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Towards the development of an online platform for an industry metabolic pathway

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ABSTRACT

This paper presents the design of a web-based decision co-creation platform to showcase water treatment technologies connected via industrial symbiosis for a circular economy approach. The platform is developed as part of the EU H2020-funded ULTIMATE project. This system initially investigates three case studies focusing respectively on: water and nutrient recovery in greenhouses, pre-treatment of wastewater from olive mills before integration into communal wastewater systems, and value-added compound recovery from wastewater in a juice factory. These cases are then merged into one abstract composite example showing all three aspects of the problem, connecting greenhouses, juice factories, and olive mills, describing a pioneering form of industrial 'metabolic network' of the circular economy. This work describes the modelling framework, the online platform and the interactive visualisations that allow users to explore the industrial symbiosis configurations enabled by the metabolic pathway. The platform thus serves as a decision support tool that merges circular economy and industrial symbiosis, as well as a pedagogical tool.

Key words: circular economy, decision support tool, industrial symbiosis, metabolic network of industries

HIGHLIGHTS

- An online decision support tool is presented.
- It links 3 case studies: a juice factory, greenhouse collective, and olive mills.
- The study merges circular economy and industrial symbiosis.
- We explore the feasibility of a nascent metabolic network of industries.

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GRAPHICAL ABSTRACT

1. INTRODUCTION

Water being at the centre of a literal nexus of services, research is understandably moving towards methodologies exploring more holistic approaches such integrated water resources management (Savenije & Van der Zaag 2008), or the concept of a dynamic metabolism modelling of urban water services (Behzadian et al. 2014; Venkatesh et al. 2014) or circular economy (CE). Industrial symbiosis (IS) can be defined as engaging 'traditionally separate industries in a collective approach to competitive advantage involving physical exchange of materials, energy, water, and/or by-products' (Chertow 2000). A clear emphasis is placed on benefits from collaboration and opportunities for convenient exchanges of useable by-products resulting from spatial proximity. CE relies on 'decoupling growth from the consumption of infinite resources, reducing waste and pollution, reusing products and materials, and the regeneration of natural systems' (Ellen Macarthur Foundation 2010). Yazan et al. (2022) reviewed decision support tools for smart transition towards CE and identified eight mainstream techniques used for analysing IS. These are: (1) agent-based modelling (Batten 2009) that simulates interactions between independent decision making entities; (2) material passports (Hansen et al. 2018) that tracks over the life cycle of an object of its circular value, and the uses for its products and components; (3) machine learning and rule-based algorithms (Van Capelleveen 2020) that utilise training data to predict outcomes; (4) environmental assessment and accounting methods from the field of industrial ecology (Daddi et al. 2017) that investigate material and energy flows; (5) game theory (Jato-Espino & Ruiz-Puente 2021) that considers the interaction between players making rational decisions based on their individual goals and interests; (6) geographical information systems (GIS)-based exploration and scoring methods (Van Capelleveen et al. 2018) that focus on region identification tools; (7) material selection methods (Ramalhete et al. 2010) that help designers select the most appropriate material candidate based on its technical properties; and (8) network and infrastructure optimisation techniques (Kastner et al. 2015) that look for ways to connect plants to facilitate and optimise the transportation of by-product exchange.

The IS support framework (Yazan *et al.* 2022) emphasises the need for modelling, in particular, agent-based models, to investigate the factors that impact on the willingness of individual businesses to co-operate, thereby improving the efficacy and sustainability of the IS solutions. Thus, a modelling solution, whether it is system dynamics, discrete-event simulation or agent-based simulation, is important for decision-makers to explore the factors that contribute to the emergence of IS,

those that are important for the potential adopters, etc. However, a challenge is the use of a simulation-based decision support system by the non-experts, which in our example, are the individual business owners. Arguably, the use of an online platform that separates the detailed simulation model (developed by programmers and simulation experts) from its intended end users, but is yet sufficiently versatile to enable novel forms of experimentation by the end users, would allow further enable the adoption of CE concepts among stakeholders. The novel forms of visualisations proposed in this paper go beyond the development of interfaces which only allow the users to change the model parameters. Indeed, and based on the domain of interest, the user interface should facilitate the development of new pathways among different businesses, whereby the waste generated by one entity becomes an input (raw material) for a subsequent entity, thereby forming a chain of input-output processes among various businesses. The input-output linkages may evolve through time. Thus, a platform targeted at end users of IS solutions should allow reconfiguration of the core model logic related to input-outputs; additionally, the platform should enable such model-level reconfiguration to be performed by non-experts through novel visualisations. Towards this, the paper extends our previous work on designing online platforms with highly visual and interactive interfaces for the NEXTGEN serious game (Evans et al. 2023; Khoury et al. 2023) that supported system dynamic models on CE of water (Evans et al. 2023). In this paper, we extend the state-of-the-art in modelling and visualisation by articulating the need for an online decision support tool that allows the stakeholders to make changes to the core model logic using novel visualisations; a tool which allows the non-experts to engage with the experimental modelling and simulation approach through novel interfaces, helping them to explore opportunities to move towards the CE of water through IS and to discover the resultant benefits.

