



TRANSCEND

Deliverable 3.2: Modeling suite prototype and sourcebook

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Executive summary

Task 3.1 conducted a desk review of methods and models for assessing the socioeconomic and ecological impacts of policies under deep uncertainty, which was presented in D3.1. The deliverable included a critical assessment of the methods used for uncertainty quantification, such as structural, parameters and input uncertainties. Building on the outcomes of Task 3.1, researchers engaged with experts and stakeholders in the living labs to develop a *blueprint* of the modeling suite tailored to the needs of each lab in the context of Task 2.1. The present deliverable D3.2, developed within the Task 3.2 building upon D3.1 and D2.1, aims to define a timeline of the steps towards assembling, calibrating and validating the actionable modeling suite for each living lab. To this end, D3.2 provides a conceptual description of the key principles guiding the modeling suite, namely uncertainty quantification (Section 2) and the protocol-based modular approach (Section 3), as well as the key methods available in the literature. Next, Section 4 describes in detail how these two principles are to be addressed in each of the seven living labs, including a description of the specific modules, models, protocols and uncertainty quantification methods, as well as an implementation timeline via a Gantt Chart.

Regarding the modules adopted, all labs will model endogenously (i.e., with an explicit model that is part of the modeling framework) the hydrologic and economic systems. All labs will model the climate system, albeit only one endogenously (the Reno, using ad-hoc statistical and dynamical downscaling) and the remaining exogenously by incorporating existing outputs from modeling and downscaling experiments such as CMIP6 and Cordex. 6 out of 7 labs will model the agricultural system endogenously (Orontes, Nitra, Júcar, Reno, Titicaca-Desaguadero-Poopo, Mahanadi), and one exogenously (Tympaki). One lab (Reno) will model the meteorological system, endogenously.

Selected models for the hydrological module include SWAT+ (Orontes, Mahanadi), HYPE (Nitra, Reno), Ribasim (Reno, as water balance model linked to HYPE), WEAP (Tympaki, Titicaca-Desaguadero-Poopo), and TETIS (Júcar); for the economic module, PMP and PMAUP (Orontes, Nitra, Reno, Titicaca-Desaguadero-Poopo, Tympaki, Mahandi) and linear models (Júcar, Mahanadi); for the agronomic module, GYMEE (Orontes), DAISY, WOFOST (Nitra), Aquacitrus (Júcar), CRITERIA (Reno), AquaCrop (Titicaca-Desaguadero-Poopo), SWAT+ tool (Mahanadi) and CMIP6 and AgMIP databases (Tympaki); for the climatic module, CMIP6 (Orontes, Júcar, Nitra, Titicaca-Desaguadero-Poopo, Mahanadi and Tympaki) and ad-hoc statistical and dynamical downscaling experiments (Reno); and for the meteorological module, the ARPAE-CO model (see D2.1 for a detailed description of these models).

Regarding the protocols and coupling approach adopted, the Orontes, Reno, Titicaca-Desaguadero-Poopo and Tympaki labs have opted for a combination of bidirectional and sequential coupling protocols, where bidirectional protocols are adopted for the coupling between the hydrological and economic module, and sequential protocols adopted for the couplings climate→hydrological, agricultural→economic, agricultural→hydrological, and meteorological→agricultural (i.e., climate and agronomic modules provide inputs to the economic and hydrological modules, which are then run iteratively). The Júcar lab has adopted a fully sequential approach, while for the Nitra the conceptual design of the coupling has been delayed until the availability of data for the calibration and setup of the proposed models is confirmed.

Regarding uncertainty quantification, all labs quantify (at least to some extent) input, parameter, and structural uncertainties (except for the Nitra for which the definition of uncertainty quantification methods has been delayed until the availability of data for the calibration and setup of the proposed models is confirmed). Input uncertainty is quantified using scenario-based approaches for all labs (excluding Nitra) and most systems, typically relying on outcomes from selected RCP and SSP scenarios; while global sensitivity analysis methods are proposed for the economic module in the Orontes, Reno, Titicaca-Desaguadero-Poopo, Mahanadi and Tympaki; and for the hydrologic module in the Orontes and Mahanadi leveraging on SWAT+ tools. Parameter uncertainty is quantified using local sensitivity analysis for the Júcar (economic and/or agricultural modules), and using global sensitivity analysis in the Orontes (economic), Júcar (economic and/or agriculture), Reno (hydrologic, economic), Titicaca-Desaguadero-Poopo (hydrologic, economic), Mahanadi (hydrologic, economic), and Tympaki (hydrologic, economic). Finally, structural uncertainty is quantified using multi-model ensemble experiments in the Orontes (economic and climate modules, as well as water use data inputs), Nitra (climate), Júcar (climate), Reno (climate, economic), Titicaca-Desaguadero-Poopo (climate, economic), Mahanadi (climate, economic), and Tympaki (climate, economic).

