2 AI SCENARIO METHODOLOGY

The methodology employed in Task 3.3 builds upon a sequential process of **mapping, stakeholder validation, experimental implementation, and scenario-based assessment**. The design of SureNexus foresees that the identification of NBS and BES in WP3 and WP4 provides the initial portfolio of options to be discussed with stakeholders, while the **results from the demonstration pilots (WP6) feed into the definition of Socio-Ecological and Technical Systems (SETs)**. These SETs, in turn, are further analysed through Artificial Intelligence (AI)–based scenario modelling in the present deliverable.

In this process, Deliverables 3.1 and 4.1 first provided a comprehensive mapping of potential solutions, creating a broad catalogue of practices for consideration. Deliverables 3.2 and 4.2 then established the methodology for identifying, proposing, and selecting a robust, prioritized set of practices, which were validated in stakeholder workshops (consolidated in D4.3).

The identification, validation, and scaling of "smart solutions", understood as best practice solutions in the WEFE Nexus require approaches that are not only technically sound but also socially robust and contextually relevant. **Co-creation through participatory methodologies ensures that multiple perspectives—scientific, technical, institutional, and community-based—are integrated into decision-making processes**. By **actively involving stakeholders**, solutions are more likely to reflect local needs, build ownership, and enhance legitimacy, thereby increasing the likelihood of successful adoption and long-term sustainability.

In the SureNexus project, **co-creation is operationalized through a combination of participatory tools and advanced digital innovations**. In this section, we introduce four core participatory processes that provide the methodological foundation for planning and management within the WEFE Nexus Framework. Together, they create a transparent, evidence-based process that links stakeholder priorities to model-supported decisions and implementation roadmaps:

Multi-Criteria Assessment (MCA): Following a careful **mapping of bioeconomy options and Nature-based Solutions (NbS),** a participatory MCA was conducted to enable stakeholders to evaluate and prioritize practices against a shared set of criteria (e.g., water productivity, energy intensity, climate resilience, cost-effectiveness, GHG reduction, biodiversity co-benefits, social acceptance, and implementation risk). The MCA yields a **ranked shortlist of best practices**, with explicit trade-offs and justifications that can be tracked through subsequent planning phases.

Conceptual AI Model Co-development with SDL and Assumptions Document: Through structured co-creation sessions, stakeholders and experts jointly define the conceptual modelm, through the defintion of the system boundaries, blocks and processes, data sources, decision rules and constraints. These inputs are formalized in an Assumptions Document jointly developed by all stakeholders, and translated into a diagram flow formal language, using Specification and Description Language (SDL), that provides a common, visual language that makes complex WEFE interactions intelligible to non-technical audiences and directly feeds the computerized model.

Computerized model validation through SDLPS: simulation and optimization. SDL diagrams are implemented in SDLPS, which compiles the processes and signals into executable hybrid model,s that are iteratively validated in decision labs using participatory dashboards. Stakeholders review scenarios, test sensitivities, and agree on implementation pathways and KPIs. This “validate-as-you-go” approach improves trust, reduces model uncertainty, and accelerates convergence toward feasible, widely supported actions.

Digital twin with NECADA: from plan to operations. Necada is the optimization software where the final SDLPS computerized validated model for WEFE Nexus is running, to execute simulations on desktop, cluster or cloud infraestructure to explore design parameters using different solutions (NbS or BES) and find optimal configurations for WEFE NEXUS metrics.

In summary, these four tools—MCA, SDL-based co-design for conceptual model, computerized model validation using SDLPS and living-lab optimization in a Digital Twin based in NECADA— mutually reinforce one another: MCA aligns priorities, SDL formalizes the system logic, SDLPS is used for participative validation of the model, and the digital-twin process stress-tests choices with stakeholders before decisions move to implementation. All details from this roadmap are fully described in Deliverabie 7.4.

Together, **these approaches establish a dynamic environment in which knowledge co-production is continuously fostered, bridging the gap between science, policy, and practice.**

Milestone 6.3, under WP6, described the experimental schemes of the Demosites, building upon the solutions identified in WPs 3 and 4. It defined the set-up of pilots, allocation of responsibilities among partners, and expected outcomes of each intervention. For example, in Spain, the scheme foresaw the installation of cork-based constructed wetlands for winery effluents and polluted groundwaters, with monitoring of pollutants, nutrient recovery and reuse of cork by-products. In Greece, the scheme described the integration of a solar desalination unit with a tropical greenhouse and an eco-tourism lodge. In Israel, the scheme highlighted the establishment of agrovoltaic fields combining solar panels with agricultural crops and fishponds.

In Deliverable 3.3, these experimental insights are **fully analysed in detail at the technological scale**. The **final integrated assessment, including socio-economic costs as well as policy and governance aspects, is presented in Deliverable 6.2.** This deliverable defines and consolidates the final Socio-ecological and Technical Systems improved under the WEFE Nexus framework, considering all scenarios assessed.

2.1 Multi-Criteria Assessment (MCA) framework

The Multi-Criteria Assessment (MCA) methodology applied in SureNexus is **described in Deliverable D3.2**. This document defined the MCA as a participatory tool to support the prioritisation of Nature-Based and Bioeconomy Solutions (NBS/BES). The MCA framework covered eight main criteria—**water, energy, food, ecosystems, social, economic, climate, and institutional**—further divided into forty sub-criteria to capture local specificities. Each solution was assessed through stakeholder scoring against these criteria, using a structured tool that generated weighted scores and visual outputs.

The MCA process was implemented through three main steps:

1. **Internal design** of the methodology and refinement of the list of candidate NBS and BES.
2. **Consultation with Demo Site leaders and stakeholders** to customise the tool for local contexts, including the definition of criteria weights and sub-criteria.
3. **Participatory workshops**, where stakeholders applied the tool to assess and prioritise solutions.

During the workshops, stakeholders were guided through a stepwise process: selecting relevant solutions, assessing them against predefined criteria, assigning relative importance through weighting, and generating aggregated scores and rankings. This participatory approach enhanced transparency, built legitimacy, and allowed the integration of local knowledge into the assessment process.