The technical novelty of this work lies in the flexibility and modularity of the hybrid framework that combines a system dynamic modelling (SDM) simulation engine with an interactive online visualisation system. Improving on the design principles and lessons learned from the NEXTGEN project (Evans *et al.* 2023; Khoury *et al.* 2023), the ULTIMATE platform presents enhanced adaptive visualisation capabilities with flexible and modular modelling capacities. Four different interactive systems are showcased: a greenhouse located in the Netherlands, a collective olive mills wastewater transport and treatment system from Israel, a juice factory from Greece, and a hybrid abstract model combining all three systems (referred to as the integrative model). The platform is fully functional and available for all to use online (https://ultimate-www.caflood-pro.com/).

2. METHODS

This work presents a hybrid modelling framework aiming at exploring a metabolic network of industries (metabolic network as in biology where metabolic reactions produce different compounds reused by other reactions) built around technological examples of CE for water and IS. The hybrid framework integrates methods and techniques from multiple disciplines, namely, systems modelling and computer simulation, and applied computer science. While SDM is used to model the underlying system of interest (which, in our case, is IS), a plethora of techniques from applied computer science have been deployed to develop the online platform and novel forms of visualisations.

The resulting hybrid modelling framework combines multiple instances of SDMs into one seamless simulation engine and then connects it to a novel user interface enabling the flow control, activation, and chaining of these models representing industrial activities with different input/outputs.

The SDMs, used as modelling modular building blocks in our framework have four generic characteristics (Naugle *et al.* 2024):

- Models are based on causal feedback structure where feedback loops are either positive or negative loops.
- Accumulations and delays are foundational, leading to a differentiation between 'stocks' or variables in which something accumulates, and 'flow variables' that determine changes to those stocks.
- Models are equation-based and are therefore simulated by calculating the value of each variable at a starting time step, and then by updating the values for all variables at the next time step until the end of simulation.
- The concept of time is theoretically continuous. In practice, it is implemented by segmenting the conceptually continuous time horizon into common discrete time steps (i.e. hourly time steps to simulate daily rainfall events over 20 years).

The Interface is linked to the SDMs in a similar fashion as a three-tier *Model-View-Controller* as shown in Figure 1. In order to provide a targeted an informed view of IS, different models can be switched on and off, and chained to each other to give a detailed account of how various by-products from some industries can become resources to others.



Figure 1 | Schematic layout thematically inspired from model-view-controllers (MVC) of how the metabolic network of industries can be explored by linking control logic chaining user interfaces (UIs) and SDMs. There are several UIs: one for each model, and one for the overall metabolic network of models where it becomes possible to enable and connect individual models.

3. THE CASE STUDIES

One of the initial concepts within the ULTIMATE project was demonstrating novel technologies within the water cycle to showcase wastewater is not only reusable but also a resource-rich medium. To present the potential benefits of adopting a CE approach for wastewater management, three case studies were chosen: a juice factory from Greece, a greenhouse located in the Netherlands, and collective wastewater transport from olive mills and treatment system in Israel. For each of the case studies, a real-time simulation engine was developed that was based on surrogate models of technologies and processes relating to water, energy, and material reuse.

3.1. The juice factory (Greek case study)

Within the Greek case study, an advanced water treatment technology has been incorporated into juice production workflow for the processing and treatment of effluent streams. A conceptual depiction of the treatment process in this example includes as the following two parts (Figure 2).

- Value-added compounds (VACs): The initial treatment/processing of effluent produced by the juice factory focuses on the extraction of polyphenols (VACs) that potentially have extremely high monetary value with the global polyphenol market size expected to reach a value around \$2.98B by 2030 (Grand View Research 2023).
- **Treated water product**: The second stage of treatment focusses on the treatment of effluent designed to adjust pH levels to a normal range and reduce Total Suspended Solids (TSS), Total organic Carbon (ToC), and Biological Oxygen Demand (BOD) levels. The quality of the treated water based on the levels of TSS, ToC, and BOD within it will determine its suitability for other applications as outlined in Table 1.

