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# Water Cycle and Circular Economy: Developing a Circularity Assessment Framework for Complex Water Systems

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## ABSTRACT

Water – the most vital resource, negatively affected by the linear pattern of growth – still tries to find its positioning within the emerging concept of circular economy. Fragmented, sectorial circularity approaches hide the risk of underestimating both the preservation of and impacts to water resources and natural capital. In this study, a game changing circularity assessment framework is developed (i.e. MSWCA). The MSWCA follows a multi-sectoral systems approach, symbiotically managing key water-related socio-economic (i.e. urban water, agro-food, energy, industry and waste handling) and non-economic (i.e. natural environment) sectors. The MSWCA modelling framework enables the investigation of the feedback loops between the nature-managed and human-managed systems to assess water and water-related resources circularity. The three CE principles lie at the core of the developed framework, enabling the consideration of physical, technical, environmental and economic aspects. An indicators database is further developed, including all the relevant data requirements, as well as existing and newly developed indicators assessing multi-sectoral systems' circularity. The MSWCA framework is conceptually applied to a fictional city, facilitating its understanding and practical use.

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## 1. Introduction

Water in the environment follows a natural circular model that secures water resources by regulating water flow and ensuring water quality. However, in human-managed systems that follow a linear model of economic growth, water is successively qualitatively degraded after use, becoming unfit for further use both by humans and ecosystems (Stuchtey, 2015). To decouple economic growth and development from imprudent resource consumption, the alternative model of Circular Economy (CE) is been promoted aiming to achieve resource efficiency, to reduce waste production and to improve environmental, economic and social sustainability (European Commission, 2015). To stimulate CE uptake, water, phosphorous and metals have been identified by Hislop and Hill (2011) as key priority resources.

Beyond its necessary preservation, water is a carrier of energy and materials. The most obvious connection between water and CE is seen in the transition of wastewater treatment plants to resource recovery facilities, motivating the recovery and valoriza-

tion of treated wastewater, materials (e.g. nutrients, organic matter, etc.) and energy efficiency (Zhijun and Nailing, 2007; Sgroi et al., 2018; Voulvoulis et al., 2018). Other non-conventional approaches that could enhance resources circularity are the use of alternative water sources (e.g. rainwater and stormwater harvesting, etc.), the decentralized sanitation and reuse model and the ecological sanitation model (Abu-Ghunmi et al., 2016). However, fragmented management and implementation of such models is unlikely to result to desired outcomes from a CE perspective. A more holistic water circularity approach is proposed by five corporate bodies (i.e. McKinsey & Company, International Water Association, Arup, Antea Group and Ellen MacArthur Foundation) in three white papers (i.e. Stuchtey, 2015; IWA, 2016; Arup et al., 2018). The authors have identified the need for an integrated water management approach from local to river basin, encompassing different sectors (i.e. systems approach), differentiating between water functionalities (i.e. resource, consumable, durable) to enable reuse and recycling, symbiotically managing resources (i.e. water, materials and energy) and considering the multiple interactions between “nature-managed” and “human-managed systems”. Three CE principles were developed and adapted to sustainable water management – i.e. Regenerate Natural Capital, Keep Resources in Use, and Designing out

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Waste Externalities – in an effort to create a common basis for the development of a CE framework for water (Arup et al., 2018). The “Regenerate Natural Capital” principle aims to ensure functional environmental flows and stocks, the “Keep Resources in Use” principle focuses on closing the resource loops, and the “Design Out Waste Externalities” principle targets at the economically efficient reduction of waste (Nika et al., 2020).

However, such an integrated approach would require to overcome existing barriers. Integrated water management requires application of integrated models enabling systematic analyses to investigate interconnections, synergies and antagonisms between the different sectors and resources (Villarroel Walker and Beck, 2012), as well as the feedback loops between the technosphere and the biosphere. Integrated management and modelling further indicate the need for data sharing, availability and security (Ludwig et al., 2014). Moreover, successful implementation of CE in water requires innovations promoted through a social and institutional context, as well as the establishment of appropriate regulations and standards (Heshmati, 2015). Although in many cases innovative technologies are already available (e.g. resource recovery from wastewater), hindered CE implementation is attributed to the lack of planning and design methodology capable to identify the most appropriate solutions, tailored to individual cases (van der Hoek et al., 2016). Difficulties have been also identified in valuing environmental benefits against economic costs, as well as the relationship between environmental practices and corporate competitiveness and profits in an effort to find the right incentives for companies to implement CE (Sartal et al., 2020). The latter becomes more challenging for water valuation as current water pricing policies do not account for external costs (i.e. externalities) related to economic, social and environmental aspects (Greyson, 2007; Hislop and Hill, 2011).

In this study, a comprehensive analysis of water within the concept of CE is being conducted in an effort to address current challenges through the development of a game changing circularity assessment framework. The proposed Multi-Sectoral Water Circularity Assessment (MSWCA) framework follows a multi-sectoral approach, focusing on both economic and non-economic (i.e. ecosystems) sectors and symbiotically managing multiple resources. It reveals the complex interconnections and interdependencies between the different sectors. In this work, the term sector is used to group the resource-oriented activities of an area that support the economy and have a direct or indirect impact to water resources. The MSWCA applies integration of models and approaches for circularity assessment in line with the three CE principles, covering physical, technical, environmental and economic aspects. An indicator database has been developed as part of the framework, allowing data circulation and enabling comparability of different systems. A qualitative showcase of the MSWCA framework in a fictional case study is also presented in this work, allowing a better understanding of its implementation and use.

## 2. Water Circularity

### 2.1. Water in the centre of CE

Naturally, the hydrological cycle is influenced by weather, climate and physical characteristics of the area (i.e. land and soil formations, vegetation and geology), meaning that land use/land cover (LULC) and climate changes significantly impact the hydrological cycle (Ma et al., 2008). A disrupted hydrological cycle directly affects ecosystems, species and therefore biodiversity, which in turn is critical to water and nutrients cycling (Lange et al., 2019). Hydrological cycle alterations are further induced by water withdrawals resulted from the various socio-economic activities; e.g. agriculture accounts for 69% of the global water withdrawals, industries for 19% and municipalities for 12% (FAO, 2016). Addition-

ally, water with degraded quality that is returned to the basin (i.e. qualitative withdrawals) may result in substantial chemical and biological consequences to human health, ecosystems and biodiversity (Davis et al., 2016), but also to amenity and economic activity. Fig. 1 illustrates the interdependencies between the different socio-economic and non-economic (i.e. natural environment) sectors.

The feedback loops – occurring in the naturally interconnected system – show that any change has an inevitable effect to all the different components of the system (i.e. the ripple effect) (Everard, 2004). Thus, water is the ultimate systems challenge. Although this ripple effect is increasingly acknowledged in various cases, water management is still fragmented (Everard et al., 2016). Socio-economic sectors are artificially divided with water being managed at sectoral level (and seldom at river basin level) and considered as an isolated component of the ecosystem. An example of the ripple effect caused by sectoral management can be seen in China's policy to address food security by achieving self-sufficiency of 95% that resulted in irreversible depletion of water resources and in increased stresses to ecosystems and biodiversity (Ghose, 2014).

The transition to a holistic and integrated water management at river basin scale was the rationale of the European Water Framework Directive 2000/60/EC (WFD), which in spite its initial recognition as a ground-breaking environmental directive, failed to achieve the initial targets. The failure is attributed to the lack of efforts towards the implementation of the systemic approach mandated by the Directive (Voulvoulis et al., 2017). The systemic approach appears as a prerequisite for CE (EMF, 2013), raising concerns of amplified risks and not reaching the expected results to water resources, ecosystems and biodiversity in case that efforts are concentrated in sectoral rather than integrated management.