The aggregated MCA results for each Demo Site are presented in **Deliverable D4.3**, where only solutions surpassing the **threshold score of 50** were retained. In the present deliverable (**D3.3**), the MCA is not re-described in detail. Instead, we take as input the **three top-ranked solutions per site from D4.3**, which serve as the basis for the **AI-based scenario analysis**. Selected indicators from previous assessments (e.g. LCC, S-LCA) are also used as benchmarks to verify the AI outputs, ensuring methodological consistency across work packages.

For details of the MCA design and rationale, see D3.2 and D4.2. For site-specific MCA results and prioritised solutions, see D4.3.

2.2 Criteria and sub-criteria applied (WEFE Nexus perspective)

The MCA framework is built on eight main criteria, grouped into two overarching categories:

- WEFE Nexus dimensions: water, energy, food, and ecosystems.
- Sustainability and impact dimensions: social, economic, climate change, and institutional factors.

These eight criteria were selected to ensure that proposed solutions contribute not only to sectoral performance but also to broader sustainable development and climate resilience goals.

Each criterion was further operationalised through a set of sub-criteria, capturing local priorities and cross-sectoral interactions. For example:

- Water: storage, reuse, savings, wastewater treatment.
- Energy: efficiency, savings, renewable diversification, autonomy.
- Food: improved crop production and resilience, reuse of organic waste, traditional practices.
- Ecosystems: runoff reduction, restoration, biodiversity, soil quality.
- Social: food security, social acceptance of reuse, health, collective activities.
- Economic: revenue opportunities, cost reductions, circular economy approaches.
- Climate change: availability of water in droughts, reduced flood and fire risk, GHG emission reduction, microclimate regulation.
- Institutional: participatory governance, policy integration, mainstreaming of NBS/BES in local planning.

In total, forty sub-criteria were defined, enabling a fine-grained assessment of technical, environmental, social, and governance aspects. By combining these dimensions, the MCA framework ensures that prioritised NBS and BES provide co-benefits across the WEFE Nexus, support climate adaptation, and contribute to systemic transformation in the Mediterranean context.

For a full description of the methodology, the complete list of criteria and sub-criteria, and their rationale, readers are referred to Deliverable 3.2 (SureNexus, 2024).

Deliverable 6.2 introduced an additional layer of methodological robustness by applying a sustainability assessment framework that combined LCA, LCC, S-LCA and CBA. This deliverable emphasized that the evaluation of solutions could not be restricted to technical efficiency alone, but needed to account for economic feasibility, social acceptance and broader environmental impacts. In its executive summary, D6.2 stated that “the project employed Life Cycle Assessment (LCA), Life Cycle Costing (LCC), Social LCA (S-LCA) and Cost-Benefit Analysis (CBA) to evaluate sustainability dimensions, while M6.3 documented the participatory selection of NbS and BeS through Multi-Criteria Analysis (MCA).” By triangulating these methodologies, the qualification of best solutions was evidence-based and multidimensional. For the cost–benefit analysis, the appraisal employed a social discount rate of 5% and a multi-decade project lifetime in line with established guidance (Guide to Cost-Benefit Analysis of Investment Projects of the EC, 2014; Rathore et al., 2022).

The Stakeholder Platform (SHP) represented a transversal component of the methodology. As the SHP Guidelines (2025) underline, “the SHP plays a pivotal role in gathering data from its members and their local partners, validating analytical outcomes, and establishing pathways for sharing results and impacts across the region.” Members of the platform, including local producers, utilities, NGOs, research centers and government representatives, were engaged in the process of validation at multiple stages. Regular meetings at the national and regional levels were outlined in the SHP Roadmap as a means of exchanging preliminary findings, coordinating expectations, and gathering input. This ongoing discussion not only increased the project's legitimacy but also offered vital information about the opportunities, obstacles, and enabling factors for replication.

The methodological contributions of WP5, which examined enabling conditions for the adoption of SETs, were finally incorporated into Deliverable 6.2. These included institutional arrangements, financial incentives, regulatory tools, and policy frameworks. As mentioned before, Deliverable 6.2 was able to pre-define a set of SETs that are not only technically sound but also socially acceptable and institutionally feasible by integrating the data from WP3, WP4, and WP6 with the governance insights from WP5 and the participatory processes of WP7.

The project methodological framework also incorporated the examination of governance and policy aspects. The evaluation took into account the institutional frameworks mentioned in Deliverables 7.2 and 7.3 in addition to the life-cycle and economic tools previously mentioned. Deliverable 7.2's knowledge brokerage framework, which placed an emphasis on capacity-building, participatory approaches, and the creation of a digital stakeholder platform, served as the foundation for determining whether the solutions had political and social support.

By methodically examining the policy and regulatory environment across sites, Deliverable 7.3 completed this approach and ensured that the technical and economic results of WP3 were interpreted in the larger context of enabling or constraining governance conditions. The inclusion of this policy layer in the methodology ensures that the lessons learned are not just based on financial viability or technical feasibility, but also take into account the institutional and policy realities that ultimately determine replicability.

2.3 Criteria AI-driven approach to scenario analysis

Within the WEFE Nexus, the systematic identification and analysis of **trade-offs** is essential to reveal conflicts across water, energy, food, and ecosystems, quantify their impacts, and inform strategies that balance objectives or convert conflicts into synergies. **Trade-offs** describes an inherent conflict between objectives: improving performance in one dimension tends to worsen another. In the WEFE Nexus, classic examples include raising nutrient removal at the cost of higher energy demand, or increasing irrigation reliability while depleting local aquifers. Trade-offs map the feasible frontier of a system and must be recognized, quantified, and managed; they do not disappear on their own.

In the SureNexus context, **compensation** refers to design and operational mechanisms that maximize system-wide efficiency and reduce environmental impact by redeploying underused resources. In practice, it involves **reusing or redistributing surplus or residual flows—energy, water, nutrients, and by-products—within or across processes** to meet other needs on-site or nearby.

A compensation may consist of a **single technology** (e.g., heat recovery, anaerobic digestion) or a **composite process** that combines multiple technologies, operations, and activities. Its purpose is to create a **synergistic balance within the Water-Energy-Food-Ecosystem (WEFE) Nexus**, optimizing resource use by transforming outputs or surpluses from one area into valuable inputs for another, thereby increasing overall efficiency and sustainability.

