA\_TU}$  driven to the local treatment unit TU. Depending on the efficiency of the Treatment Unit, only part of the greywater flux might be recycled to the storage tank ST in two steps  $\varphi_{TU\_C2}$  and  $\varphi_{C2\_ST}$ . The collector C2 adds the harvested precipitations flux  $\varphi_{HP\_C2}$  from the node HP to the grey water flux  $\varphi_{TU\_C2}$ . Some of the harvested rainwater flux  $f_{P\_HP}$  may be directly returned to an infiltration zone IZ. The flux  $\varphi_{C2\_ST}$  is driven to the storage tank where it can directly feed the fixed undrinkable needs  $f_{ST\_C1}$  or be disposed to the biodiversity area BA ( $\varphi_{ST\_BA}$ ) when the tank is full. Modeling urban systems to graphs may require adding collector, adapter and partitioner nodes.

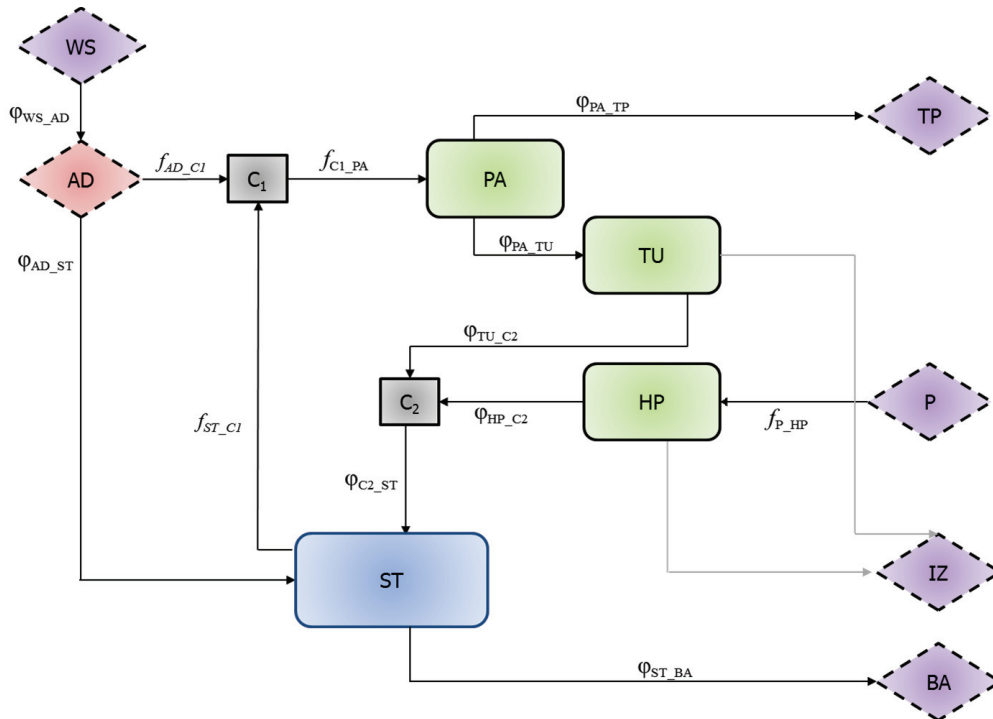


Fig. 2 Schematic network corresponding to the centralized and decentralized example of Fig. 1. The five types of nodes pictured with different colors and shapes are described in Table 1. Fluxes between nodes are labelled according to their input and output nodes with an underscore symbol in between.  $f$  and  $\varphi$  fluxes refer respectively to fixed fluxes (forcing terms) and computed fluxes. Fluxes in grey will not be taken into account in the simulations

### 2.4. MATHEMATICAL FORMULATION

The mathematical formulation is obtained by using the information contained in the infrastructure elements and in the graph described in the two previous sections. It is performed in two steps. The first step consists in labelling and numbering the fluxes so that all nodes get well identified input and output fluxes. We call  $n_f$  and  $n_\varphi$  respectively the number of fixed and computed fluxes. Fluxes labelling is fundamentally a network-scale task that does not require any knowledge of the internal structure of the nodes. It will thus be performed within the graph structure of the network.