In this context, the development of a holistic circularity assessment framework is required that would enable and support a strategic circular water management approach. The MSWCA framework is encompassing both socio-economic (i.e. water, energy, agro-food, other related industry and waste handling) and non-economic (i.e. ecosystems) sectors, to overcome the issue of fragmented water management.

### 2.2. Circularity Prerequisites

The effective implementation of circularity involves the identification of clear circularity pathways, e.g. water circularity focuses on using the right water from multiple water sources (i.e. surface and groundwater, desalinated water, industrial brine and wastewater, rainwater and stormwater, greywater and blackwater) for the right purpose to the right users in a synergetic combination of centralised and decentralised water systems. Such approach implies the application of different water functionalities (Stuchtey, 2015) that enable a targeted and effective multi-sourcing, recycling and reuse of water. However, in many cases, the circular models do not fit as the arisen challenges are not technical but rather policy related, leading to difficulties to make a step change. Therefore, the actual implementation of water functionalities requires the establishment of water quality standards and appropriate policies and regulations at both the centralized and decentralized levels, supporting the concept of water circularity.

Circularity performance assessment additionally requires the specification of clear circularity targets, presented as CE principles by Arup et al. (2018), i.e. *Regeneration of Natural Capital*, *Keep Resources in Use*, and *Design out Waste Externalities*. The CE principles indicate the consideration of environmental, technical, physical and economic aspects in the assessment, as well as the symbiotic management of water-related materials and energy. The World Forum on Natural Capital defines natural capital as “the world's stocks of

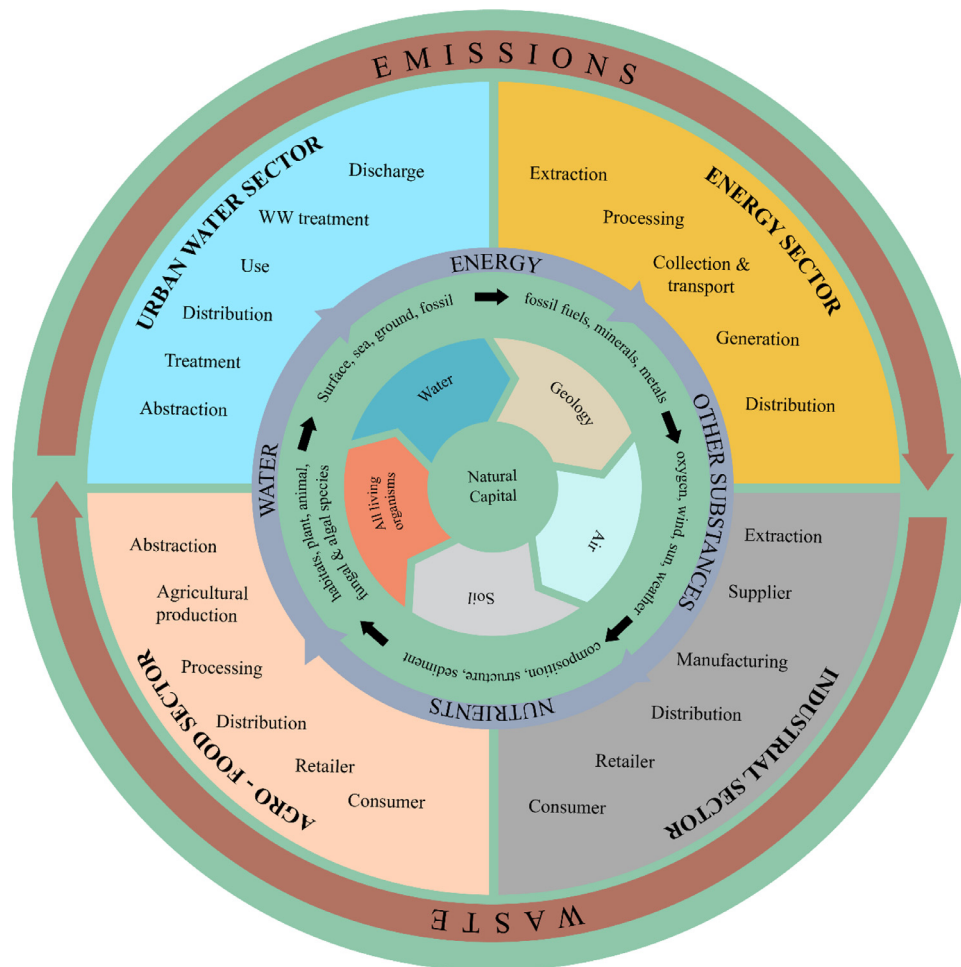


Fig. 1. Multi-sectoral process diagram illustrating the interdependencies between the different sectors and the natural environment in terms of water and other resources.

natural assets, which include geology, soil, air, water and all living things". The Natural capital principle aims to ensure functional environmental flows and stocks. "Keep resources in use" CE principle targets the reduction of extraction/abstraction of natural resources and minimization of waste generation by closing the water, water-related materials and energy loops within the system. The 'Design out Waste Externalities' principle targets the reduction of negative externalities by turning them into positive outcomes. Externalities can be both positive (e.g. monetary value attributed to clean water, biodiversity etc.) or negative (e.g. monetary value attributed to pollution) and result from producing or consuming a good or service. Any kind of waste and/or emissions (solid, liquid, gaseous) potentially causes environmental impacts translated to negative externalities. Thus, waste reduction and reuse result in reduction of negative externalities and in potential increase of positive externalities.

The MSWCA framework enables the incorporation of the three principles to holistically assess the target system.

### 2.3. Symbiotic Management of Resources and Dynamic Interactions

Water feedback loops and the associated ripple effect require the implementation of systems approach by using multi-sectoral analysis. However, water can be seen not only as a resource but also as a carrier, both in the human-managed and nature-managed systems; e.g. nutrients are diluted in water, thus their transport, fate and natural cycling is controlled to a high extent by water, while in the human-managed systems various substances (includ-

ing nutrients, minerals, metals and other) are concentrated in used water, which can be seen either as a cause of pollution or as an opportunity for resource (other than water) recovery, valorisation and reuse. Energy embodied in water can also be recovered and used.

Holistic multi-sectoral assessment implies the simultaneous investigation and management of multiple resources (i.e. water, energy, nutrients and other materials) as they flow through the different socio-economic and non-economic sectors. However, symbiotic management of resources at multi-sectoral systems increases the complexity of managing supply and demand, due to numerous supply and value chains; more complicated and dynamic interactions and incorporated processes between them; and various environmental, economic, social and regulative aspects.

To adequately describe the behaviour of the system and enable the circularity assessment, covering all different aspects, integration of methods, models and metrics is required (Nika et al., 2020). The intrinsic purpose of circularity is to reduce the amount of resources used by increasing their recirculation and reuse (i.e. closing the resources loops), which indicates the need for quantification (Saidani et al., 2019). Therefore, Material Flow Analysis (MFA) and Substance Flow Analysis (SFA) are widely used to assess circularity (Pauliuk, 2018; Moraga et al., 2019). They systematically quantify the flows and stocks of materials in systems, differentiating between flows of goods (e.g. drinking water) and flows of substances contained within these goods (e.g. nitrogen) (Pivnenko et al., 2016). On the other hand, the effects resulted by closing the resources loops (i.e. consequential circularity) need to

be investigated as well, which has led to an increased use of LCA-based methods to assess this aspect (Saidani et al., 2019). While MFA can be applied at different levels of sophistication enabling its use in complex systems, LCA generally neglects the feedback loops between the anthroposphere and the biosphere (Weidema et al., 2018) hindering its use in complex systems where interactions between socio-economic and ecological systems are of major importance. Feedback loops are observed at different time scales, resulting from “fast” (i.e. occurring over days and years) and “slow” (i.e. occurring over decades and centuries) processes (Ward et al., 2019). A “fast” process is water withdrawal or crop yield, while a “slow” process is change in biodiversity. Consequential circularity is therefore suggested to be assessed by coupling natural and human system models in an effort to investigate and predict complex system behaviour, emerging from non-linearities, time lags and unexpected results caused by feedback loops. Natural system models are referred here as numerical models to simulate the natural system’s behaviour and dynamics. Nika et al. (2020) presented a variety of hydrologic and biogeochemical models to simulate water and nutrients (or solutes) transport, fate and cycling. Other types of natural system models including ecological models, such as modelling of biodiversity change, or water quality models, etc. also exist and may be required to be coupled. On the other hand, human system models vary from analytical tools – such as MFA and LCA – and more complex agent-based models to capture human system’s dynamics by incorporating market processes, human decision making and behaviour.