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1. Introduction

This deliverable D3.2 presents the modeling suite to be adopted and developed in each lab to support the identification of robust Transformational Adaptation Policies (TAP) by stakeholders. The modeling suite adopts a protocol-based modular approach. Modularity means that models at each system level in the suite are to be i) run independently in modules, and ii) connected through sets of bidirectional protocols. These are defined as rules to manage interrelationships among systems' modules, i.e. two-way feedback. This conceptual model is combined with uncertainty quantification methods to sample and analyze structural, parameter and input uncertainties, and thus explore plausible futures that support the identification of robust TAP. To this end, each module is to be populated with multiple models of climatic (CMIP6 and downscaled projections in CORDEX), hydrologic (e.g. SWAT, HYPE), agricultural (e.g. AquaCrop-OS, DSSAT, APSIM, WOFOST), microeconomic (econometric and mathematical programming models such as PMP, PMAUP, LP) and macroeconomic systems (input-output and computable general equilibrium models, e.g. CMCC's ICES), as well as models of other relevant systems (e.g. CMIP6, ISIMIP) identified during co-development, to quantify structural uncertainties. Sensitivity analyses of key parameters and inputs will be also run to identify input and structural uncertainties. Leveraging data provided by the water accounting and monitoring toolbox developed in T4.3, we will parameterize, calibrate, and validate the modeling suite in each living lab. Moreover, we will also reduce uncertainty where possible by incorporating more accurate data inputs generated in WP4 to modeling.

This document provides a conceptual description of the key principles guiding the modeling suite, namely uncertainty quantification (Section 2) and the protocol-based modular approach (Section 3), and the key methods available in the literature. Next, D3.2 describes in detail how these two principles are to be addressed in each of the seven living labs, including a description of the specific modules, models, as well as protocols, uncertainty quantification methods, and an implementation timeline via a Gantt Chart (Section 4).

2. General principles of the modeling suite I: Uncertainty quantification

2.1. Modeling under deep uncertainty

SES (Socio-Ecological System) models play a pivotal role in understanding water availability, water uses, and their trends (Alcamo et al., 2003); identifying key socioeconomic and environmental drivers of scarcity, as well as their interactions; and informing the design of water management policies that can mitigate the impacts of growing water scarcity (Franzke et al., 2022; Westerberg et al., 2017). SES quantitative models articulate the complexity of the real world into manageable mathematical structures that can be used to transform exogenous shocks (e.g., climate change, a policy) into a prediction. Model predictions have great value: they should be (although sometimes they are not) transparent, easy to understand, faster than comparable heuristic reasoning (in fact some model

processes exceed the capacity of the human brain), and based on the scientific method (unlike guesses or opinions, models and their predictions are built on repeatable experiments or observational studies that test scientific theories) (Lempert, 2019; UNDRR, 2021). Despite these advantages SES models are not infallible, and their predictions are subject to uncertainties (Griffith, 2012). Confronting and addressing these uncertainties is important to provide a better understanding of the complexities in water resources management, and thus facilitate better decisions (Saltelli et al., 2020).

We define uncertainty as a situation where “it is not possible to identify all plausible futures or assign a probability to each identified plausible future” (Walker et al., 2003). Note that this definition explicitly excludes probabilistic risk. Although both risk and uncertainty preclude knowledge of the future and are often used interchangeably, their treatment in SES modeling is significantly different. Risk can be delimited using probabilistic functions and confidence intervals, which in turn can be updated and reduced as more evidence and information is made available using Bayesian inference (Lempert, 2019). On the other hand, the defining feature of uncertainty is that it cannot be delimited with probabilities (Knight, 1921). Moreover, while the epistemic elements of uncertainty related to (the lack of) knowledge itself (such as the processes and models used to represent SES) can be potentially reduced, the ontological elements arising from the inherent variability of SES cannot be reduced as in probabilistic risk (e.g., *what entities will inhabit our world and how will they interrelate?*) (Walker et al., 2003).

Numerous factors contribute to the emergence of uncertainty in SES models, ranging from input errors (Puy et al., 2022b) to output inaccuracies (Saltelli et al., 2020). Building on the taxonomies by Marchau et al. (2019) and Walker et al. (2003), and the literature review in Section 2, in this report we identify the following sources of modeling uncertainty (see Deliverable 3.1 for a more detailed description of this taxonomy):

- 1) *Input uncertainty* is the uncertainty associated with data inputs and underlying assumptions. It emerges from i) the external driving forces, or *forcings*, that have an influence on the system model (e.g., alternative policy designs, climate change scenarios, emissions scenarios); and ii) the data inputs that describe the baseline situation and quantify relevant features of a system (e.g., water use data, land use data, economic data).
- 2) *Parameter uncertainty* is the uncertainty associated with the data and methods used to calibrate the model constants, or parameters. While some parameters are regarded as certain, such as the mathematical constant π , or the acceleration of gravity, others can be discretionarily fixed to a certain value *a priori* or calibrated by comparing model outcomes to observed values in historical data series (typically by minimizing the difference between the two), which leads to uncertainty.
- 3) *Structural uncertainty* emerges from an insufficient understanding of the relationships between inputs, variables, and outputs within models. Structural uncertainty can emerge from “an incorrect definition of the system boundary, functional forms [...], variables and parameters, equations, assumptions and mathematical algorithms”, both within a system model or between system models (coupling design) (Walker et al., 2003).