The central goal is to **maximize the intelligent use of available resources** to lower consumption and minimize environmental impacts. This is achieved by:

(i) reusing or redistributing leftover or unused energy and resources within a system;

(ii) mitigating negative impacts—or enhancing benefits—in one element of the nexus through the efficient management of another; and

(iii) **converting potential problems** (such as waste) **into solutions** (such as energy or nutrients).

Ultimately, a compensation is a **practical mechanism** for mapping and managing interconnections among key resource flows. It prioritizes system-wide efficiency, loss reduction, and smart flow management—helping transform liabilities into assets and supporting long-term socioecological sustainability, even when not all resources are generated in-house. In this sense, a compensation serves to represent and quantify the interconnections and exchanges between vital resources. It is fundamental for designing strategies that address resource scarcity and ensure long-term socio-ecological sustainability.

Trade-offs are system-level conflicts revealed by analysis; compensations are the technologies and processes we deploy to mitigate those conflicts and, where possible, convert them into synergies.

Accordingly, the SureNexus project developed a **Compensation Block**—a decision-support module that identifies and prioritizes context-appropriate alternatives (solutions, practices, and technologies) across the WEFE Nexus, tailored to each demonstration site. Initial application scenarios include: (a) selecting the most effective water treatment; (b) recovering and conserving energy; and (c) recovering and valorizing agricultural bioproducts.

For the selection of solutions implemented in the compensation block, preliminary databases were developed where the main technical parameters for each of the aforementioned cases (water, energy, bioproducts) were defined, and integrated within the NECADA software, in different compensation lists including the main solutions related to water, energy, and bioproducts (https://necada.com/compensations), including the name of the selected compensation, along with a brief description, the cost, and associated maintenance cost.

The preliminary databases were fed with the solutions previously determined with a participatory methodology developed under the SureNexus project, the Multicriteria Assessment tool (MCA), to assess the potential contribution of each Solution to the WEFE Nexus approach including the **8 principal dimensions of the WEFE Nexus: Water, Energy, Food, Ecosystem, Social impact, Economic impact, Climate change impact and Institutional impact** This methodology has been incorporated into an on-line NBS/BES tool[1] that allows assessing and selecting practices and technologies appropriate to local contexts.

[1] NbS/BeS tool, https://tool.surenexus.eu/page0.html

In parallel, these criteria are encoded in the NECADA Digital Twin, which runs scenario simulations to explore design parameters across alternative interventions (e.g., Nature-based or bio-engineered solutions) and to optimize WEFE-Nexus performance metrics. Once the top options are identified, the module quantifies cross-dimension “compensations” (trade-offs and synergies), formalizes the linkages among Water, Energy, Food, and Ecosystems, and enables stakeholder-driven stress-tests—examining sensitivity, robustness, and failure modes—so choices are validated and de-risked before implementation.

The SureNexus **AI WEFE Nexus Tool** was co-designed with stakeholders (as explained in detail in Deliverable 7.4), from day one and is continuously co-developed and validated through iterative cycles. Communities, utilities, farmers, regulators, and researchers co-define objectives, assumptions, data sources, and KPIs, ensuring the model reflects real constraints and priorities—not just theory. Each iteration captures new evidence (sensors, costs, policies), updates the assumptions document, and revalidates outputs in workshops, making the tool both scientifically rigorous and socially legitimate.

This participatory pipeline turns complexity into clarity: it reveals where consensus exists, where risks remain, and which configurations perform best under uncertainty. By coupling codesign with living documentation and repeatable stress-tests, SureNexus AI WEFE NEXUS Tool delivers decisions that are technically sound, context-aware, and implementation-ready.

2.4 Compensations Data Base in Necada Digital Twin

NECADA is an advanced computational modelling platform designed by Inlab research group at UPC with the collaboration of the UNESCO Chair on Sustainability, to evaluate, simulate, and compare sustainable solutions across the Water–Energy–Food–Ecosystems (WEFE) Nexus. Built around a multi-agent system and powered by artificial intelligence, NECADA integrates environmental, technical, and socio-economic parameters to assess the performance of nature-based solutions, bioeconomy practices, and technological interventions under different scenarios. The platform provides quantitative outputs—including energy generation or consumption, greenhouse-gas mitigation, water storage, biomass and crop production, and pollution removal—allowing users to visualise trade-offs, identify synergies, and support evidence-based decision-making.

The **AI WEFE Nexus tool Digital Twin (DT) permits rigorous comparison of alternative technologies via the Compensation Block**. Through the Compensation Block, NECADA enables users to design tailored combinations of solutions adapted to local contexts, thus positioning NECADA as a versatile tool for planning, optimisation, and demonstration of integrated Nexus strategies.

The NECADA Digital Twin's compensation view delivers a standardised, side-by-side assessment across harmonized WEFE metrics, quantifies trade-offs and synergies, applies stakeholder weightings, and aggregates outcomes into a balanced, decision-ready score that can be stress-tested across scenarios and uncertainty.

The **AI WEFE Nexus Tool uses these databases to compare solutions** within an end-to-end decision environment that integrates heterogeneous datasets—hydrology, energy use, agronomic data, costs, and environmental indicators—into a single, traceable, and fully auditable workspace. Through Digital Twins, the platform applies predictive analytics to forecast demands, emissions, and ecosystem responses under varying climate, policy, and operational conditions, with all assumptions, formulas, and data sources fully versioned to ensure complete reproducibility. Deliverable 7.4 provides a detailed overview of the AI WEFE Nexus Tool's capabilities regarding the NECADA Compensation Database, including data integration, predictive analytics, scenario modelling, resource optimisation, and impact assessment.

Considering the pre-selected solutions for each demonstration site (Figure 1), the required information was incorporated into the NECADA Compensation tool. Initially, the aim was to **test three solutions for each of the four demosites (12 solutions in total).** However, by the end of the project we had evaluated 37 different solutions, each adapted to the specific context and characteristics of the respective demosite. Figure 7 shows the NECADA interface where all tested compensation options are available and can be executed for simulation and scenario comparison.

FIGURE 1. PRORITISED SOLUTIONS SELECTED IN THE PARTICIPATORY PROCESS FOR EACH DEMOSITE.