Within the hybrid modelling framework, the key output from the Greek case study is that of the treated water product. The treatment technology used within the GtG system follows an adaptive approach whereby the energy, chemicals, and materials used for the treatment of juice effluent adapt according to the pH, ToC, and TSS of the effluent. With the model analysed in the Netherlands case study, the water is only stored in the 'Mixing Tank', outlined in Figure 3, if the quality meets the standard for greenhouse irrigation.

3.2. The Greenhouse (Netherlands case study)

The Netherlands case study investigates the potential of electrodialysis (ED), aimed at reclaiming water and assessing the feasibility of nutrient recovery from wastewater discharged by a collective of greenhouses. ED is an innovative electrochemical membrane technology that can be a low-energy-cost alternative for treating wastewater for this application. To simulate



Figure 2 | Schematic layout of the GtG juice processing case study.

Table 1	Water reus	e potentia	based on	ToC ranges
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ToC (mg/L)	Potential use case
<6.6	Irrigation of nearby fields ^a
1–20	Irrigation of greenhouses
5–10	Reuse by fruit company (cooling)
10–30	Reuse by fruit company (washing)
6.6–500	Discharge to wastewater treatment plant (WWTP) ^b

^aLegislation requires BOD < 25 mg/L.

^bWastewater BOD < 500 mg/L.





this, a demand-driven mass-balance model was developed (Figure 3). To provide a baseline comparison between energy use for specified water recovery rates the electrochemical membrane technology is compared against a reverse osmosis approach for water treatment/recovery.

This model is demand driven whereby water and nutrient demands are determined by the greenhouse characteristics such as crop types, irrigation methods, area, etc. To meet the water demands the original model had access to a combination of water sources: harvested rainfall, surface water, reclaimed treated water and other water. From the nutrient aspect the model only considers nutrients via fertigation whereby these originate from an external additive sources within the mixing tank and via any reclaimed nutrients present within the treated drainage water. While the water reclamation approaches allow for the recovery and reuse of water, some losses still occur within the system relating to evapotranspiration, plant take up, and discharged water, where the quality of discharged water cannot be reused for irrigation within the system without additional treatment.

To simulate the demand within the system, the inputs relating to water and nutrient demand estimates were derived from selected crop types. Ten types of nutrients (nitrates, ammonium, phosphate, potassium, calcium, magnesium, sulphur, chlorides, sodium, and sodium tolerance limit) are tracked through the system. The mmol/L requirements for fertigation water are estimated from literature along with percentage uptake rate estimates that can be customised by the user of the model to infer values of nutrients present in the collected discharge water that is to be treated. Utilising laboratory data, percentage-based recovery parameters for different nutrients are estimated for different water recovery rates and target conductivity/water quality values (Table 2).

The model allows the user to select the desired quality (in terms of conductivity levels) of the treated water for reuse, which subsequently determines the quantity of nutrients being recovered, and energy required to recover this volume of water at this quality.

While the parameters affect the quality of recovered treated water, they also determine the quality of the discharged water that cannot be reused directly within the Netherlands case study. From the individual model perspective this discharged wastewater would need to undergo additional treatment prior to being discharged to a municipal wastewater treatment plant (WWTP).

3.3. The olive mills (Israel case study)

The modelling framework within the Israel case study centres on the reduction/mitigation of wastewater shock loading at the municipal WWTP that can occur during olive harvest season due to the illegal discharge of olive mill wastewater (OMWW) into the domestic sewer system. OMWW has an organic load of around 27,000 mg/L that can be treated to <5,000 mg/L using Advanced Anaerobic Treatment (AAT; Sobhi *et al.* 2007). While this approach allows for the safe disposal of OMWW it still poses an additional logistical problem in getting the OMWW to the AAT facility. The proposed solution to this issue was for the transportation of OMWW via trucks to a decentralised WWTP. Figure 4 outlines the schematic layout of the Israel case study model. Within this model, OMWW produced by individual olive mills is transported by a tanker to a location, where it is mixed with domestic wastewater, and then treated by the AAT.