Scientists have been progressively enhancing their toolkit for quantifying these sources of uncertainty. This includes uncertainty analyses to quantify input and parameter uncertainties (Bankes, 1993; Lempert et al., 2013), and multi-model ensembles that quantify structural uncertainty (AgMIP, 2024; HEPEX, 2024). Uncertainty analysis¹ and multi-model ensemble forecasting have been combined in “grand ensemble” experiments that simultaneously quantify uncertainties emerging from inputs, model parameters and model structures across one or multiple systems, both ecological (CMIP, 2024; ISIMIP, 2024) and (albeit less frequently) socioecological systems (Basheer et al., 2023; Gold et al., 2022; Schmitt et al., 2021; Smith et al., 2022; Zatarain Salazar et al., 2017). Beyond the quantification of cascading uncertainties, the systematic exploration of uncertainty across multiple interconnected systems and the wealth of coupling methods developed in SES research (such as Coupled Human and Natural Systems (CHANS) and socio-hydrology science) has shown potential towards identifying the emergence of nonlinearities (Bartusek et al., 2022; D’Amario et al., 2019).

Despite notable scientific advances on various fronts, there appear to be still significant gaps concerning how and which sources of uncertainty are incorporated into SES models for water resources planning and management. In fact, research on the topic has repeatedly deemed the integration of uncertainty assessments into models for water resources management “insufficient” (Di Baldassarre et al., 2016; Gain et al., 2021; Partida et al., 2023; Saltelli et al., 2020). These authors object that most uncertainty assessments focus on limited aspects of input and parameter uncertainty (e.g., local uncertainty analyses of climate change scenarios), while there remain significant knowledge gaps around how uncertain inputs other than climate change scenarios (e.g., water use estimates), as well as the design of human and water system models (including model coupling), influence modeling outputs and policy recommendations. For example, in a review of mathematical programming models, Saltelli et al. (2019) find that up to 65% of the “highly cited” papers in the review “do not properly explore the space of the input factors” and/or “use inadequate methods (i.e., varying one input factor at a time)”, expressing concern that the overall problem is worse considering these highly cited papers represent the “upper end of methodological rigor”. Uncertainty quantification is even more limited where model parameters and structures are concerned, as shown by Deliverable 3.2 of the TRANSCEND project, which comprised a literature review of 198 hydroeconomic models of which 148 quantified input uncertainties, 40 quantified parameter uncertainties and 7 quantified structural uncertainties.

Growing evidence has shown that disregarding modeling uncertainties in research and policy making can have substantial costs for ecosystems (Grafton et al., 2018), income (Parrado et al., 2019), employment (Groves et al., 2015), capital value (Adamson and Loch, 2021), insurance industry (Agudo-Domínguez et al., 2022), or sovereign creditworthiness (Standard & Poor’s, 2015), to name but a few. In this context, incorporating uncertainty quantification into SES models has become a prerequisite towards the development of robust science and policy (Puy et al., 2022a).

¹ Uncertainty analysis is often equated to sensitivity analysis. In reality though, uncertainty analysis focuses on quantifying uncertainty in model output; while sensitivity analysis takes uncertainty analysis one step further to study “how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input” (Saltelli et al., 2008). Thus, uncertainty analysis precedes sensitivity analysis.

2.2. Methodological framework and principles for uncertainty quantification

A foundational principle of TRANSCEND is that uncertainty quantification is a prerequisite to validate any model, before it can be subsequently used to inform robust policies, including Transformational Adaptation Policies (TAP). Note that validation is understood here not as proving the model true beyond doubt, but instead as extensively corroborating the model by surviving a series of tests (formal, of internal consistency, or relative to their predictive capacity). These tests must be extensive and account for all relevant uncertainties (Saltelli et al., 2008). In an “ideal” uncertainty quantification, heterogeneous uncertainty sources are propagated through the model to create an empirical distribution of the output (see grey curve in Figure 1). A comprehensive uncertainty quantification incorporates an uncertainty analysis of parameters, inputs, and model structures. The resulting uncertainty in the output, captured for example by its variance, can be then further elaborated into a sensitivity analysis where these outputs are apportioned to modeling inputs/decomposed according to source (Saltelli et al., 2019).