From the 37 final solutions tested, 20 correspond to Nature-Based Solutions for water treatment and supply, 5 correspond to bioeconomy-oriented solutions, and 12 are energy solutions, primarily involving solar panels designed to compensate for and reduce GHG emissions compared to grid-based systems.

Table 1 details the final solutions and practices (named in the AI WEFE Nexus as compensations), tested in each demonstration site, grouped as follows: A) Water Treatment (in blue) and B) Bioeconomy (in orange). The NECADA code shown corresponds to the final identification number assigned to each solution within the Compensation Block of the NECADA Digital Twin.

In this deliverable, we focus on the **bioeconomy solutions** that were tested, while presenting a **methodological approach that is common to all types of solutions** assessed in the project. The detailed analysis of the results for **water treatment solutions and practices** is provided separately in **Deliverable 6.2**, to avoid duplication and ensure a more in-depth discussion of each thematic block.

It is important to stress that compensation databases in SureNexus are **living assets** that are continuously updated to reflect new evidence, changing contexts (rural/urban, arid/temperate), and application scales (unit, facility, basin). In line with the project’s open-science ethos, all non-sensitive knowledge should be **free and openly accessible** to stakeholders across sectors.

Living, open compensation databases

While the conceptual model developed in SureNexus is ultimately **a single integrated WEFE Nexus model**, it has been designed to operate under a **wide range of conditions and contexts**. To achieve this, the model incorporates a **final fine-tuning step through the use of a compensation block**, which can be configured—or kept unchanged—depending on the local context, **allowing the integration of locally adapted solutions and practices**.

The key advantage is that the **compensation block is structurally separated from the core model**. It behaves as an independent module that can be modified without changing the general architecture. By adjusting this block, we can:

- Incorporate **site-specific parameters** and constraints (climate, crops, technologies, socio-economic conditions, etc.),
- Represent **alternative solutions or scenarios** for comparison, and
- Calibrate the model to **any demonstration site or new context** beyond the original demos.

In practice, this modularity means that the **core WEFE Nexus model remains stable and comparable across sites**, while the compensation block provides the necessary flexibility to adapt the simulations to diverse realities and explore different compensation strategies.

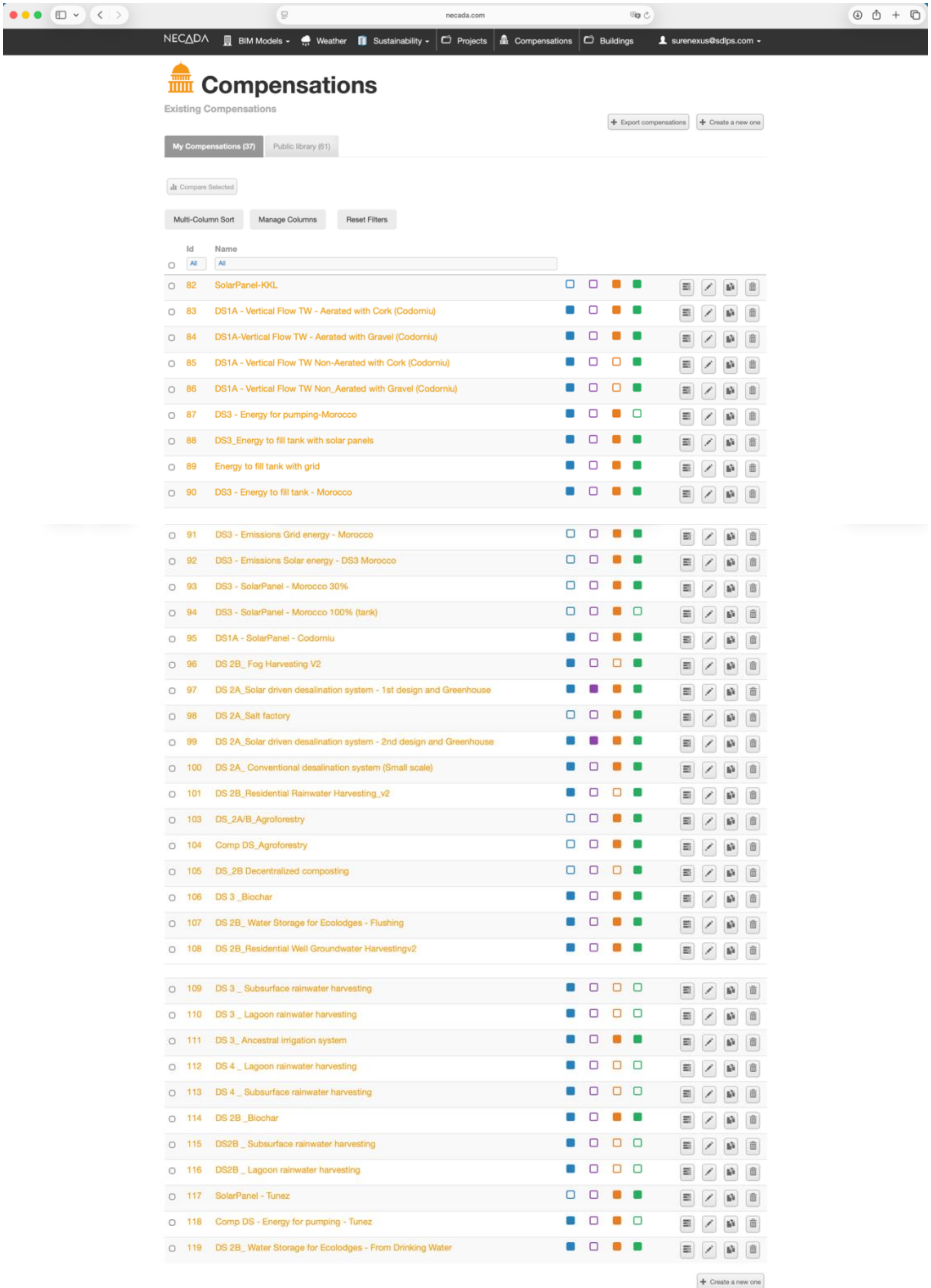

FIGURE 2. ARRAY OF COMPENSATIONS FINALLY TESTED IN THE NECADA COMPENSATION DATABASE.