	Target conductivity	Nutrient recovery (%)							
Water recovery		NO ₃	NH ₄	PO ₄	к	Ca	Mg	Na	SO4
60%	5 mS/cm	14	0	4	29	10	13	53	3
	2 mS/cm	4	0	0	6	0	0	16	0
	<2 mS/cm	1	0	0	1	0	0	4	0
80%	5 mS/cm	9	0	2	27	9	12	51	0
	2 mS/cm	5	0	1	10	3	4	25	0
	<2 mS/cm	1	0	2	1	0	0	4	0
90%	5 mS/cm	10	0	2	29	10	13	54	0
	2 mS/cm	4	0	0	7	2	3	20	0
	<2 mS/cm	1	0	0	1	0	0	3	0

Table 2 | Nutrient recovery percentage for different water recovery and quality metrics (Guleria et al. 2024)



Figure 4 | Schematic layout of Israel's OMWW treatment case study.

Within the singular model setup OMWW is mixed with domestic wastewater at a ratio of 0.5 m^3 of OMWW to every 95.5 m^3 of domestic wastewater treating around 120 m^3 per day. This mix is anaerobically treated at the decentralised AAT to reduce its COD value to acceptable levels prior to being discharged into the sewer system to continue to the municipal WWTP. In addition to the COD reduction, the anaerobic treatment of the OMWW and domestic WW produces biogas at a volume ranging from 8 to 15 m^3 /day.

As an additional advantage of this decentralised treatment approach, the treatment facilities are not constrained to the proximity of the municipal WWTP and instead can be theoretically located anywhere in the region in proximity to the sewer network. Figure 5 highlights the spatial distribution of olive mills within the modelled region and the respective municipal WWTP at Karmiel and a proposed optimum location for the AAT derived via cumulative travel distance analysis of tucks from each olive mill using the road network. In this example the proposed AAT location would reduce the cumulative travel



Figure 5 | Location of olive mills with respect to municipal Karmiel WWTP and proposed location of decentralised AAT.

distance between all olive mills (based on the assumption of uniform OMWW production by each mill) by 26% thus reducing the overall fuel consumption for the transport of OMWW.

The three case studies have demonstrated the modelling of different CE applications. These applications could be further linked as a CE system that the outputs of one model could serve as inputs or complementary inputs to the other. An integrative model, that combines the three case studies can be applied to analyse the overarching CE system.

4. IMPLEMENTATION OF THE HYBRID MODELLING FRAMEWORK

An online decision support tool for a collective (such as a group of greenhouse farmers) requires a responsive interface that must be able to send back results to the user quasi-instantly. This requires an SDM to run in the background and compute the solution of a given problem on demand with minimum latency. Furthermore, some portion of a given model would have to be reused as a component in a different model later, so there is a need for a modular reusable structure. The simulation engine running the SDMs was therefore implemented in the Julia programming language (Bezanson *et al.* 2012), a recent scripting language with sufficient speed and flexibility to satisfy both requirements. As mentioned in Section 2, out hybrid modelling framework that integrates techniques from SDM and applied computer science (online platform, visualisation) is based on the Model-View-Controller architecture.

4.1. Design considerations for the UI

Experts in each case study have asked for the ability to visualise the impact of changes directly during a presentation, may it be online or via some in-person demonstration on a common screen. They also underlined the usefulness of being able to access the system from different devices ranging from a laptop to a smartphone so that participants might be able to concurrently explore different sets of operational parameters, compare possible outcomes and discuss pros and cons.

In response, an adaptive interface (shown in Figure 6) was developed allowing users with a sufficiently large screen to interact with a zoomable and pannable (i.e., ability to be moved as in a panorama) interactive map-board. Users with a very narrow screen can view the same information as a series of more 'smartphone-friendly' interactive tables with icon-based popup menus.

Note that there is also a system/options box that allows the user to mute audio voice comments and switch between the present 2D projection and an isometric projection of the interactive board. There is also a 'style' switch that allows to change



Figure 6 | The adaptive interface shows a zoomable/pannable board/map if the screen is sufficiently large (left), or folds to a smartphonefriendly table-based view with a popup menu if the screen is narrow (right).

from a 'corporate' visual style suitable for a business-oriented audience to a 'cartoon' visual style more relatable to the general public.

4.2. The juice factory UI (Greek case)

The juice factory interface has five input parameters (water quality, resources, operations, energy, and VACs) and a large results section as shown in Figure 7. In terms of water quality, users can change the required water quality in terms of COD and ToC (different usages such as irrigation, discharge, cooling or washing in the fruit juice factory will have different tolerances). The ability to change the quantity of consumables (such as resins and chemicals) involved in the treatment of the wastewater (such as for example changing the pH) and the VAC extraction process is paramount when considering cost reduction. The Greek VAC recovery technology is still at a pioneering stage. Therefore, operational parameters such as the flow rate of treatment, the probability of a disruption event, or the average recovery time after a disruption are crucial to informing any decision related to its adoption for full-scale deployment as an industrial process.