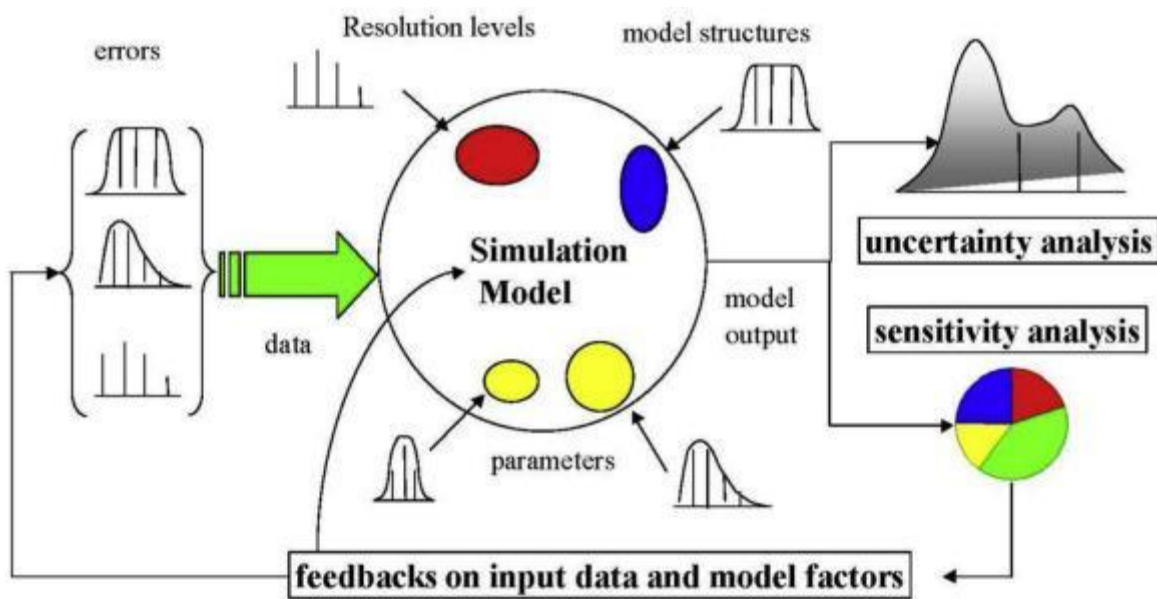


Figure 1. Idealized uncertainty and sensitivity analysis. Taken from Saltelli et al. (2019)

In cases where the model is deterministic (i.e., it always produces the same output from a given initial state, as opposed to randomness), evaluating the uncertainty in the output essentially involves propagating the uncertainty from the input variables to the output. This can be achieved by iteratively running the model with various values for the uncertain inputs within their feasible ranges, such as through a Monte Carlo simulation or ad hoc methods, resulting in a distribution of potential model outcomes (illustrated as the shaded area in Figure 1). Uncertainty analysis may also entail extracting metrics like the mean, median, and variance from this distribution, and potentially establishing confidence intervals, such as for the mean. Once this initial analysis is completed, the subsequent step might involve utilizing sensitivity analysis to attribute this uncertainty to the input variables (e.g., "a

specific variable is solely accountable for 70% of the uncertainty in the output”) (Saltelli et al., 2019). Sensitivity analysis here serves primarily as a tool to quantify the contributions of model inputs, or subsets of inputs, to the uncertainty in the model output, so as to identify which input variables have the greatest influence on model uncertainty (“prioritizing factors”), allowing for the collection of additional information about these parameters to diminish model uncertainty, or identifying variables that have minimal impact and can potentially be adjusted (“fixing factors”) (Puy et al., 2022a).

One can anticipate four key issues in the design of uncertainty and sensitivity analysis. The *first* one relates to the number of factors (inputs, parameters, structures) considered in the analysis: having incorporated all uncertainties, the model output may vary “so wildly as to be of no practical use” (Saltelli et al., 2008). In other words, the conclusions of any sensitivity analysis will be robust enough “if the number and range of input values is wide enough to be credible and narrow enough to be useful” (Leamer, 1985). However, as noted by Saltelli et al. (2008) and in line with previous work by Beven and Binley (1992) and Beven and Freer (2001) that introduced the equifinality concept (i.e., distinct configurations of model components such as inputs, parameters, or structures, can lead to similar or equally acceptable representations of the real-world process of interest), this “trade-off may not be as dramatic as one might expect, and that increasing the number of input factors does not necessarily lead to an increased variance in model output.” Typically, a few inputs create almost all the uncertainty, and the majority make a marginal contribution.

The *second* issue refers to local v. global analyses. As noted by (Saltelli et al., 2019):

“A local method in its simplest form yields the partial derivative of the model with respect to one of its input factors, i.e. $\partial y / (\partial x_i)$. Two notable deficiencies of this definition of sensitivity are that first, if f is nonlinear with respect to x_i , then its partial derivative will change depending on where in the range of you choose to measure. Second, and more generally, if there are interactions between model inputs, then $\partial y / (\partial x_i)$ will change depending on the values of the remaining input factors as well. In short, first partial derivatives are only a valid measure of sensitivity when the model is linear, in which case will remain constant for any x .”

The corollary is that local methods can only work properly for linear models. Let us illustrate this with a common variation of the first partial derivative, a local method usually referred to as the one at a time (OAT) approach. OAT designs cannot effectively explore a multidimensional space, as graphically illustrated by Saltelli et al. (2019) (Figure 2):

“Imagine that the input space is a three-dimensional cube of side one. Moving one factor at a time by a distance of $\frac{1}{2}$ away from the center of the cube generates points on the faces of the cube, but never on its corners. All these points are in fact on the surface of a sphere internal and tangent to the cube, as illustrated in [Figure 2]. The volume of the sphere divided by the volume of the cube is about $\frac{1}{2}$. If we increase the number of dimensions this ratio goes towards zero very quickly. In ten dimensions, the volume of the hypersphere divided by the volume of the hypercube is 0.0025, one-fourth of one percent. In practice, it is even more restrictive than that because the OAT design does not even explore inside the hypersphere and is limited to a “hypercross”. In other words, moving factors OAT in ten dimensions leaves over 99.75% of the input space totally unexplored. This under-exploration of the input space directly translates

into a deficient sensitivity analysis and is but one of the many incarnations of the so-called “curse of dimensionality”, and the reason why an OAT SA is perfunctory, unless the model is proven to be linear.”