Once fluxes labelled, the derivation of the equations is a node task. Each node has been designed as shown in section 2.2 to be independent of the other ones. The system of equations is filled by a simple loop over the nodes. For each node the corresponding equation or system of equations given by Table 1 is integrated in the system. Additional variables are added to the system like the volume  $v$  of the tank. We note  $n_v$  the number of such additional variables. As shown by Table 1, the system is made up of differential and algebraic equations. The differential part

comes from inertial variables like the volume of the storage tank while algebraic equations come from simpler flux balance equations without any node insertion. The full system of equation results in the following set of Differential Algebraic Equations (DAEs):

$$M\dot{Y} = g(t, Y) = - \begin{bmatrix} A_{V\phi}(Y) \\ A_{\phi\phi}(Y) \end{bmatrix} \phi - \begin{bmatrix} P_{VF}(Y) \\ P_{\phi F}(Y) \end{bmatrix} F(t) \quad \text{with} \quad M = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \quad (4)$$

This system of equations is of size  $(n_D + n_A)$  where  $n_D$  and  $n_A$  are respectively the number of differential and algebraic equations. The matrix  $M$  is of dimensions  $(n_D + n_A) \times (n_v + n_\phi)$ ,  $I$  is the identity matrix  $(n_D \times n_D)$ ,  $Y$  is equal to  $[V, \phi]^T$ . The matrices  $A_{V\phi}(n_D \times n_\phi)$ ,  $A_{\phi\phi}(n_A \times n_\phi)$ ,  $P_{VF}(n_D \times n_f)$  and  $P_{\phi F}(n_A \times n_f)$  are matrices expressing the connectivity of the system where. Their coefficient may depend on the system state  $Y$  as for the tank. The vectors of forcing and computed fluxes  $F = [f_1 \dots f_{n_f}]^T$  and  $\phi = [\phi_1 \dots \phi_{n_\phi}]^T$  are of sizes  $n_f$  and  $n_\phi$  as previously mentioned.

At this stage, it is checked that the number of equations  $(n_D+n_A)$  is equal to the number of variables  $(n_v+n_\phi)$  ensuring that the system is well determined. We choose to maintain the DAE system under this form (4) to solve it for the following reason. We have seen that the temporary storage tank adapt its behavior to the water availability and demand leading to different regimes. The regime is differential when the level in the volume is intermediary (neither empty nor full). The regime is algebraic when the volume is either empty or full. With the equations described in Table 1 and the smoothing functions (1) and (2), the behavior of the volume is fully described by a system of equations that does not degenerate (its rank remains constant whatever the regime). However some of its coefficients can become equal to zero depending on the regime preventing substitution to systematically work. The differential algebraic form is well adapted to those types of highly evolving systems with strong non-linearity and threshold effects. Under this formulation, the system can be integrated using adapted numerical schemes including the evolving order ODE solver of Matlab® ode15s [9].

The DAE expression is not only a formal and mathematical convenience but a reliable and robust way to follow the evolution of the urban water system in all regimes. Because the system of equation never degenerates, it remains fully integrable at any time without any modifications. The quality of the solution can be easily adapted using order and time step controls. The steepness of the solution especially around the transition between regimes can also be adapted through the smoothness of the partitioning functions  $s$  and  $i$  (1,2). Other studies in different contexts including reactive transport in porous media [10, 11] have shown that this approach remains well suited for high dimensional systems made up of a large number of differential and algebraic equations.

While robustness is ensured by the non-degenerated DAE formulation detailed above, flexibility comes from the adapted object oriented framework where elementary infrastructure tools, network, and system of equations are encapsulated in three different classes. Each of the classes can be independently enriched to add new node types, new graph structures and new time integration schemes. Such an organization is well adapted to benefit from advanced capacities in related scientific fields through software integration.

### 3. RESULTS

We simulate in this section the behavior of the combined centralized and decentralized system presented in section 2.1 with a parametrization derived from a recently built urban cluster in France (ZAC “les portes de la Seiche”, Chartres de Bretagne). Parameters have been normalized by the number of persons in the urban cluster to be expressed on a person basis. The daily average consumption per person  $f_{AD,C1}$  is set at 0.1 m<sup>3</sup>/d. Its variability is modelled by a simple sinusoidal function of period 1 day with a maximum in the day time and a minimum of zero in the night time. Consumption is divided into drinkable needs (25% of the total consumption) and undrinkable needs (75%). Once consumed, the used water is divided into black water and grey water. The proportion  $r$  of grey water in the total used water (grey and black) will be taken between 0.25 and 0.8. It is the main parameter of this study. We assume in this illustrative example that all the grey water can be treated and recycled, and that the treatment is sufficiently fast so that the grey water is directly available for the undrinkable needs.

Precipitations are set as 1000 mm/yr as typically measured in this region of France. Precipitations are simulated on a daily basis using a simple exponential distribution with a mean value modulated by the period of the year to model

the seasonal variability (Fig. 3). The surface where precipitations can be harvested is set at 10 m<sup>2</sup> per person. Both grey water and harvested precipitations are driven to the temporary storage tank, which has a capacity of 0.05 m<sup>3</sup> (50 l). When starting the simulation, all fluxes are initially equal to zero and the tank is empty. As detailed in other studies on overflowing storage ode15s solver of Matlab [9] with relative and absolute tolerances set to 10<sup>-9</sup> and 10<sup>-6</sup>. Simulations take a couple of seconds for a one year period of time.