Integrated modelling or nexus approaches to deal with interdisciplinary issues emerging from CE and water-related concepts (e.g. Sponge City) or even from water management are increasingly acknowledged in the recent literature. For example, available tools investigating interlinkages between different sectors are suggested to be used as city circularity tools in the review paper of Paiho et al. (2020). However, the reviewed tools mainly focus on the socio-economic sectors, while natural environment is underestimated by not being an integral part of the analysis. On the other hand, Nguyen et al. (2020) incorporate ecosystem services in the developed integrated assessment framework but as the focus is on Sponge Cities, it lacks models or approaches targeted at assessing circularity in human-managed systems. Li et al. (2018) developed a watershed modelling framework to “represent the coevolution of the water-land-air-plant-human nexus in a watershed”,

but the investigation of circularity is again out of the scope of this study.

Working towards the direction of integrated approaches, the MSWCA framework allows the assessment of multi-sectoral systems characterized by interdependencies and feedback loops. It suggests the integration of MFA, LCA and economic models for the socio-economic sectors (i.e. human system), and hydro-biogeochemical model(s) and ecological indicators/modelling for the natural/biophysical system to investigate the natural system’s dynamics and behaviour, within a single modelling framework. However, the purpose of the developed framework is not to specify the exact models (both the number and the modelling software) to be used, but rather to recommend concepts and modelling approaches that are required for a multi-sectoral systems assessment. There is not a unique combination of models and tools, as the most appropriate natural and human system models are case-specific. For example, if natural ecosystems (such as forest) form a major component of the studied system, then biogeochemical models, considering macropore flow of phosphorus, may be more appropriate compared to the studied system in which agriculture plays a major role with conventionally tilled soils where macropore flow is less pronounced (Pferdmenges et al., 2020). Additionally, the number of the models and tools to be coupled should be decided with cautious. The higher the number of coupled models and tools, the higher the complexity of the integrated model is, impeding its application.

Therefore, the MSWCA framework considers the interconnections between the different sectors in terms of water, energy, nutrients and other substances/materials flows and enables the incorporation of feedback loops – in terms of physical responses and not human behaviour – between the different socio-economic sectors and between the anthroposphere and biosphere as well. More complex agent-based modelling that investigates the human system’s dynamics can be coupled to the integrated model at a later stage (if necessary).

#### 2.4. Common Baseline for Data Requirements

The effectiveness of integrated water management depends on accurate information resulted from a holistic assessment; while the effectiveness of the assessment framework depends on securing access to accurate data from different sources (Fig. 2). Collection,

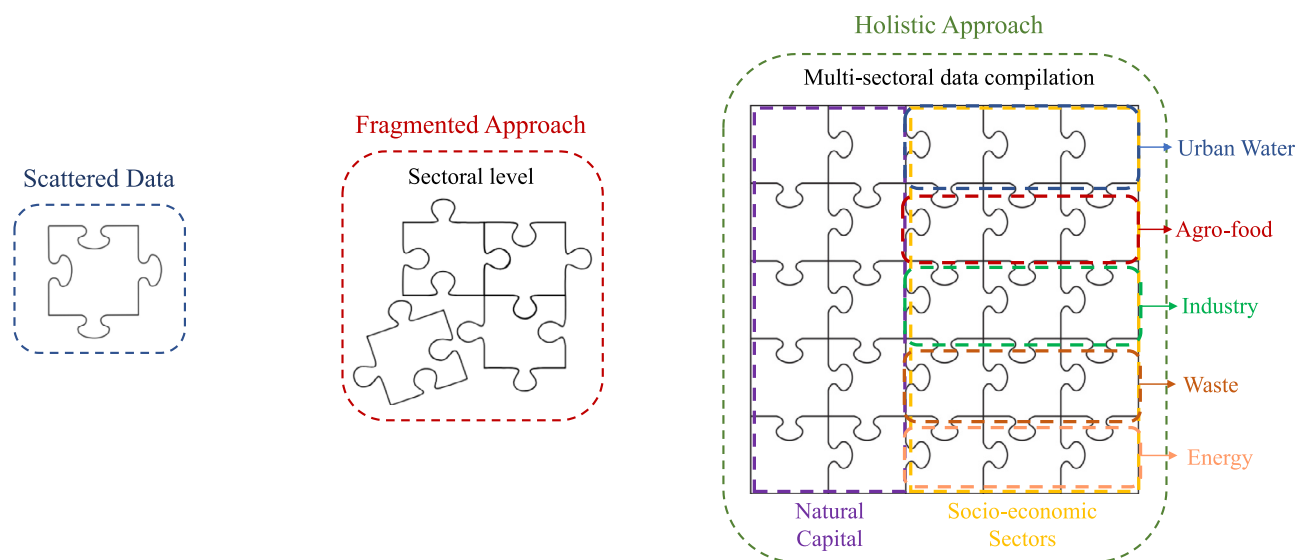


Fig. 2. Data requirements for building the puzzle.



standardization, homogenization and exploitation of the multiple heterogeneous and fragmented data sources that are required for a holistic multisector circularity assessment is not trivial.

Historical data are conventionally collected for different purposes from diverse disciplines following various methodologies and structure resulting in inconsistent forms, resolution and terminology. Water data are currently trapped in silos, rising issues of data accessibility, ownership, trust, interorganizational-competition, security and privacy for data-sharing among the interested parties. In many cases, there is also a lack of consensus on relevant data needed to feed the frameworks, resulting from different philosophies in data importance. Regarding environmental data related to nature-managed systems, there is a two-tier data regime. There are fields with very good protocols and metadata (e.g. weather and climate), whereas there are fields that are underdeveloped in terms of data requirements and reporting (e.g. nutrients cycling, ecosystem services, etc.). Therefore, decision-makers are often hindered to compare management options, make informed decisions balancing economic, social and environmental interests, and subsequently evaluate and prioritize potential solutions.

To overcome this bottleneck, common data policies, data management infrastructures and shared data systems are required between public and private decision-makers, stakeholders and practitioners. Therefore, an indicators database, including every data instance required for a holistic approach, is developed within the MSWCA framework.

## 2.5. Data Gathering and Models Uncertainty

There are several levels of uncertainty associated with the modelling process, from the input data (i.e. quality, reliability, data processing protocols) to the model or sub-models structure (i.e. conceptualization inaccuracies, omission of significant mechanisms, ill-defined boundary conditions) and the linkage between different water-subsystems or between human sectors and the natural environment (i.e. gaps in knowledge on the interactions between human-natural systems and their boundaries, issues with the integration of fast and slow process dynamics between natural and human systems). The robust quantification of uncertainties and risks of the model outputs increases the predictability and practicability of the model and helps decision makers to develop an understanding of the reliability and impact of the uncertainties on the model estimations.