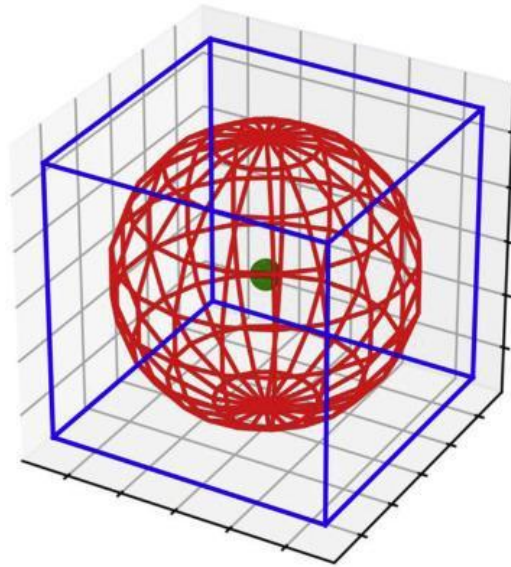


Figure 2. Local v. global sensitivity analyses. Taken from Saltelli et al. (2019)

In sensitivity analysis, global analyses can be categorized into either random, quasi-random, or space-filling designs, or into orthogonal array-based designs that are replicated across various points within the input space (e.g., derivative-based measures, Monte Carlo estimation of variance-based sensitivity indices, and elementary effects, among other applications).

Summing up, when performing uncertainty and sensitivity analyses in TRANSCEND, the recommendation is to adopt global analyses that more comprehensively sample and assess uncertainty. A non-exhaustive list of uncertainty and sensitivity analyses techniques is provided in the next section.

The *third* issue refers to computational cost. Computational cost may pose a challenge in conducting uncertainty and sensitivity analyses where 1) each model run demands a considerable amount of time, stretching from minutes to hours or even longer, especially in the case of highly intricate models; and/or 2) where the model encompasses numerous uncertain inputs, which expand exponentially the computational cost with the increase in the number of inputs—a phenomenon known as the curse of dimensionality. Addressing computational expenses is crucial in many practical sensitivity analyses. Strategies to mitigate this burden include employing emulators or metamodels driven by machine-learning techniques that are particularly suitable for large models (Storlie et al., 2009), and employing screening methods to reduce the dimensionality of the problem such as High-dimensional model representations (Li et al., 2006).

The *fourth* issue refers to correlated inputs. Although, in some cases inputs can exhibit significant correlations, sensitivity analysis techniques typically operate under the assumption of input independence. Addressing this issue remains a relatively nascent area of research, and definitive methodologies have yet to be firmly established. One approach is to establish relatively simple rules (e.g., when quantities supplied decrease, prices must increase, perhaps within a predetermined range) that manage the correlation. An alternative is to create scenarios using external sub-models (e.g., a CGE model that can generate ranges for price responses to changes in supply – which nonetheless may add further uncertainty and computational costs to deal with it (see issue number three in the previous paragraph).

A *fifth* issue relates to boundaries for the uncertainty quantification. At some point, modelers must decide on the inputs, models, etc. and that will condition the outputs of the modeling exercise. For example, data constraints or gaps at a local level can be addressed using global datasets that may be less accurate. Also, modeling structures are decided by modelers, and biases may also emerge here. While uncertainty quantification should also explore these aspects, and in TRANSCEND we will explore them as far as possible (e.g., with multi-model ensemble experiments to quantify structural uncertainties), some limits must be defined to not generate computational costs we cannot afford. For example, we cannot test the sensitivity of outputs to each decision made in the structure of a model, but we can compare alternative modeling structures to identify vulnerabilities/decisions to which outputs are highly sensitive.

2.3. Uncertainty and Sensitivity analysis

The bare minimum threshold for uncertainty quantification in TRANSCEND SES modeling and TAP assessments in each living lab is the quantification of uncertainty in model output. This can be done by leveraging on various methods, which we discuss below. Some of them, such as the scenario analysis or derivative-based local methods, can be strictly catalogued as tools for uncertainty quantification, since they quantify uncertainty in model output without necessarily providing information on how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input. Some others combine uncertainty analysis with sensitivity analysis, by quantifying first uncertainty in the output to then apportioning output uncertainty to sources of input uncertainty. Moreover, the detail in the attribution of input uncertainty to output uncertainty varies for each method, and some sensitivity analysis methods can be combined to gain detail (e.g., factorial experiments can be combined with Analysis of Variance/ANOVA to provide variance-based measures).

TRANSCEND SES modules may comprise alternative model structures, each of which rely in turn on more than one input or parameter. This calls for sensitivity analysis techniques focusing on assessing multiple factors (i.e., global). Yet, due to the computational and resource constraints of the project, the use of local methods (e.g., derivative-based methods, simple scenario analysis) or the combination of global methods with heuristics (e.g., factorial experiments guided by scenario analysis) can be warranted under specific circumstances.