Table 1. Final solutions and practices tested in each demonstration site, grouped as follows: A) Water Treatment (in blue) and B) Bioeconomy (in orange). The NECADA code shown corresponds to the final identification number assigned to each solution within the Compensation Block of the NECADA Digital Twin.

Compensation	NECADA	DS1A Codorniu DS1B Torre Marimon	DS2A Agios Fokas Greece	DS2B Tinos Ecolodge Greece	DS3 INRA Morocco	DS4 KKL Israel	CompDS Tunisia
Vertical Flow TW Aerated with Cork	83	Tested Ok					
Vertical Flow TW Aerated with Gravel	84	Tested Ok					
Vertical Flow TW Non-Aerated with Cork	85	Tested Ok					
Vertical Flow TW Non-Aerated with Cork	86	Tested Ok					
Residential Rainwater Harvesting	101		Tested Ok			Tested Ok	
Residential Well Groundwater	108		Tested Ok			Tested Ok	
Subsurface Rainwater Harvesting	115(DS2B) 109(DS3) 113(DS4)			Tested Ok	Tested Ok	Tested Ok	
Underground Irrigation	csv						Tested Ok
Lagoon Rainwater Harvesting	110		Tested Ok	Tested Ok	Tested Ok	Tested Ok	Tested Ok
Ancestral irrigation systems	111				Tested Ok	Tested Ok	
Solar driven vapour condensation 1^{st} design	97		Tested Ok		Tested Ok		
Solar driven vapour condensation 2_{nd} design	99		Tested Ok		Tested Ok		
Salt Factory	98		Tested Ok		Tested Ok		
Conventional Desalination System RO	100		Tested Ok		Tested Ok		
Water Storage (for Ecolodge, flushing)	107			Tested Ok			
Water Storage (for Ecolodge, irrigation)	119			Tested Ok			
Fog harvesting	96			Tested Ok			
Agroforestry	103(DS2AB) 104 (Tun)		Tested Ok	Tested Ok	Tested Ok		Tested Ok
Conservation Agriculture (mulching)	csv				Tested Ok		
Biochar application	114(DS2B) 106(DS3)			Tested Ok	Tested Ok		
Decentralized composting	105(DS2B)			Tested Ok			

2.5 Experiments and Scenarios Definition in Necada

Once the computerized model has been validated by the different stakeholders and calibrated with real data (a process described in detail in Deliverable 7.4), and once the context-specific compensation options have been defined, the next step is to **test the key challenges previously identified by all stakeholders**. At this stage, the power of AI lies in the ability of the WEFE Nexus model to support decision-making in the following four main areas:

A) **Scenario Modelling & Simulation**. Anticipates outcomes from changes in water allocation, variations in agricultural yields, or modifications in energy production under different climatic or political conditions.

B) **Resource optimization**. Identify optimal strategies for sustainable allocation and management.

C) **Impact Assessment**. Evaluates the environmental and socio-economic impacts of any project.

D) **Dialogue Facilitation**. Provides an objective basis for dialogue on shared trade-offs between countries, facilitating collaborative decision-making

The images in Figure 3 and Figure 4 illustrate the **sequential workflow for configuring and executing a WEFE Nexus experiment** within the NECADA AI digital twin platform. The process begins in the *Projects* section, where the user creates a new project or selects an existing one. At this stage, the platform captures the basic metadata that defines the experiment's context, including the project name, description, geographical or thematic scope, and the type of WEFE Nexus intervention to be analysed. This establishes the **core environment from which experiments and compensation blocks will be managed.**

Once the project is created, the next step is to associate it with the relevant compensations selected from those previously defined in the Compensation Block. This module contains the comprehensive database of nature-based solutions and bioeconomy practices available in the system. By linking the project to the appropriate compensations, the model activates the specific parameters, processes, and performance metrics associated with each solution, ensuring that the subsequent simulations reflect the real operational behaviour and expected Nexus impacts of the selected practices.

Once the project is created, the next step is to **associate it with the relevant compensations selected from those previously defined in the *Compensation Block***, where a data base with the nature-based solutions and bioeconomy practices are located.

The Compensation Block is a modular add-on, external to the core WEFE model, that allows the user to adapt the simulation to specific local conditions—such as alternative technologies, resource constraints, environmental parameters, or socio-economic settings.

Through the interface, the user can browse existing compensations, **select one or several (group-compensation scenarios),** or create new ones. This modular design provides high flexibility: any scenario can be customised by combining compensations that best represent the intended intervention or context.

Once the project is created, the next step is to **associate the relevant compensations chosen from all the previously defined in the compensation block** (Figure 3, lower part). Compensation block is a modular add-ons external to the core WEFE model that allow the user to adapt the simulation to specific local conditions—such as alternative technologies, resource constraints, environmental parameters, or socio-economic variations. The interface allows the user to browse existing compensations, select one or more compensations (in a group compensation scenario), or create new ones. This modular design provides flexibility: any scenario can be customised by combining compensations that best represent the intended intervention or context.