The complexity of an integrated circular water management assessment model increases with the increase of sectors and components (i.e. agro-food, energy, waste, natural capital). Mapping of the uncertainty sources, their magnitude and their relationships is a significant step in the analysis (Uusitalo et al., 2015). The holistic model should consider uncertainties from the different water sub-systems modeled and uncertainties due to the coupling of the sub-systems (Tscheikner-Gratl et al., 2019). However, there are differences in the perception of uncertainties across the environmental modelling and integrated water modelling community and across the different water sectors and a standardized methodological approach to identify, quantify, reduce, report and communicate uncertainties is still missing (Bach et al., 2014; Montanari, 2007; Vanrolleghem et al., 2011). An overview on uncertainty sources for the integrated water modelling can be found in the study of Tscheikner-Gratl et al. (2019), whereas a practical approach for the quantification of uncertainty in integrated water models is proposed by Tscheikner-Gratl et al. (2017). Five generic steps have been identified for handling uncertainties in Integrated Environmental Models (IEMs) incorporating ecosystem services (Baustert et al. (2018)): 1) location, 2) identification, 3) characterization, 4) treatment and 5) communication of the uncer-

tainties in a cyclic and iterative process. Techniques commonly applied in each of these steps are also discussed.

In the current work, the following techniques are suggested to be implemented for the assessment, reduction and control of uncertainties (Li et al., 2018): i) application of a data-model fusion and data assimilation framework to integrate heterogeneous data into the required spatial and temporal dynamics and constrain the used water models (Keenan et al., 2011; Li et al., 2018; Liu and Gupta, 2007), ii) application of multi-objective and multivariate calibration techniques to reduce the bias of the model (Rouholahnejad et al., 2012; Zhang et al., 2013) and iii) implementation of global sensitivity analysis in which the variation range of all input parameters is considered simultaneously; the contribution of input parameters to the total model error is assessed for the entire range space of the input parameter (Borgonovo and Plischke, 2016; Gan et al., 2014; Sarrazin et al., 2016)

It is also suggested to expand the boundaries of the uncertainty assessment beyond the calibration/validation and uncertainty assessment phases. Uncertainties can be located, identified and mapped during the model conceptualization stage considering the model goal and scope, the model structure and required parameters (considering acceptable uncertainty ranges while accounting related risks). Specific consideration is required for the efficient and standardized communication of the uncertainties to the relevant stakeholders Baustert et al. (2018).

## 2.6. Valorisation of Resources and Market Analysis

The Principle No. 4 of the Dublin Statement on Water and Sustainable Development (International Conference on Water and the Environment, organized by the United Nations; Dublin, Ireland, January 1992) highlights that “not recognizing the economic value of water generally leads to wasteful and environmentally damaging uses of the resource. Managing water as an economic good is an important way of achieving efficient and equitable use, and of encouraging conservation and protection of water resources”. Therefore, value “of water” and “in water” is included in the MSWCA framework, revealing and assessing the economic aspects of the CE principles: *Design Out Waste Externalities* (e.g., optimization of water resources use through sufficient and correct valuation of water); *Keep Resources in Use* (e.g., optimization of resource yields obtained from water – energy, nutrients, minerals and chemicals – and water reuse); *Regenerate Natural Capital* (e.g., correct valuation of natural capital through non-market methods, such as pollution prevention, natural capital restoration, etc.).

### 2.6.1. Value of Water

In order to adequately value water, different types of uses in market and non-market sectors must be characterized. Water as an economic good in market sectors, can be considered as an intermediate or a consumption good. Intermediate goods are employed to make final products (e.g., agriculture, industry), while consumption goods provide direct human satisfaction (e.g., water used by households). In the case of intermediate goods, the economic theory of a profit-maximizing producer provides the conceptual valuation framework, while in the case of consumption goods the theory of the utility-maximizing consumer is used (Young and Loomis, 2014; Spellman, 2015). As with any other environmental resource, economic value is measured by the aggregation of many users' revealed preference or willingness to pay (WTP). WTP is straightforward elicited in the case of market prices, since prices set by market equilibrium show the WTP by the buyer at the margin. Similarly, for non-marketed goods, the WTP elicitation constitutes the theoretical basis to calculate “shadow prices”. The theoretical foundations of nonmarket economic valuation of environmental resources are well developed (Freeman, 2003). Since market valua-

tion varies according to spatial, qualitative and temporal attributes, non-market valuation (or 'shadow pricing') of water should follow similar rules. Economists additionally consider the existence of other non-use values, such as future option, existence and bequest values, however, the focus of this study is on the economic valuation of use values as an instrument to consider in circularity assessment.

The conventional demand or marginal benefit function is the concept measured in economic valuation approaches. For sectors such as agriculture (i.e., irrigation), industry and households (or residential use), an abstract demand function can be formulated in order to connect water use (demanded quantity) and price, together with other factors influencing demand (e.g., income, temperature). Water services (e.g., provision, urban sanitation and treatment) are generally provided under monopoly (public, private or both) and prices do not generally change enough to elicit a demand function. In this case, a great amount of observations on transactions is needed in order to have sufficient variation in price. Additionally, cross-sectional data from different water service suppliers in different municipalities or locations may also offer sufficient price variation. Under this approach, parameters of demand functions can be estimated by using statistical inference and econometric techniques. An alternative valuation approach for sectors using water as intermediate good (or service), such as agriculture and industry, bases on the residual value. If appropriate prices (as determined by the market) can be assigned to all inputs but one, the remainder of total value of product is imputed to the remaining or residual input, water.

Non-market valuation approaches can be divided into either "revealed preference" or "stated preference" approaches, which are both used to elicit the value of water in different sectors (including the environment) and to economically assess environmental positive and negative externalities from economic sectors affecting water resources (e.g., ecosystem degradation, water pollution). As in the case of market valuation (based on eliciting a demand function upon observed behavior), these methods also base on observed behavior of water users. Revealed preference methods rely on observations of actual expenditure choices made by users (revealing their preferences) and approach market valuation by inferring the net WTP upon observed changes in user's expenditure for different levels of the environmental resource (i.e., quantity, quality). This approach generally uses travel cost, hedonic pricing, and choice modelling methods. Under the assumption of utility maximization, users' WTP can be inferred upon their revealed preferences. In the case of stated preference, methods base on the simulation of a hypothetical (non-existent) market in which respondents (or users) are asked to express WTP for existing or potential environmental features. The deployed methods are choice modelling – in this case when hypothetical alternatives are ordered by respondents' preferences – and contingent valuation method (CVM). CVMs are based on a survey to a sample of respondents (water users) with the aim to elicit how much money respondents will be willing to pay or willing to accept (WTA) to maintain the existence of (or to be compensated for the loss of) an environmental resource or service. Stated preferences of the surveyed individuals are thus obtained.

The proposed MSWCA framework accounts for different methodologies to assess the value of water, since an adequate implementation of the CE principles require the use of both, market and non-market valuation methods depending on the considered sector and the service/externality to be valued. Specifically, market valuation method will be used to estimate demand curves upon available data in the different sectors and nonmarket valuation will be preferably performed based on stated-preference methods, though depending on the specific case-study, revealed-preference methods could also be adequate. It is worth noting that nonmarket valuation faces some potential weaknesses, which need to be

considered. Though evidence suggests that stated preference methods are able to provide valid and reliable estimates, a carefully designed survey and sampling procedure to gather the required information are of extreme importance. Hypothetical bias, aggregation bias, moral satisfaction, and scope sensitivity represent some of the main limitations that stated preference methods need to handle (Kahneman and Knetsch, 1992; Morrison, 2000; Harrison and Rutström, 2008). In the case of revealed preference methods, though widely accepted by economists as reliable valuation methods, observed behaviors do not usually provide all information needed to deliver valid estimates in all cases (Haab and McConnel, 2002). Consequently, the use of both methods is usually recommended when sufficient data is available. Additionally, commented limitations are more likely to occur in the case of non-use values (which are not the focus of the proposed framework).