Below we briefly present some uncertainty and sensitivity analysis techniques, including local (which are recommended only for assessments of a key variable/scenario or for those specific cases where models are linear) and the preferred global designs. The list is non-exhaustive, and alternative techniques can be adopted where suited better to the purpose at hand. For an exhaustive description of sensitivity analysis techniques and some applications, the reader is directed to Saltelli et al., (2008). For additional applied sensitivity analyses, the reader is directed to Saltelli et al. (2004).

Among the *local designs*, which are recommended only for assessments of a key factor/scenario or for those specific cases where models are linear, sensitivity analysis techniques include:

Derivative-based local methods, which involve calculating the partial derivatives of the output with respect to each input variable at a fixed point in the input space. These methods are computationally cheap but also suffer from the limitation of not fully exploring the input space (see Figure 2).

The one-at-a-time (OAT) method is a straightforward and commonly used local approach where each input variable is individually altered while keeping others at their baseline values, then returning the variable to its original value before repeating the process for other inputs. This method allows for measuring sensitivity by observing changes in the output, typically using techniques like partial derivatives or linear regression. OAT is favored by modelers for its practicality, as it enables easy identification of the input factor responsible for any observed failure in the model. However, OAT does not fully explore the input space as it overlooks simultaneous variations in input variables, thus failing to detect interactions between them and proving inadequate for nonlinear models. Moreover, the portion of the input space explored with OAT diminishes drastically with an increase in the number of inputs, making it inefficient for complex systems (see Figure 2).

Linear models or regression analysis is another approach where a linear regression is fitted to the model response, and standardized regression coefficients are used to measure sensitivity. This method is suitable for linear models and offers simplicity and low computational cost. However, it requires the model response to be truly linear, which may not always be the case in practice.

Scenario analysis, scenario thinking, scenario planning, scenario method, or scenario prediction are all strategic planning methods that are suitable for its use in stakeholder engagement processes such as those conducted in TRANSCEND. This approach identifies the key sensitive inputs, and sometimes also their range, relying on heuristics. Depending on the way the scenario is designed, the approach can be local or global. For example, if the scenario includes two key variables (input prices and crop prices) and one is changed while the other is kept constant, the approach would be similar to OAT and thus could be labelled as local design. On the other hand, if the effect of all possible input combinations on outputs are explored, the approach would qualify as global design (factorial experiment). Scenario analysis is flexible and can be combined with other uncertainty and sensitivity analyses, both local and global, such as OAT, linear models, derivative-based methods, factorial experiments, etc.

Among the *global designs*, which are those recommended for most SES models and frameworks, except in those cases where the models adopted are linear and local techniques can be adopted, selected sensitivity analysis techniques include experimental designs, namely full factorial experiment, fractional factorial experiment, random sampling, and Latin hypercube sampling; variance-based methods; Elementary Effects Method; and Group Sampling.

Full factorial sampling. A full factorial experiment involves multiple factors, each having various possible values or "levels." The experiment explores the outcome for every possible combination of these levels across all factors. This type of experiment enables researchers to analyze the impact of each factor on the response variable, as well as the interactions between different factors on the response variable. Employing a full factorial design provides data to estimate the average response variable for each level of every parameter. This estimation is achieved by averaging over simulations where all other parameters vary across their possible combinations of high and low values. However, a drawback of employing a factorial design is the extensive number of simulations required. For instance, with only two levels (i.e., two alternative values for each factor, which can be a parameter or input), analyzing 10 parameters would necessitate 2^{10} (or 1024) simulations, and for 20 parameters, over a million simulations would be needed. Researchers can mitigate this challenge by selecting a subset of simulations to create a more manageable design that still yields valuable insights, for example using a fractional factorial sampling.

Fractional factorial sampling. In statistical analysis of factorial experiments, the system tends to be influenced primarily by main effects and interactions of lower orders, i.e., single factors and two-factor interactions are show the most prominent responses observed in a factorial experiment and thus drive output variability and uncertainty. Higher-order interactions between main effects (e.g., three factors) are typically negligible. In fractional factorial sampling, a deliberate selection is made to use only a portion (fraction) of the experimental runs included in a full factorial design. This approach aims to unveil crucial insights into the key aspects of the problem being studied, while significantly reducing the number of experimental runs and resources required compared to a full factorial design. Essentially, it leverages the realization that numerous experiments within a full factorial design are frequently redundant, offering minimal or negligible additional information about the system.