In the results section of the interface, a table visible in Figure 8 shows a cost-benefit analysis of VAC recovery wastewater filtration technology from the perspective of polyphenols extraction, water reuse, and related to energy and consumable expenditure.

4.3. The greenhouse UI (The Netherlands case)

The Netherlands greenhouse interface has input parameter areas connected to a large result section as shown in Figure 9. Users can change input parameters, i.e., increase/decrease yearly rainfall, the efficiency of the irrigation systems in use, change the surface area of the greenhouse, choose several types of crops to cultivate and their prevalences, as well as select their associated irrigation technology. In the results section of the interface, one can first see a small table visible in Figure 10 showing a cost-benefit analysis of the new treatment technology (ED) and compare it to the widely used treatment technology (reverse osmosis). Estimated costs of water supply, energy, and water treatment are shown for both technologies. Total costs are visible, as well as savings on fertiliser costs, and total savings.

Additional results are shown as animated charts to users:

- The average yearly use of rainwater,
- Treated drain water, and other sources (such as tap water),
- The nutrient levels in pre-treatment water as well as water quality before reuse and after discharge,



Figure 7 | A zoomed-out view of the different components in the Greek juice factory connected to a large results section.

/benefits analysis		Treated wastewater reuse potential
Costs	Benefits	Yearly volume of juice effluent treated:
Energy expenditure for	Value of Value Added	3,681,720 L/year
areatment: 39,210 €/year	Compounds obtained: 14,818,440 €/year	Treated water that is suitable for irrigation of fields: 3,681,368 L/year (100%)
Resin expenditure: 30,711 €/year	Maximum potential value of reusable water : 2,945,341 €/year	Treated water that is suitable for irrigation in greenhouses: 3,681,368 L/year (100%)
Hydrogen Peroxide expenditure: 2,107,136 €/year		Treated water that is suitable for cooling processes in fruit factor: 3,681,368 L/year (100%)
Sulphuric Acid expenditure 30,979 €/year		Treated water that is suitable for washing in fruit factory: 3,681,368 L/year (100%)
Sodium Hydroxide expenditure: <mark>3 C/year</mark>		Remaining treated water that is suitable for discharge to WWTP: 0 L/year (0%)
Total cost: 2,208,045 €/year	Net benefits: 15,555,736 €/year	Yearly volume of water that would rerquire further treatment or dillution prior to discharge: 352 L/year (0%)

Figure 8 | A view of the results part of the interface showing a cost/benefits analysis.



Figure 9 | A zoomed-out view of the different interactive components in the Netherlands greenhouse interface – three input areas (rainfall, irrigation efficiency inputs, and greenhouse cultivation parameters) are connected to a large results section.

Electrodialysis	Reverse osmosis
Water supply cost: 7,011 Euros/year (-77.4%)	Water supply cost: 31,029 Euros/year
Energy use: 588 kWh/year Water treatment cost: 418 Euros/year (-94.9%)	Energy use: 11,470 kWh/year Water treatment cost: 8,143 Euros/year
Total cost: 39,569 Euros/year	Total cost: 64,348 Euros/year
Fertiliser Saving: 1,003 Euros/year	
Total Saving: +25,783 Euros/year	

Figure 10 | Zooming on the cost/benefits analysis section of the results part of the interface showing energy, water, and fertilisers footprint when using electrodialysis (as opposed to reverse osmosis).

- Sankey diagrams that illustrate the flows of consumed and reused water and nutrients,
- The resulting quantity of fertilisers used and saved.

4.4. The olive mills UI (Israel case)

The Israel olive mills UI has five input parameters/areas (olive mills, wastewater transportation, wastewater treatment, seasonal scheduling, and mills selection and relocation) connected to a large results section as shown in Figure 11.

OMWW is highly toxic, only a limited amount can be spread on fields per hectare per year (users can set the amount spreadable on fields), and if discarded in water bodies without pretreatment, it can cause severe problems for the aquatic environment and can prevent normal wastewater treatment plants to function properly. Users are therefore being allowed to change parameters related to how concentrated the produced wastewater is through seasonal scheduling, and how it is transported and treated. There is also the possibility of creating a new abstract olive mill with new characteristics such as the distance to the Karmiel AAT plant, the distance to the new decentralised AAT plant, the daily wastewater production, and the olive fields area in order to evaluate changes in results such as transportation costs.