### 2.6.2. Value in Water

The proposed MSWCA framework takes also into account the value in water. Recoverable materials carried by water and recovered energy depend on the water source (e.g., hydrologic system, waste water, reclaimed water), the specific market needs and regulations, and production process requirements of the system. Valorization of these resources is straightforward based on market valuation techniques since market prices exist for all these materials/resources. Extraction and conveyance costs should be valued. The benefits of resources incorporation (e.g., energy from thermal sources, nitrogen for agricultural uses) can be assessed by Life Cycle Assessment (LCA) approaches, through evaluating the environmental positive impacts achieved by using these reclaimed resources (compared to alternative sources) in all the stages of a product's life. Additionally, using alternative "in water" resources can provide cost savings in the production process (e.g., energy savings), which can be assessed by Life Cycle Cost (LCC) economic analysis (Marín, 2015). Environmental benefits, such as reduction/elimination of negative environmental externalities related to mineral extraction (e.g., water, soil and air pollution), achieved savings in energy power from polluting sources, avoidance of excess nutrient loads in water bodies, etc., can be economically valued by non-market approaches, as described in previous section. In this sense, LCC helps to identify and assess circularity measures to be implemented in complex water systems. Although LCC economic analysis is simple to understand and perform, and helps to assess circularity and resource efficiency, it also has some limitations. On one hand, it is mainly valid on the micro level (e.g., specific production processes), where data scarcity and calculation uncertainty may represent relevant limitations. On the other hand, LCC is inadequate for assessing environmental impacts (mainly due to market and information failures), being recommended the use of LCA to complement LCC (Kambanou and Sakao, 2020). In this regard, it is worth noting that though LCA might imply higher implementation complexities in terms of inputs and resources needed, studies such as Walker et al. (2018) and Potting et al. (2017) assert that circularity indexes should be supported by LCA approaches. The circularity assessment approach proposed in this study takes into account the use of both analytical approaches, LCA and LCC, with the aim to assess the value in water.

### 2.7. Measuring and Assessing Circularity

Circularity assessment involves a complex multi-sectoral systems analysis managing different resources and considering feedback loops and interdependencies. Such a complicated analysis inevitably produces complicated results, which require simplification in order to facilitate communication and comparison. The use of indicators is a common practice in complex systems to simplify results visualization (Lu et al., 2019).

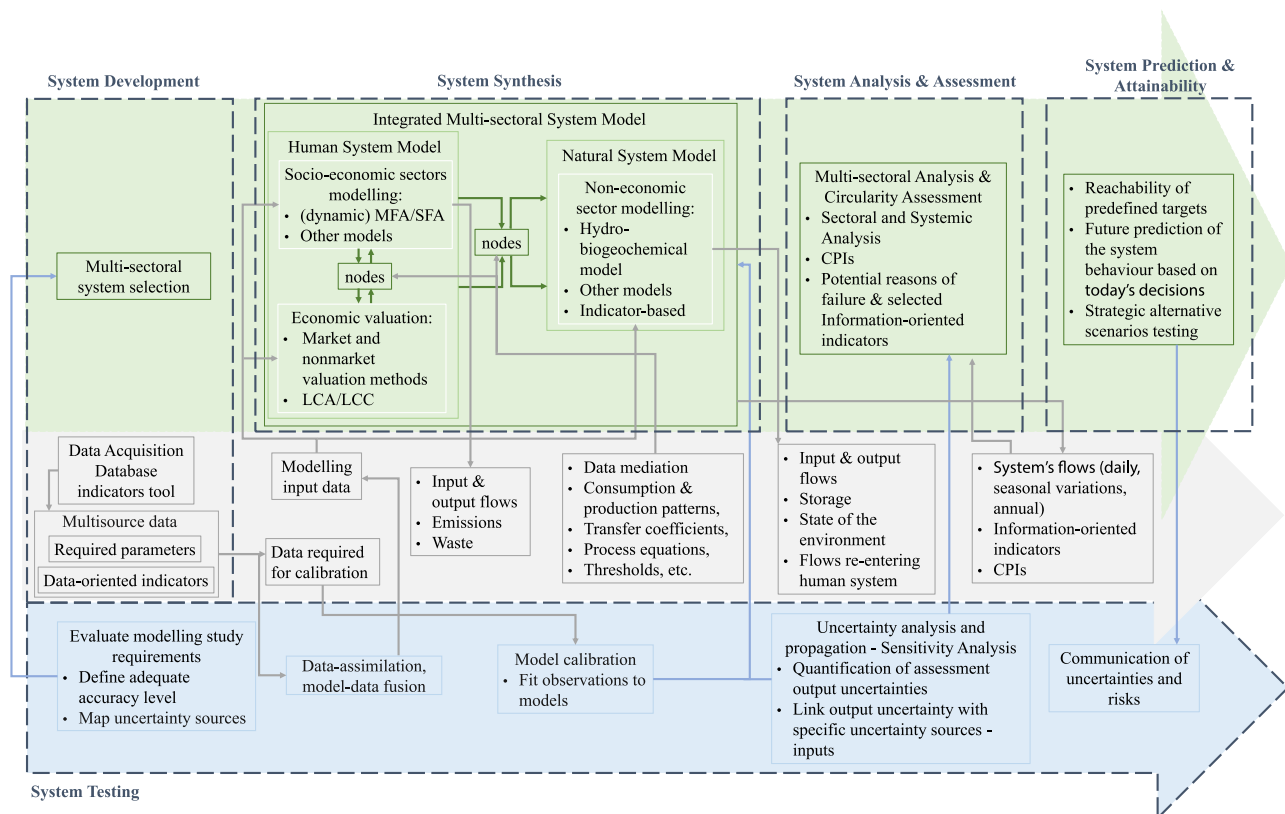


Fig. 3. The MSWCA framework illustrating the different modelling phases and data flows (within the grey arrow in the middle).

In the developed indicators database (Section 4), the selection of appropriate existing and newly developed indicators targets at a holistic evaluation of the three CE principles, i.e. three different sets of indicators, one indicator set per principle. The indicators are further differentiated in data-oriented indicators (i.e. indicators provided by stakeholders), information-oriented indicators (i.e. calculated indicators from modelling) for system's understanding, and action-oriented indicators (i.e. Circularity Performance Indicators calculated from modelling) for circularity assessment. Thus, information overload is avoided but at the same time access to information-oriented and data-indicators offer the possibility of understanding underlying factors, processes, or interactions that are linked with circularity.

### 3. The MSWCA framework

In this section, the conceptual Multi-Sectoral Water Circularity Assessment (MSWCA) framework is presented, aiming to bridge gaps and synthesise highlighted aspects mentioned in previous sections. The framework (Fig. 3), includes five distinct phases namely, system development, system synthesis, system analysis, assessment and system testing. The main components of MSWCA are MFA, natural systems models and economic valuation. Information-oriented and Action-oriented (i.e. Circularity performance indicators, CPI) indicators, as well as sensitivity and uncertainty analyses are incorporated into a modelling framework. MSWCA follows a multi-sectoral systems approach similar to the one developed by Villarroel-Walker (2010). MSWCA considers different socio-economic (i.e. urban water, energy, food/agriculture, industry, waste handling) and non-economic (i.e. natural environment) sectors and targets the symbiotic management of resources (i.e. water, energy, nutrients and other materials) as they flow through the different sectors. The modelling approach enables the

investigation of the feedback loops between the socio-economic sectors and the environment, as well as of the complex interactions between them. Therefore, synergies and antagonisms among the different sectors are revealed and a balance between socio-economic activities and environmental resilience is promoted. The MSWCA is developed in line with the following principles:

- To unlock data trapped in silos and overcome data inefficiencies by developing an indicators database;
- To promote systems approach by assessing multi-sectoral systems incorporating various resources, making natural capital an integral component of systems circularity;
- To estimate both the value in and of water by considering both market and non-market sectors;
- To holistically assess the circularity performance of multi-sectoral systems – both at systems and sectoral levels – considering sensitivity and uncertainty analyses; and
- To evaluate the impact of future interventions to achieve future circularity targets.