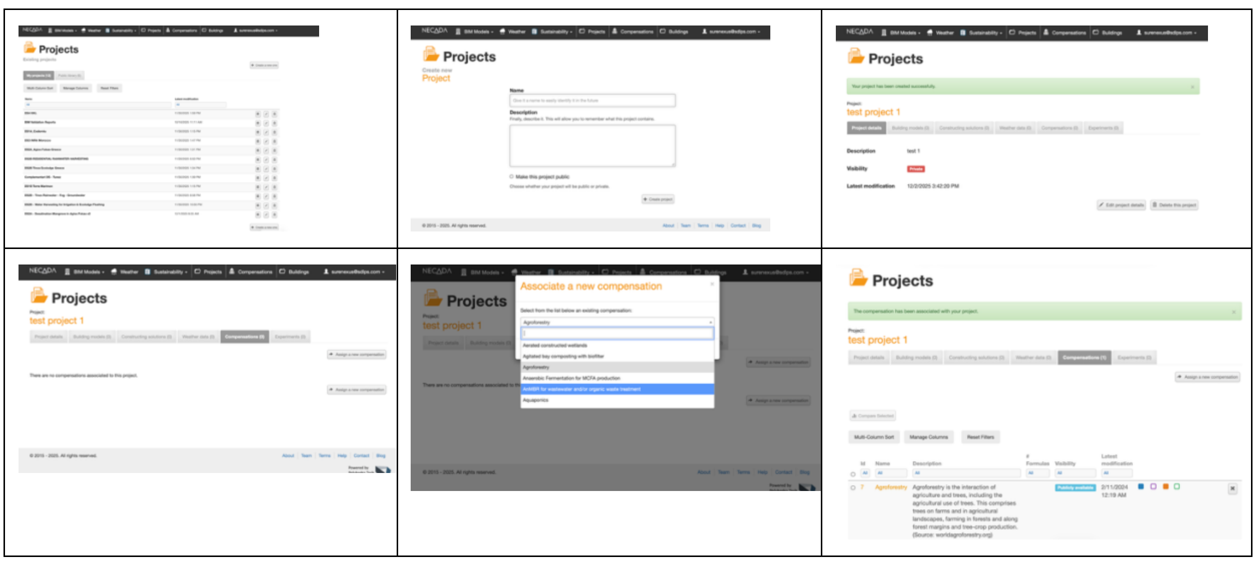

FIGURE 3. STEPWISE PROCEDURE FOR CONFIGURING AND RUNNING NECADA AI WEFE NEXUS EXPERIMENTS USING COMPENSATION BLOCK. PART I, PROJECT CREATION AND LINKING TO REQUIRED COMPENSATIONS.

After associating the compensations, the workflow continues in the **Experiments** tab, where the user defines the actual simulation experiment (Figure 4). In this section, the user specifies the parameters to be tested, including the selected compensations, the experiment description, and its objectives.

A complementary area for input data entry, called **Farm**, is also available. Here, site-specific information related to the four WEFE Nexus dimensions (food, water, energy and, ecosystems) is uploaded in CSV format. The most relevant datasets typically include:

I. **Crop** – yield and production data.
II. **Kc** – crop coefficients for each plant type.
III. **Fertilizer** – quantities and types of fertilizers applied.
IV. **Temperature** – all variables required to compute potential evapotranspiration, including temperature, precipitation (maximum, minimum, and average), and extraterrestrial radiation.
V. **Wastewater** – source water quality data, including key pollutants such as nitrogen, COD, BOD, etc.

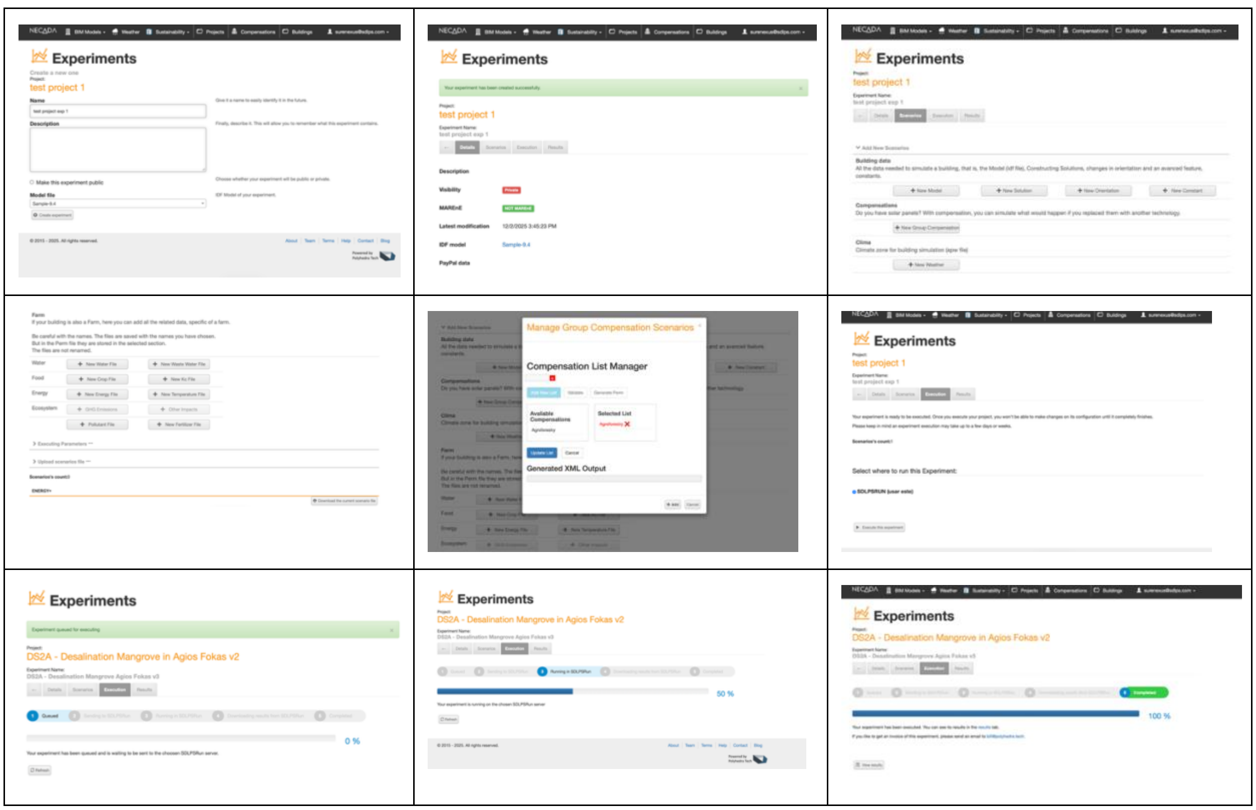

FIGURE 4. STEPWISE PROCEDURE TO CONFIGURE AND RUN NECADA AI WEFE NEXUS EXPERIMENTS USING COMPENSATION BLOCKS

Following experiment definition, the system moves to the **scenario management interface**, where each compensation scenario can be individually adjusted. Users can modify values inside a compensation block, load alternative blocks, or verify that all required inputs are consistent with the underlying digital twin model. NECADA automatically validates compatibility between the core model and the chosen compensations, ensuring that the experiment is correctly parameterized before running the simulation. This step is essential because it guarantees that the model is aligned with the specific conditions the user wants to explore.