In the result section of the interface presented in Figure 12, one can first see a small table showing a cost-benefit analysis of the implementation of the AAT in Karmiel. This is contrasted with the new site located in an optimum location minimising the average travelling distance to all olive mills. Accumulated travelling distance, fuel consumption, and yearly fuel costs are displayed in both cases.



Figure 11 | A zoomed-out view of the different components in the Israeli olive mills industry connected to a large results section.

Accumulated distance: 3,816 kms/yearAccumulated distance: 1,604 kms/yearAccumulated fuel use: 1,247 L/yearAccumulated fuel use: 524 L/yearAnnual fuel costs per mill: 1,247 Euros/yearAnnual fuel costs per mill: 524 Euros/yearAnnual fuel costs: 2,096 Euros/yearAnnual fuel costs: 881 Euros/year	Karmiel	New Site		
Accumulated fuel use:Accumulated fuel use:1,247 L/year524 L/yearAnnual fuel costs per mill:Annual fuel costs per mill:1,247 Euros/year524 Euros/yearAnnual fuel costs:Annual fuel costs:2,096 Euros/year881 Euros/year	Accumulated distance: 3,816 kms/year	Accumulated distance: 1,604 kms/year		
Annual fuel costs per mill: Annual fuel costs per mill: 1,247 Euros/year 524 Euros/year Annual fuel costs: Annual fuel costs: 2,096 Euros/year 881 Euros/year	Accumulated fuel use: 1,247 L/year	Accumulated fuel use: 524 L/year		
Annual fuel costs: Annual fuel costs: 2,096 Euros/year 881 Euros/year	Annual fuel costs per mill: 1,247 Euros/year	Annual fuel costs per mill: 524 Euros/year		
(-58%)	Annual fuel costs: 2,096 Euros/year	Annual fuel costs: 881 Euros/year (-58%)		
Saving: 1,215 Euros/year		Saving: 1,215 Euros/year		
	igas generation & value Aud	,		
Biogas production VAC recovery	Biogas production	VAC recovery		
Biogas production VAC recovery Average daily BioGas Annual VAC Mass	Biogas production Average daily BioGas	VAC recovery Annual VAC Mass		
Biogas productionVAC recoveryAverage daily BioGasAnnual VAC Massproduction:Produced:	Biogas production Average daily BioGas production:	VAC recovery Annual VAC Mass Produced:		

Production	Treatment & disposal
Olive mill wastewater produced yearly: <mark>874 m3/year</mark>	Olive mill wastewater spread over fields yearly: 6 m3/year
olive mill wastewater that needs to be treated per year: 868 m3/year	Average volume of treated wastewater per year: 179 m3/year (20.60%)
Number of times per to COD alerts/year	year COD threshold is exceeded :

Wastewater treatment & disposal

Figure 12 | Zooming on the cost-benefits analysis section of the results.

Estimate annual value

of VACs obtained:

0 Euros/year

In the results section of the interface, a table visible in Figure 12 shows a cost-benefit analysis related to wastewater transportation, treatment and disposal, as well as associated biogas generation and possible VACs recovery as it can use the same filtration system as the juice factory.

Average annual BioGas

production:

1,505 m3/year

5. DESIGN OF THE INTEGRATIVE MODEL, THE METABOLIC NETWORK OF INDUSTRY INTERFACE, AND EXPERIMENTATION

To help with decision support in IS involving models from the three case studies seen above, a simulation engine running a hybrid model is created and is connected to a bespoke user interface, leading to explore the space of solutions via experimentation.

5.1. The integrative model

To create an integrative model (i.e., a combined model that captures the processes related to the three case studies) for capturing a metabolic network of industries, the outputs and inputs of respective models and a chain of operation should be considered. For example, with two hypothetical processes in a CE, process A and process B, treated water output from process A could be at a sufficient quality standard for use as input to process B; however, treated water from process B may not be at a sufficient quality standard for use as an input to process A.