MSWCA stages include:

**System development:** This phase involves the **selection of the multi-sectoral system**. All the involved socio-economic sectors are specified and the system boundaries are expanded to include the physical boundaries of the surrounding natural environment. The sectors include all the relevant unit processes (process diagrams of the selected socio-economic sectors - Fig. 1) and consider the flows of the targeted resources (i.e. water, energy, nitrogen, carbon, phosphorus, other materials). The inclusion or not of other materials/resources, such as metals, minerals, cellulose etc. depends on the market needs and the additional industrial sector of interest in order to utilize and valorise the specific material.

The second phase of **data acquisition** is of major importance as it directly affects the quality, accuracy and precision of the re-

sults. Data acquisition enables the calculation of natural and anthropogenic flows of resources, therefore general data (e.g. climate, geomorphology, LULC), water, energy, nutrients/other materials uses, soil and water quality, resource recovery, etc. are required. Additionally, the state of certain ecological parameters is required to enable correlation between them and natural resource cycles. Several sources of information may be used to obtain the required data. The source of information is related to the uncertainty level of the model and therefore to the sensitivity analysis. In order to form a common baseline for data acquisition related to multi-sectoral systems an indicators database is developed, correlating the required data – obtained in terms of required parameters and data-oriented indicators – to information-oriented and action-oriented indicators for circularity assessment (Section 4).

**System synthesis:** The first phase of system synthesis involves the geospatial representation of the studied multi-sectoral system, i.e. land use land cover of the system, including number and type of buildings (in their actual location) and population.

The next phase – built upon the previous one – is the development of the integrated model for the multi-sectoral system that includes four modelling components, i.e. the socio-economic sectors, the non-economic sector (i.e. natural environment), their nodes of intersection, and the system as a whole. The socio-economic sectors are modelled using MFA based on developed mass balances. The resource flows (i.e. water, nutrients, energy and other materials) required to solve the mass balances are calculated based on available data, consumption and production patterns, mass transfer coefficients and process equations. The establishment of resource patterns, transfer coefficients for each process and the application of different products lifetime functions enable the establishment of dynamic MFA that would facilitate the integration to the natural system models. Computational models can be also used to estimate specific resource flows or air emissions in case that higher precision is required. The developed resource balances – for each of the socio-economic sectors – result in quantification of inputs and outputs, waste (including emissions to air, water and soil), accumulation, internal resource reuse/recycling and resource/materials to be recirculated to another socio-economic sector. At this stage, the information to be transferred from each socio-economic sector to the others, as well as to the natural environment (i.e. input to the natural system model) is specified. The different socio-economic sectors are interconnected in the model via nodes, indicating their physical interactions. The nodes can be simulated using linear, nonlinear and differential equations, thresholds, if-then rules and demand-supply functions, integrating market simulation that is based on economic valuation and analysis. The nodes also act as modules performing data mediation (both semantically and structurally interoperable data flows, according to Wang and Grant, 2019) to enable data transfer from one model to the other. The complexity of nodes simulation increases significantly if complex agent-based models (ABM) are integrated that can be used to simulate diffusion of innovation and adoption, changes in policies, individual behaviour, etc.

The non-economic sector, i.e. the natural environment, is modelled using natural system models and input data resulted from the human system models (e.g. water withdrawals, irrigation water, nutrients inputs, emissions, etc.) and entering the natural system models via the feedback loop nodes. Static data (e.g. soil and management conditions, soil type and formations, hydraulic conditions, etc.), as well as dynamic data (e.g. weather conditions) obtained through data acquisition procedure are also used as model inputs. Hydro-biogeochemical modelling – enabling an integrated investigation of water, carbon, nutrient and sediment dynamics – is suggested to simultaneously simulate the water and nutrients transport, fate and cycling. Mass transfer is at the core of such models using a series of (differential) constitutive equations based on vari-

ous processes (e.g. diffusion, reaction etc.) and their corresponding coefficients (e.g. diffusion or mass transfer coefficients). Forces and fluxes are computed to solve field balance equations. Additionally, ecological parameters, such as biodiversity, soil erosion, etc. are included in the model in the form of indicators. As their relationship with the water and nutrients cycles is not straightforward, statistical approaches can be used to investigate correlations. The modelling output is mainly the quantification and qualification of different resources flows that re-enter (via the feedback loops nodes) or affect the socio-economic sectors.

Integrated modelling is interacting – via the nodes – with market analysis and **economic valuation**. For the non-economic sector of natural environment, non-market valuation approaches, i.e. revealed preference and stated preference methods, are deployed for the economic valuation of water resource. For the socio-economic sectors, the economic valuation targets water as an intermediate good, water as a consumption good, and indirect resources recovered from water, using market valuation techniques. For the recovered resources, LCA and LCC, physical, chemical, and mechanical properties and regulatory standards are included in the analysis. Therefore, this phase focuses on the elicitation of the value of water and of recovered resources in the different sectors and on the investigation of positive and negative externalities occurred from the socio-economic sectors, affecting the natural capital.

At this stage, the multi-sectoral system's model is solved and calibrated (see the following section of *System testing*) for the year of data acquisition and the identified indicators are calculated.

**System analysis:** The results of the integrated model are interpreted. Graphical representations, flow diagrams, table matrices, etc. are created, enabling the **multi-sectoral analysis** of the system in terms of holistic performance, synergies, antagonisms, feedback loops and identification of hotspots. The system analysis phase is completed with the circularity assessment based on specific circularity metrics (i.e. **Circularity Performance Indicators** – CPIs). The CPIs consist of a set of whole-of-system and sector-specific indicators and are categorized based on the CE principle that they target, holistically assessing circularity of multi-sectoral systems incorporating various resources.

**System testing:** Activities to identify, characterize, treat and communicate the uncertainties of the MSWCA are dynamic and run in parallel to all MSWCA stages, from the selection of the multi-sectoral system and conceptualization of the modelling study, to the model integration and evaluation of the assessment outputs. In the initial phases of the system development, uncertainty sources are mapped (qualitatively or quantitatively) and prioritised. Acceptable levels of uncertainty are also defined in this phase. This can help evaluate the system boundaries selected, the completeness of sectors and flows considered in the assessment and guide the data collection (i.e. identify data that will impact significantly the assessment output focus effort to improve their quality) and model section processes (i.e. identify the requirements and the temporal and spatial resolution of the models). The uncertainties map can be updated during model development.

The integration of data and models used in the assessment is an important step in the analysis and needs to follow a systematic data assimilation framework, to combine the heterogeneous streams of data with the models accounting for the related uncertainties in a transparent and statistically robust way. During the integrated modelling phase, special attention is required to the calibration techniques followed; the parameters of the model need to be selected to maximize the fit of the model with the data. It is suggested either to calibrate the integrated model simultaneously (can be computationally expensive) or to calibrate the upstream model (e.g. the natural system model) and gradually integrate and calibrate the downstream modules (e.g. the human system model, etc.).