Finally, once everything is configured, the user launches the simulation. The last images in the sequence show the **progress bar and the execution status**, which evolve as NECADA processes the compensation-enhanced model. When the run reaches 100%, the **simulation results become available for analysis—allowing the user to compare scenarios**, **evaluate the performance of different compensation strategies, and extract the WEFE Nexus indicators needed for decision-making**. This stepwise approach ensures that experiments are transparent, reproducible, and fully adaptable to different environmental and operational contexts.

The **computation time** depends mainly on the number and complexity of scenarios tested. As a reference, a typical batch of simulations can be completed in **around 20 minutes** when executed via the web interface. Running the model on a local computer can reduce this time, but the web-based execution offers important advantages in terms of **accessibility, scalability, and collaborative use**: multiple users can launch experiments from different locations, results are stored in a common environment, and hardware requirements on the user side are minimized.

On top of this data foundation, the tool supports scenario modeling and resource optimization. Users can compare Nature-based and bio-engineered solutions, stress-test them against uncertainty, and evaluate trade-offs and synergies across Water-Energy-Food-Ecosystems KPIs. Multi-criteria analysis helps rank portfolios by cost, performance, and risk, while the compensation logic quantifies cross-dimension effects to maintain WEFE balance.

2.6 Results Analysis

In the **Results** section, a selector at the top allows the user to choose the type of output to be displayed and immediately visualise all results in HTML format (Figure 5, upper part). Just below this selector, a button enables the **download of all digital data generated by the AI WEFE Nexus model, including all CSV files and the corresponding** trace.xml files. With this information, any additional post-processing, analysis, or visualisation can be carried out using external tools (e.g. spreadsheets, statistical software, or figure graphical software). Below the download button, all **permutations—representing the different scenarios tested**—are listed in detail, together with information on the associated files, including the CSV inputs and the compensations applied in each case.

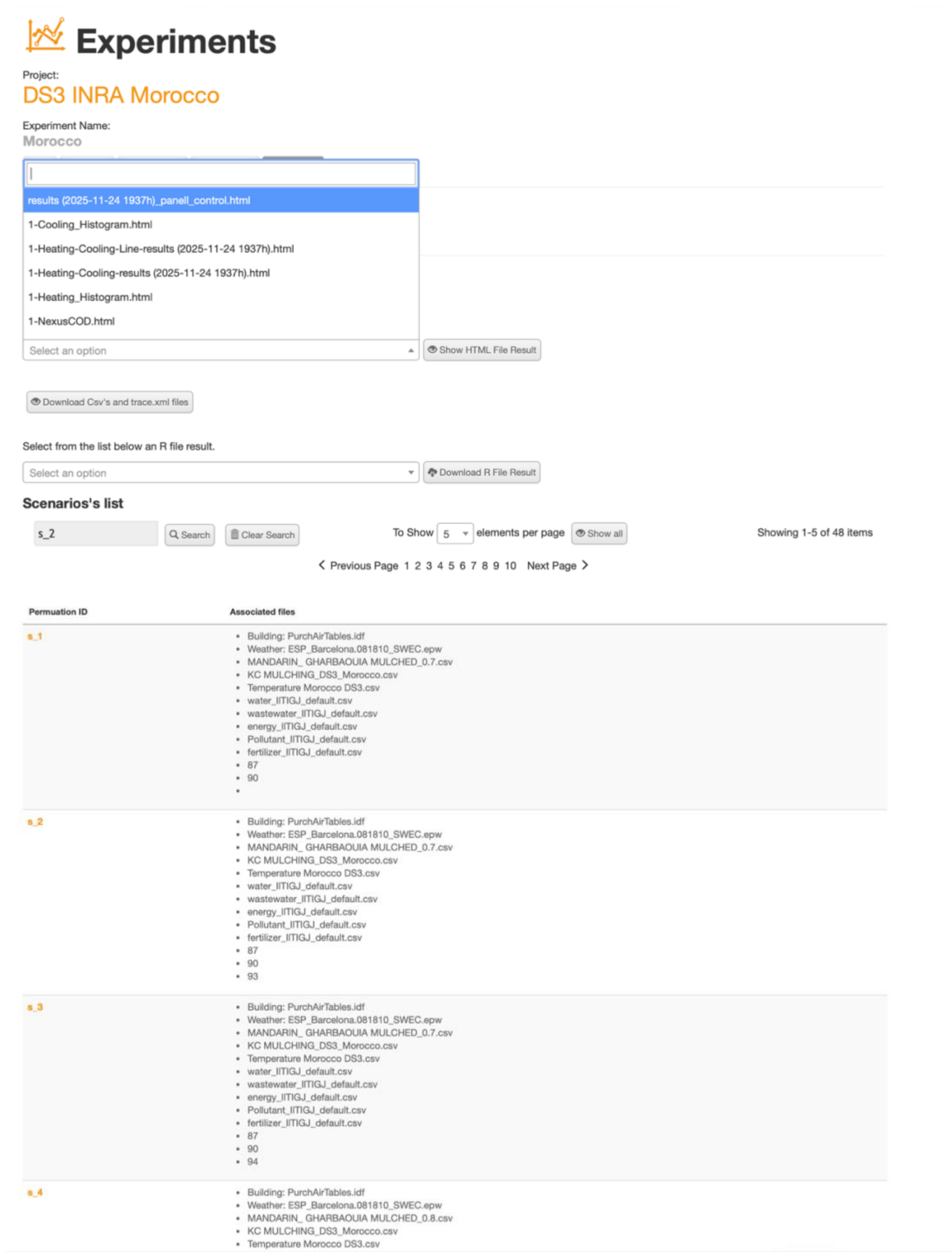

FIGURE 5. RESULTS SECTION IN THE NECADA DIGITAL TWIN, WHERE ALL OUTPUTS AND SCENARIO PERMUTATIONS (I.E., ALL TESTED CONFIGURATIONS) ARE DISPLAYED.