Based on the water use and quality, and wastewater effluents of the three case studies, the proposed configuration chain is as follows: Juice factory \rightarrow Greenhouse \rightarrow Olive mills. In this configuration, treated water from the juice factories is assumed suitable for greenhouse irrigation, which becomes an alternative water supply for the greenhouses. The concentrated discharged wastewater from the greenhouses can then be mixed with domestic wastewater and OMWW, prior to treatment by the AAT facility. Wastewater from AAT processing is finally treated at a municipal WWTP. Figure 13 depicts the schematic layout of the integrated model being proposed. In this figure we see a simplified view of the three industries with intermediary storage tanks situated between them that provides an alternative source of water for the preceding model.

Having built a simulation engine running the SDMs, the next step is then to design a bespoke user interface that can support symbiosis decision making where whole businesses can join or leave. We refer to this combined interface as the metabolic network of industries interface, and which is discussed next.

5.2. The metabolic network of industries UI

The UI (as shown in Figure 14 and Figure S16, Supplementary material section) needs to enable users to:

- · Activate/deactivate industrial symbiotic links (via a series of clearly labelled switches),
- Visualise the resulting metabolic pathway of industries (activating different IS should show a different pathway graph)
- Change the scale of considered technologies (to explore the feasibility of a solution when going from experimental to production scale),
- In this hybrid model, we consider water availability, wastewater toxicity, potential benefits i.e. monetary value of saved water and other by-products as well as the avoidance of potential fines, and additional transport costs for olive mills wastewater.



Figure 13 | Schematic layout of the integrative model illustrating the chain of input–output operations for the juice factory, the greenhouse, and the olive mills.



Figure 14 | A zoomed-out view of the different components in the integrative model that shows a metabolic network of industries.

5.3. Experimentation

Users can choose to activate or deactivate the IS between the juice factory and the greenhouse (where the partially treated wastewater can be reused for irrigation), or between the greenhouse and the AAT treatment unit (where the wastewater discharged by the greenhouse can be used to dilute the highly toxic OMWW and facilitate downstream domestic wastewater treatment). Figure 15 shows two diagrams of what the resulting metabolic network of industries looks like when all industrial symbioses are activated as opposed to none. Table 3 lists how the outputs (water availability, wastewater toxicity, benefits, and additional transport costs) are impacted by four different ways of enabling IS between the juice factory, the greenhouse, and olive mills. Regarding additional transport costs, we hypothesise in our abstract case that they are negligible regarding wastewater transportation between the juice factory and the adjacent green house as IS usually arises from physical proximity, but that there is a distance of about 50 kms between the olive mill and the AAT plant where wastewater transportation needs to be done by road with trucks of average carrying capacity of 17 m³.

5.4. Deployment

The decision support tool, which is based on the hybrid modelling approach (Section 2), is comprised of a frontend web page (or client) that interacts with a remote server running the SDMs. The simulation engine consists of three models running concurrently in a Docker container, meaning that all the code, libraries, and dependencies are packaged in a self-contained virtualised unit that is easy to run on different systems without needing tailored installation.

The web programming technology is based on JavaScript open source visualisation libraries (such as D3js and MaterialUI) integrated within the React framework, an industry standard for creating reusable components for user interfaces. The modular aspect of the code allows us to easily create new variations of decision systems for future work.

Having learned lessons from the deployment experience of the past NEXTGEN project (https://nextgenwater.eu/), we have decided to avoid running the server through cloud services due to the prohibitive costs for long-term hosting (beyond 2 years), the complexity of the installation process, and the added maintenance work due to compulsory and unwanted 'upgrades' to the system. Instead, we have chosen to revert to hosting the platform on an Ubuntu Linux server, in the end, it proves to be an overall much simpler and more cost-effective solution.

6. RESULTS & DISCUSSION

Exploration via the user interface shows that the benefits obtained when considering each industry in isolation are somewhat different from the benefits obtained by enabling IS.

When looking at each industry separately:



Figure 15 | There are four different ways of enabling IS, of which two cases are illustrated; (top) when there is no symbiosis between the three industries – (bottom) when there is IS between the juice factory, the greenhouse, and the olive mills.

- The greenhouse case study shows (see Figure 10) substantial benefits in terms of water and energy savings can be shown (saving 70% of the water and 90% of the energy footprint linked to water treatment) while using the decision platform due to the use of ED as opposed to reverse osmosis.
- The juice factory case study shows that VAC recovery technology holds promise when extracting polyphenols from orange wastewater (with an estimated added value of 15 million euros/year for one factory as seen in Figure 8).