Random Sampling and Monte Carlo methods. Random sampling uses brute computational force to create a set of random numbers for inputs that can be used to quantify uncertainty on outputs. This does not offer any guarantee on the final output being a good representative of the real output uncertainty, unless a sufficiently high number of simulations is performed (on average, the approximation improves as more simulations are performed). As a result, random sampling particularly in complex SES models can be computationally very expensive. The Monte Carlo method stands as a prevalent method for random sampling, and essentially involves sampling input parameters from probability density functions. The model is then executed iteratively, tens, hundreds, or even thousands of times, each time with different sets of sampled parameters. Parallel computing tools can be employed to accelerate the calculations, benefiting from the embarrassingly parallel nature of the experiment (i.e., little or no effort is needed to separate the problem into several parallel tasks). Note that this approach is different to scenario analysis: in the scenario analysis method the researcher asks herself the question "what if" to produce a point-prediction, while in Monte Carlo Experiments

the researcher explores randomly the range of plausible inputs to explore output uncertainty. The output of Monte Carlo experiment comprises numerous realizations (see Figure 1), which can be subsequently analyzed using statistical techniques. The key steps in conducting an uncertainty analysis of inputs and parameter uncertainties involve:

- Identifying all structures, parameters and inputs potentially contributing to model prediction uncertainty.
- Establishing the underlying structures/parameter/inputs distributions, either through expert judgment or empirical evidence, capturing their mean, standard deviation, and ranges. Where probabilities are not known, expert judgement or uniform probability density functions are also feasible (equal probability for each input value).
- Propagating the uncertainties of the factors (structures/inputs/parameters) through the model(s) via (probabilistic) simulations, using a global design.
- Extracting, where possible, central tendency measures from the output distribution of predicted values (e.g., mean) as well as confidence limits and intervals to quantify uncertainty in the model prediction.

In some cases, probability density functions cannot be attributed, which may warrant an unweighted approach. This may be the case of inter-model comparison experiments where each model is run separately. This does not preclude the feasibility of a Monte Carlo experiment, which can be run on inputs and parameters for each model structure separately. Moreover, it has been argued that when “probabilistic information is not considered, each potential vulnerability is equally important on the overall robustness, which can also be interpreted as an implicitly equal weighting” (Taner et al., 2019), which could be used to assign an equal probability to each model in the Monte Carlo experiment. Yet formally speaking we cannot strictly claim that each model has an equal weight where probabilities are essentially unknown.

Latin Hypercube. Latin hypercube sampling is a methodical sampling approach employed to decrease the number of simulations required for assessing response uncertainty, thereby cutting down on computational expenses. Instead of randomly selecting samples across the entire input space, this method partitions the input space into distinct "strata" and chooses a representative value from each stratum. These representative values cover the entire domain without duplication, ensuring thorough coverage in the complete simulation while significantly reducing redundancy. Dutta and Gandomi (2020) describe the following steps in Latin hypercube sampling:

- *“Step 1. Partition the input sample space of each random variable (RV) into L ranges of equal probability = 1/L. It is not necessary to divide the domain with equal probability;*
- *Step 2. Generate one representative random sample from each range. Sometimes, the midvalue is used instead of a random sample from range;*
- *Step 3. Randomly select one value from L values of each RV to get the first sample s1*
- *Step 4. Randomly select one value from the remaining L—one value of each RV to get the second sample s2, and so on up to L sample sL*
- *Step 5. Repeat Steps 1 to 4 for all the RVs*
- *Step 6. The rest sampling technique is the same as in MCS”*

Dutta and Gandomi (2020) also provide MATLAB built-in functions for Latin hypercube execution.

Variance-based methods. Variance-based methods belong to a category of probabilistic techniques used to characterize both input and output uncertainties by representing them as probability distributions. These methods analyze the output variance and decompose it into components attributed to individual input variables and their combinations. Consequently, the sensitivity of the output to a particular input variable is evaluated based on the extent to which variations in that input contribute to the variance observed in the output. Variance methods can be applied on top of other sensitivity analyses, for example, by conducting an ANOVA on top of a factorial experiment, Monte Carlo experiment or Latin hypercube experiment. Using variance-based methods we can calculate the main effect or contribution to the output variance of the main effect of a factor, by measuring the effect of varying that factor alone, but averaged over variations in other factors; or the total effect that captures the contribution to the output variance of a given factor, including all variance caused by its interactions, of any order, with any other factor. This requires a large number of simulations, and the computational burden can rapidly escalate, particularly if each individual model run consumes a considerable amount of time. In such scenarios, several methods exist to alleviate the computational expense associated with estimating sensitivity indices, including the Fourier Amplitude Sensitivity Test (FAST) or metamodels/data-driven approaches such as High Dimensional Model Representation (HDMR).

3. General principles of the modeling suite II: modularity and protocols

Reflecting scientific advances, TRANSCEND modeling suite adopts a protocol-based modular approach that captures the two-way feedbacks between socioeconomic and ecological systems (multi-system). **Modularity** means models at each system level will be run independently in modules; and then connected through sets of **protocols**, which are defined as rules designed to manage interrelationships (where feasible through two-way feedbacks) among systems' modules (Csete and Doyle, 2002). Modules will be populated with alternative models in inter-model comparison experiments. Through co-creation (WP1-2), we are working alongside stakeholders in living labs to explore the relevant models to be included in each module, identify critical parameters and conduct sensitivity analyses. Detailed progress on model co-creation is reported in *D2.1 - Blueprints of the modeling suites by lab*.

The two subsections below present the modules in the suite, and the protocols used for interconnecting them using a i) time-invariant and ii) time-variant setting.