When the user activates the **selector to display the HTML results**, a new screen appears showing all figures generated by the model. It is important to highlight that the **AI WEFE Nexus tool can directly create visual outputs from all results produced by the SDLPS (computerised) model, covering every scenario tested.** For example, Figure 6 presents the GIR (Gross Irrigation Requirement) results for 48 different scenarios, corresponding to various mandarin and orange varieties, with and without mulching, and comparing grid-powered pumping with solar panels. On the left side of the interface, all scenarios are listed with their specific details; in the centre, a **Link List** provides access to the different result sets; and on the right, the selected figure from the Link List is displayed for visual analysis

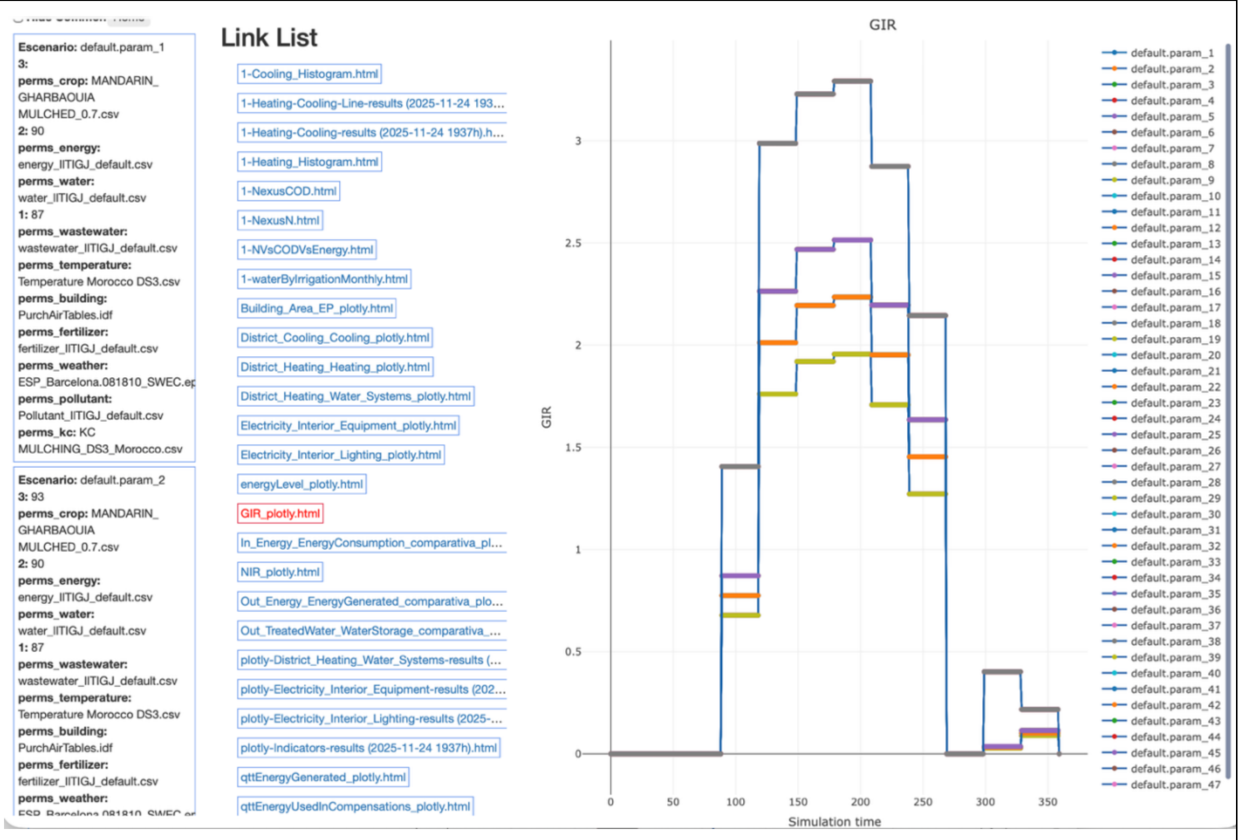

FIGURE 6. RESULTS SECTION IN THE NECADA DIGITAL TWIN, WHERE ALL OUTPUTS AND SCENARIO PERMUTATIONS (I.E., ALL TESTED CONFIGURATIONS) ARE DISPLAYED.

2.7 Postprocessing of Results Analysis

As mentioned above, the AI WEFE Nexus Digital Twin (DT) tool is capable of directly generating results for all tested scenarios. However, these raw outputs are not always immediately understandable for stakeholders or end users. To "translate" the model results into a form that is more accessible and decision-oriented, a dedicated post-processing phase was developed. This post-processing step is therefore essential in order to:

I. **Provide a comprehensive WEFE performance analysis for end users**, aggregating model outputs into clear indicators/KPI (e.g. water productivity, energy intensity, GHG emissions, ecosystem impacts, and food production metrics) that can be easily interpreted.

II. **Standardise and normalise results across scenarios**, for instance by expressing all key variables per hectare, per cubic metre of water, or per unit of product, which allows fair comparison between technologies, practices, and demonstration sites.

III. **Generate intuitive visualisations and summary dashboards**, such as bar charts, radar plots, and comparative tables, where the performance of multiple scenarios can be quickly compared and the best-performing options identified.

IV. **Support stakeholder dialogue and decision-making**, by condensing complex simulation outputs into a limited set of KPIs and graphics that can be used in workshops, policy briefs, and co-creation sessions, thus bridging the gap between the AI model and practical implementation.

The following section presents the analyses carried out for the five Demo Sites (Spain, Greece, Morocco, Israel, and Tunisia), combining the outcomes of the stakeholder workshops (Deliverable 4.3) with the Artificial Intelligence (AI)-based scenario development. For each Demo Site, the structure is as follows:

- Context and challenges: a brief introduction to the local conditions and Nexus-related pressures.
- Top three prioritised solutions: the best-performing practices identified through the participatory Multi-Criteria Assessment (MCA), summarised from Deliverable 4.3. Only the top three are retained, as these were selected as inputs for the scenario analysis.
- AI-based scenario results: exploration of how the three solutions perform under different conditions, highlighting synergies, trade-offs, and potential co-benefits across the Water-Energy-Food-Ecosystem (WEFE) Nexus.
- Discussion: reflection on the local implications and lessons learned.

This approach ensures continuity with previous deliverables while avoiding duplication. Whereas D4.3 provided a comprehensive overview of all solutions considered in the workshops, D3.3 focuses on the priority options and their projected performance through AI modelling. The combination of participatory evaluation and predictive analysis allows the project to validate solutions in context while anticipating their scalability and long-term impact.