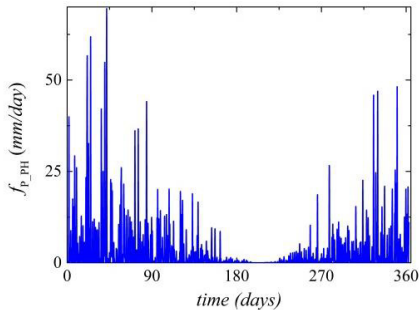


Fig. 3 Precipitations time series in mm/day/pers

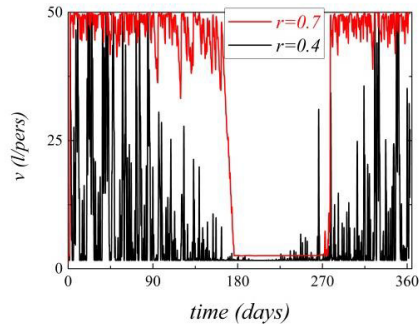


Fig. 4 Volume of the temporary storage in l/pers depending on the ratio of grey water in waste water

For two ratios  $r$  of grey water over the total used water of 0.4 and 0.7, the volume of water stored into the tank changes significantly over the year. For  $r = 0.7$ , the volume is full most of the year (Fig. 4, red curve). In this case, 70% out of 75% of the undrinkable water needs are constantly provided by the recycled grey water and the 5% remaining needs are easily met by the precipitations outside of the summer period (absence of precipitations). The water volume is almost always full with some high frequency variations close to the maximum of 50 l coming from the precipitation variability. For  $r = 0.4$ , only 40% out of the 75% of the undrinkable water needs are provided by the recycled grey water. The tank is hardly fully filled outside of high precipitation events. The water volume in the tank is highly variable with filling and emptying periods closely following the precipitation variations with some damping of their amplitude coming from the buffering capacity of the tank.

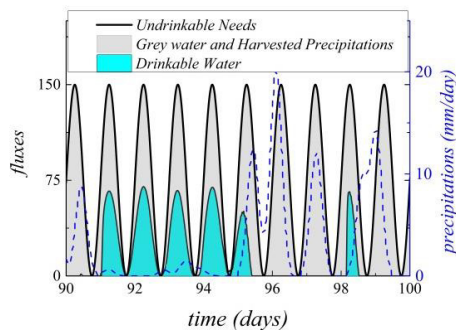


Fig. 5 Grey water and harvested precipitations (grey color), optional drinkable water (light blue) and precipitation chronicle (dashed blue curve) for a ratio of grey water in waste water  $r = 0.4$

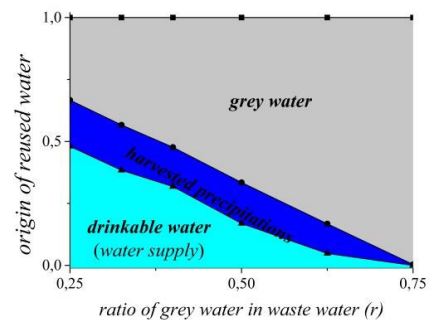


Fig. 6 Ratio of grey water, harvested precipitations and optional drinkable water for undrinkable needs

Looking more in details at the origin of the undrinkable needs in the 90-100 days period (Fig. 5), most of the demand is met by grey water recycling and harvested precipitations (grey area) at and after precipitation events (dashed blue curve). Drinkable water fluxes taken for undrinkable uses (light blue area) become necessary shortly after the precipitations have stopped. The water stored in the tank can complement the grey water availability to meet the undrinkable needs for around one day and a half when starting from a full reservoir for the ratio  $r$  of 0.4.

We determine the efficiency of the system by computing the origin of the undrinkable water needs over a 1-year

period as a function of to the ratio of grey water in the total used water ( $r$ ) (Fig. 6). The proportion of harvested precipitations is relatively constant as long as the ratio  $r$  remains smaller than 0.6, showing that the use of harvested precipitations is limited by the storage capacity rather than by the harvesting capacity. The 0.050 m<sup>3</sup> tank volume would be optimal only for relatively high ratios of grey water recycling around 0.6.

#### 4. CONCLUSION

This example illustrates the potential interest of exploring different urban water designs. Investigations could be readily extended to more advanced urban structures, infrastructure tools diversity and climate scenarios to explore the adaptation capacity of competing urban designs. Such simulation could also be coupled with optimization algorithms to systematically search the most adapted design and parameters for well-identified objectives. The flexibility and robustness of the simulations will be critical to ensure the convergence of the optimization algorithm and the selection of the most suited urban organization.

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