To investigate how the variability of input conditions and how uncertainties of the inputs and models are translated into uncertainties of the integrated model outputs, **uncertainty and global sensitivity analyses** are performed. The sensitivity analysis indicates important parameters that significantly affect the reliability of the assessment results. Uncertainty analysis is used to obtain probability distributions, the integrated model outputs and indicators based on the probability distributions of the input data. The uncertainty of the model's output due to the uncertainty in the model's parameters and other input data is calculated, using a set of uncertainty levels based on the quality, range and the applicability of different sources of information. Finally, clear communication of the uncertainties and reliability of the assessment results (in a qualitative and quantitative way) is vital to create trust in the assessment results and support decision making of the pathways to achieve the predefined circularity targets.

The final phase of MSWCA is the **assessment** by investigating the **attainability** of specific circularity targets, in terms of CPIs. The goal of this phase is twofold; to assess the circularity performance of the current system and to predict by understanding potential future behaviour of the system based on today's decisions (i.e. the model is run again to predict future system trajectories and assess the ability of the system to reach the circularity targets). In case that the system does not reach the quantifiable circularity targets, strategic alternative scenarios can be tested.

#### 4. Circularity Performance Indicators (CPI)

The developed excel tool (Supplementary Materials) includes an indicators database for holistic circularity assessment of multi-sectoral systems, enabling information sharing for integrated management of resources. It includes requirements on data that should be measured and collected for the quantification of the CPIs.

The tool differentiates between required parameters and three types of indicators, i.e. data-oriented, information-oriented and action-oriented (i.e. CPIs) indicators. Parameters (i.e. data requirements) and data-oriented indicators (i.e. DOI) are based on information coming from different stakeholders and sources, allowing the integrated modelling of the system. Parameter is defined as a factor that can be measured or observed. DOI are indicators that can provide information on matters of wider significance or make perceptible a trend or phenomenon that is not immediately detectable (Hammond et al., 1995). The DOI can be provided by stakeholders. For example, water demand/use by sector is defined as a state indicator (e.g. by UNIDO and by European Environment Agency) for recognising potential water conflicts. An estimation of water demand can be provided by relevant stakeholders (e.g. municipalities). Another example is the water supply service coverage or proportion of population served by the water supply industry that is defined by UNSD, 2008 as an indicator for water accessibility and its estimation can be provided relevant stakeholders as well. Information-oriented indicators (i.e. IOI) consist of a long list of indicators that are resulted from modelling calculations – based on parameters and DOI – during the implementation of the framework and they are not directly used in, but rather support the assessment. The assessment is based on action-oriented indicators (i.e. AOI), named here as CPIs. AOI or CPIs are derived from the integrated modelling and are calculated from further processing of IOI, DOI and parameters. CPIs are used for communication of the results and consist of a short list of indicators targeted at the three CE principles to reduce the number of indicators used for circularity assessment. The IOI are indicators measuring circularity aspects indirectly and therefore, are used to explain the outcomes of the assessment. The IOI are not used for communicating the results of the assessment but they are accessible to the inter-

ested parties for informative purposes. The tool includes existing and newly-developed indicators.

The indicators tool is tailored to the multi-sectoral system approach by differentiating between whole-of-a-system and sector-specific indicators, i.e. indicators related to the system as a whole, and to the urban water, agro-food, energy, industrial, waste handling sectors and natural capital. The tool also provides information about the units, methodological aspects (i.e. methodology, equation, or reference in order to calculate the indicator), typology (differentiating between descriptive, efficiency and performance indicators), level of measurement (i.e. a 1<sup>st</sup> level indicator is a value derived from parameters, a 2<sup>nd</sup> level indicator is derived from further processing a 1<sup>st</sup> level indicator into an equation or model, and so on), description and goal of the indicator. The indicators are further categorized based on the type of information they provide, i.e. generic, economic, information related to water, nutrients & substances, energy, biodiversity, and information related to the CE principles. *Regenerate Natural Capital* and *Design Out Waste Externalities* principles contain consequential CPIs, while *Keep Resources in Use* principle is measured with intrinsic CPIs.

#### 5. Conceptual Example – A Circular City

The MSWCA framework is applied in a conceptual example of a small city. The imaginary city's electricity source is from renewables (i.e. solar and wind energy), the urban water sector consists of centralized water supply to meet the drinking water demands of the area using a surface natural resource, centralised wastewater treatment receives only blackwater, while greywater from the sinks and taps is treated separately (decentralised greywater treatment) and in combination with rainwater harvesting is used to meet the domestic demands (i.e. toilet flushing, washing machines and irrigation of gardens). The centralised wastewater treatment is performed in one treatment plant and the treated effluent (after disinfection) is sent to a set of natural and humanmade wetlands. The wetland system supplies the local agricultural water requirements. The agro-food sector consists of agriculture (both livestock and crops) and the agricultural production is sold in local markets. The waste handling sector receives the produced sludge, which is composted and used as soil amendment, while livestock manure, food and green waste are composted and sent back to agriculture for fertilization purposes. All other types of waste are disregarded in this example.

The required information is collected in the form of parameters and data-oriented indicators via the proposed Indicator Tool. The configuration of the multi-sectoral system is illustrated in Fig. 4.

The next step of the framework includes the development of the integrated model. Parameters and data-oriented indicators are used as inputs to the model. For each one of the socio-economic and non-economic sectors, mass balances are developed and model inputs are used to calculate all the required resource flows and to solve the developed mass balances for all the incorporated resources.

For the urban water sector, daily water rates – for water treatment, use, greywater and blackwater production, treatment, recycling and discharge – are used in combination with precipitation data and catchment area (for rainwater harvesting), water resources, permanent and seasonal population, centralized and decentralized water users to calculate all the daily water flows in terms of inputs from the natural environment (i.e. water withdrawals from the natural resource, harvested rainwater), internal recirculation (for domestic water requirements), storage (in case of excess water), and outputs to the natural environment (discharge to the wetlands, leakages, and irrigation of gardens). The nutrient flows of the urban water sector are calculated based on data from nutrient concentrations in raw water, blackwater and greywater, on