Table 3	Impacts on the	water availability,	wastewater t	oxicity, benefi	ts, and transportation	n costs caused b	y enabling IS	between t	he juice
	factory, the gre	enhouse, and the	olive mills						

	Water availability		Wastewater toxicity	Potential benefits	;		Transport costs
Symbiosis	Potential volume of treated water using GtG technology that is suitable for irrigation.	Volume of treated water from GtG used in greenhouse for irrigation.	Average COD of treated effluent from advanced anaerobic wastewater treatment	Water savings for greenhouse	Potential benefits from Value- Added Compounds	Potential avoidance of fines linked to toxicity of discharged wastewater	Additional wastewater transport costs from olive mill to AAT by truck (about 76 × 50 km long trips per year)
Juice factory Greenhouse Olive mills	3681.3 m ³ /year	2429.1 m ³ / year	922 mg/L	2,502 euros/ year	14,808,440 euros/year	yes	2,096 euros/ year
Juice factory Greenhouse Clive mills	3681.3 m ³ /year	2429.1 m ³ /year	1051.3 mg/L	2,502 euros/ year	14,808,440 euros/year	no	no
Juice factory Greenhouse Olive mills	3681.3 m ³ /year	0 m ³ /year	924.9 mg/L	2,502 euros/ year	0 euros/year	yes	2,096 euros/ year
Juice factory Greenhouse	3681.3 m ³ /year	0 m ³ /year	1045.6 mg/L	0 euros/year	0 euros/year	no	no

• The olive mills case study shows that the cost associated with the transportation and treatment of OMWW can also be significantly reduced when optimising the placement of a decentralised AAT plant (Figure 12).

When connecting all three previous case studies to explore the viability of a nascent 'metabolic pathway' of industries, what looks like initially modest benefits points towards potential gains of a greater magnitude. From the point of view of water availability, the decision support tool shows that enabling IS between the juice factory and the greenhouse increases the amount of reused wastewater, and therefore lowers the overall consumption of surface and tap water. IS also shows promise to lower the toxicity of the wastewater discharged to domestic WWTPs (by using partially treated wastewater from another source to dilute olive mills discharges) in the case of olive mills. There are probably many possible similar ways to use partially treated wastewater to lower the toxicity of discharges in other industries and hence avoid potential fines or penalties.

If each industry is a node that can be linked by IS to other nodes or industries (by reusing locally available by-products), greater benefits start to appear when increasing the number of connected nodes.

If industries (or connected nodes) within a catchment are all reusing wastewater discharged by each other, the sum of the volumes of wastewater reused by each node will rise dramatically and easily surpass the total volume of freshwater abstracted from the river. With a growing number of connected nodes, IS would greatly increase efficiency not only in term of water reuse, but also for other by-products such as nutrients, heat, and materials. Metals, for example, have a high potential as reusable by-products due to their high concentration in domestic wastewater and continuously increasing thermodynamic rarity (the energy required for mining a mineral from the earth core, as well as smelting and refining it). Concentrations of metal in

domestic wastewater shown in Appendix Table 4 built from literature (Sewage sludge management in Germany 2013; Westerhoff *et al.* 2015) can potentially rise from 1 to 4 orders of magnitude when mixing with industrial wastewater. Reusing metals found in runoff water in a metabolic network of industries could become for example a potent way to lower carbon emissions.

7. CONCLUSIONS

The web-based decision co-creation platform shows substantial advantages from a water, energy, and nutrient reuse perspective to making use of ED in the case of a greenhouse. Similarly, the use of VAC recovery technology shows a reduction in overall water footprint due to the capability to reuse some of the partially treated water discharged by the juice factory, and presents a significant opportunity to extract expensive VACs at a reasonable cost. This technology can also be used to greatly reduce the high toxicity of OMWW using AAT in a cost-effective way.

These three separate examples of industrial activities, when linked together in the decision support tool, interconnected by the physical exchange of materials, water, and other by-products – help users uncover the usefulness of what might be the basis for a metabolic network of industries (as in biology where metabolic reactions produce different compounds reused by other reactions).

The potential for IS is not just limited to the exchange of water or wastewater, but also heat, nutrients, metals and all sorts of local by-products. The resource efficiency of such a metabolic network of industries is also very likely to grow significantly with the number of industrial nodes connected.

As future work, we intend to go beyond the scope of the ULTIMATE project and present the co-creation decision platform to major actors in the pharmaceutical and food industries in Europe, as well as farmers, and see if they can be engaged into starting a nascent metabolic network of industries based on water reuse and nutrients, metals, and VAC recovery.

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DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

CONFLICT OF INTEREST

The authors declare there is no conflict.

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