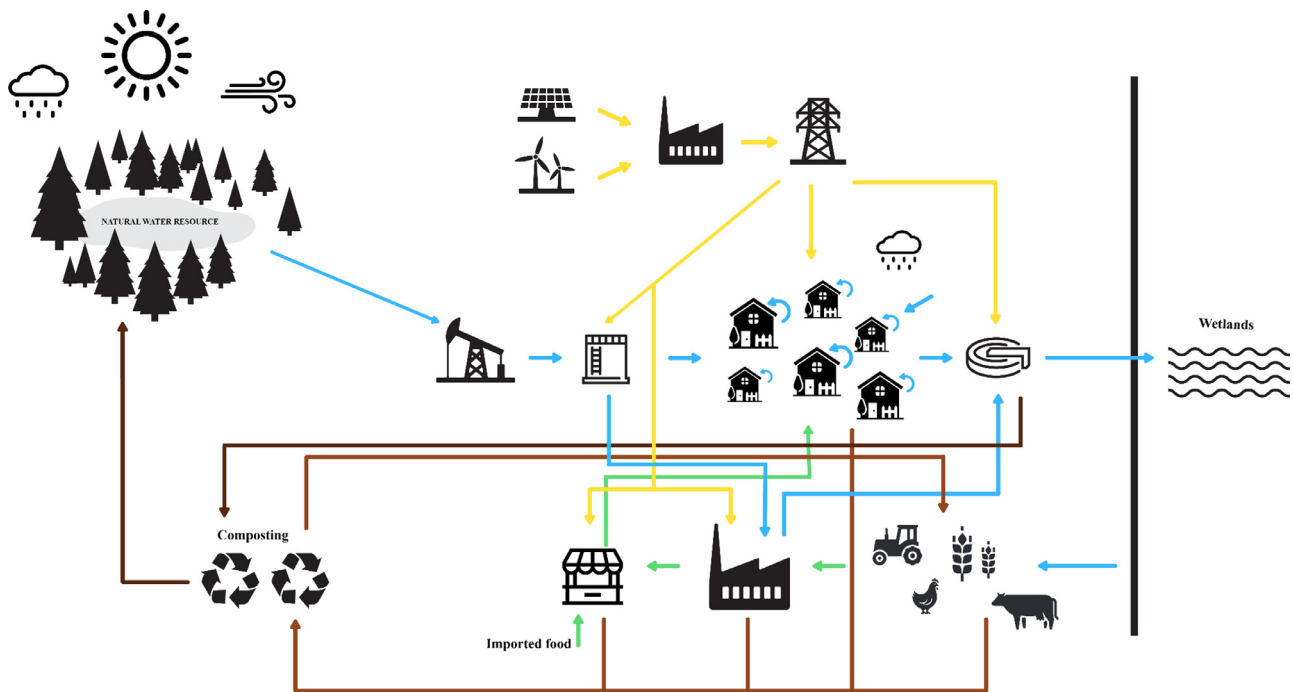


Fig. 4. Configuration of the system.

the incorporated water volumes, and treatment rates. The calculations result in daily nutrient inputs (from the natural environment and the agro-food sector), internal recirculation (i.e. nutrients incorporated in the recirculation of domestic water), storage and outputs to the environment (in terms of emissions and discharge or disposal) and to waste handling sector (nutrients in sludge). Water flows are also accompanied with other critical substances (e.g. chemicals used for treatment, pathogens and other pollutants) and their flows are also calculated based on their concentrations in water, waste or usage rates. The energy consumption in centralized and decentralized water and wastewater treatment are also calculated.

For the agro-food sector, nutrient and water flows incorporated in the local agricultural production are calculated based on hydro-biogeochemical modelling using soil condition, soil type and formations, hydraulic conditions, management practices, weather data, fertilizer inputs, etc. The quantification of water (e.g. infiltration, evapotranspiration, irrigation, runoff, etc.) and nutrient (e.g. nutrient surplus, nutrient in crops, nutrient in residuals, gaseous emissions etc.) flows are the modelling outputs. The local market receives locally produced food yields and imported food. The green and food waste resulted in the agro-food sector, as well as the nutrient content in the waste are also calculated. The energy consumption is calculated as well.

For the waste handling sector, daily inputs of sludge and manure, green and food waste received as well as their nutrient content are calculated. The outputs include daily amount of produced compost to be recirculated to the agricultural sector and to the natural environment, nutrients amounts in the produced compost, and nutrient outputs diluted in produced wastewater (in case of dewatering) and fate, nutrient emissions, nutrient leakages, nutrients in residual waste from screening and fate, water vapour, etc. Energy requirements are calculated as well.

Hydro-biogeochemical modelling is deployed to reveal the state of the natural environment in terms of nutrients and water cycles, soil condition and biodiversity as well. The quantification of water (e.g. infiltration, evapotranspiration, water withdrawals, runoff, etc.) and nutrient (e.g. nutrient surplus, nutrient in crops, nutrient

in residuals, gaseous emissions etc.) flows are the modelling outputs, as well as the state of soil and biodiversity condition, quality and quantity of water bodies, and air quality or emissions. All the quantified final outputs of the human system model serve as inputs to the natural system model, while the calculated natural capital flows leaving the natural environment, re-enter the human system model.

The economic simulation is based on economic valuation of market and non-market services and is run in tandem, revealing economic changes in values (either positive or negative) due to the behaviour of the physical multi-sectoral system.

The final step is the integration of all the different models by using developed equations, functions and rules that describe the feedback loop and socio-economic nodes. These nodes determine the amount and frequency of the resource flows entering and leaving each modelling component. The integrated system model is run, solving the whole-of-a-system daily, seasonal and annual mass balances and revealing potential changes to the natural capital due to fast processes. This is the completion of the first simulation loop. Sensitivity and uncertainty analyses are performed to investigate the uncertainty of the modelling outcomes and communicated to the relevant parties.

After ensuring the computability of the integrated model, the information-oriented indicators that were not used to solve the mass balances and the action-oriented indicators are calculated. In this conceptual example, some of the IOI that are used to solve the water balances in the integrated modelling procedure include rainfall volume, infiltration, evapotranspiration, runoff, change in soil moisture, water demand per sector, actual irrigation water demand, and others. However, the IOI of irrigation efficiency is not required to solve the water balances, but it is further calculated – as a ratio of water supplied for irrigation per actual irrigation demand – to evaluate if the agricultural system is overwatered, underwatered, or sufficiently irrigated. Similarly, the AOI of regenerative capacity index for water requires further calculation; the total quantitative and qualitative water withdrawals of the system are compared to the natural water recharge (volume of water of improved quality that is stored to the water bodies due to natural

hydrological water cycle) taking also into consideration the volume of water (of the same quality) that is returned to the water bodies from the anthropogenic water system.

After having calculated all the IOI and AOI/CPIs, the results are presented and assessed. The first step of the assessment is the presentation, analysis and evaluation of the CPIs. The analysis reveals the extent of achieved intrinsic circularity of the different resources, the consequent environmental and economic effects, the synergies and antagonisms between the different sectors in terms of resources consumption and circularity and the identification of hotspots (both current and future). After the identification of system's hotspots, the relevant information-based indicators (i.e. the ones connected to the CPIs) are analysed to understand the reason of system's failure and what actions are required to improve circularity. The reasons might be technical, physical, economic, social, regulatory or policy and they should be communicated to the relevant parties to take appropriate actions. For example, if one of the identified hotspots is the gross P balance, IO indicators related to P cycling are analysed to understand if the reason is overfertilization, low retention capacity of soil, overwatering, etc. Or if water stress is severe, IO indicators of environmental water use, environmental water requirements, water provisioning capacity, alternative water use, internal and intersectoral water recycling, water intensity, water demand requiring drinking water standards, etc. are further analysed to understand the reason of failure. The analysis is performed internally and only the most probable reasons of failure are presented to the relevant stakeholders.

## 6. Conclusions

To address water circularity, fundamental changes are needed in the way water is managed and valued, and in the way, data is shared among practitioners, policies, regulations and assessment frameworks. The proposed MSWCA framework approaches circularity from a multi-sectoral perspective following a systems approach that symbiotically manages key water-related socio-economic and non-economic sectors. A visualization of the MSWCA's application to a fictional city is presented to enable the understanding of the framework and its practical use.

Whilst developing the MSWCA framework, we identified a number of hurdles. The consistency and valid flow of input information is one of the identified hurdles. To overcome this problem, we suggest the *indicators tool*. The tool establishes a common baseline for data requirements and indicators to be used for the assessment. The next identified issue is the economic valuation of nonmarket goods. To overcome this issue the MSWCA framework suggests the use of both revealed and stated preference methods. The third issue relates to feedback loops and interdependencies between different sectors and the natural environment. This framework offers a novel methodology to link natural environment to human system models. Integration also entails seamless data exchange between different system components, making data interoperability a necessity. The MSWCA framework provides the environment for the interaction of data from multiple sources thus facilitating integrated modelling integration. Increased data volume and modelling complexities creates uncertainties, the proposed framework also suggests qualitative and quantitative methods to manage uncertainty in the framework.

## Declaration of Competing Interest

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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## Supplementary materials

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