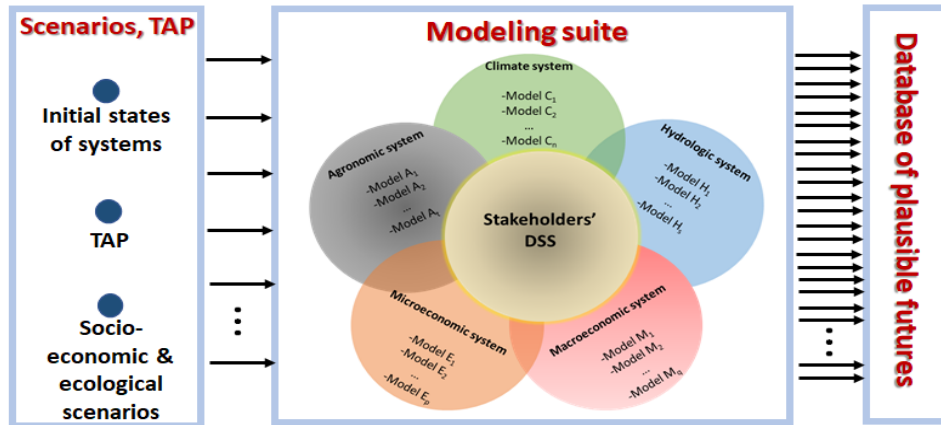


Figure 3. TRANSCEND modeling suite.

3.1. Modules

Each system/module in TRANSCEND is populated with one or multiple models (multi-model), which we use to study the impacts of multiple inputs including TAP (multi-scenario). Specifically, the suite will include models of climatic (CMIP6 and downscaled projections in CORDEX), hydrologic (such as SWAT), agricultural (such as AquaCrop-OS), microeconomic (econometric and mathematical programming models such as PMP, PMAUP, LP), and/or macroeconomic systems (CMCC & USAL input-output and computable general equilibrium models, e.g. ICES), depending on the lab needs; as well as other models (see e.g. CMIP6, ISIMIP) and systems deemed relevant by scientists and stakeholders during co-creation (see D2.1 - *Blueprints of the modeling suites by lab*). A detailed description of each module is provided in Annex I to this report.

3.2. Protocols

The modules presented above are interconnected via protocols, which are rules designed to manage interrelationships (where feasible through two-way feedbacks) among systems' modules (Csete and Doyle, 2002). By building links among modules, using two-way or single-way protocols, we define a hierarchy of modules that can be run to assess the impacts of a given shock over all relevant systems. The hierarchy is activated after a shock/forcing affects one of the modules, and the effects are subsequently propagated throughout the remaining modules of the framework via the established protocols. Shocks/forcings involve a policy/TAP and/or a scenario or set of scenarios (notably climate change scenarios).

Protocols for interconnecting modules in TRANSCEND can adopt two alternative settings: i) time-invariant and ii) time-variant. Note that this setup also affects outputs and contributes to uncertainty, so a potential uncertainty quantification exercise may also address this contextual/structural uncertainty (see D3.1).

If we adopt a **time-invariant** setting the analysis is circumscribed to a specific period and an iterative process is activated and repeated until convergence is reached, at which point predictions are stable and consistent, allowing for a comparative statics analysis. Convergence can be assessed through a convergence test (Hasegawa et al., 2016; Ronneberger et al., 2009). This time-invariant static approach is typically used to assess changes in the equilibria of systems following a shock through comparative statics (Bosello et al., 2012a; Dixon et al., 2012; Parrado et al., 2020, 2019; Pérez-Blanco et al., 2016; Taheripour et al., 2016).

On the other hand, under a **time-variant** setting, information is carried forward in time from one module to another for a predetermined number of years. While convergence could be part of the analysis the time dimension opens the possibility to explore adaptive pathways of specific shock or policies without the need to achieve convergence, by slightly modifying the protocols to allow for a time lag in the feedback processes of the system. Time-variant settings are particularly useful to explore *dynamically robust strategies*, that is, a set of possible actions designed to allow the policy maker to adapt dynamically from one action to another over time in response to how the future unfolds (Walker et al., 2010). Dynamically robust strategies can be developed using modeling approaches such as Dynamic Adaptive Policy Pathways (DAPP) (Haasnoot et al., 2013) or Real Options Analysis (ROA) (Steinschneider and Brown, 2012). In essence, modeling approaches such as DAPP or ROA represent decision makers' evolving hypotheses about the most important uncertainties, relationships, measures and decision levers, where decision levers represent policies that can be taken to influence the system, with the aim of “finding a plan that is successful in a wide variety of plausible futures” that happen *in succession* (Kwakkel et al., 2015). Another option is to use backcasting “hierarchies”: starting from a desired agricultural extension scenario, we can assess what crops and what distribution or value channels we want and explore what this would require in terms of prices, regulatory setting and water allocation/sharing.

Both time-variant and time-invariant approaches are designed to be flexible, and protocols will change depending on the systems considered and the models explored within each module. Below we present two illustrative cases of a i) time-invariant (Figure 4) and ii) time-variant protocol setting (Figure 5).

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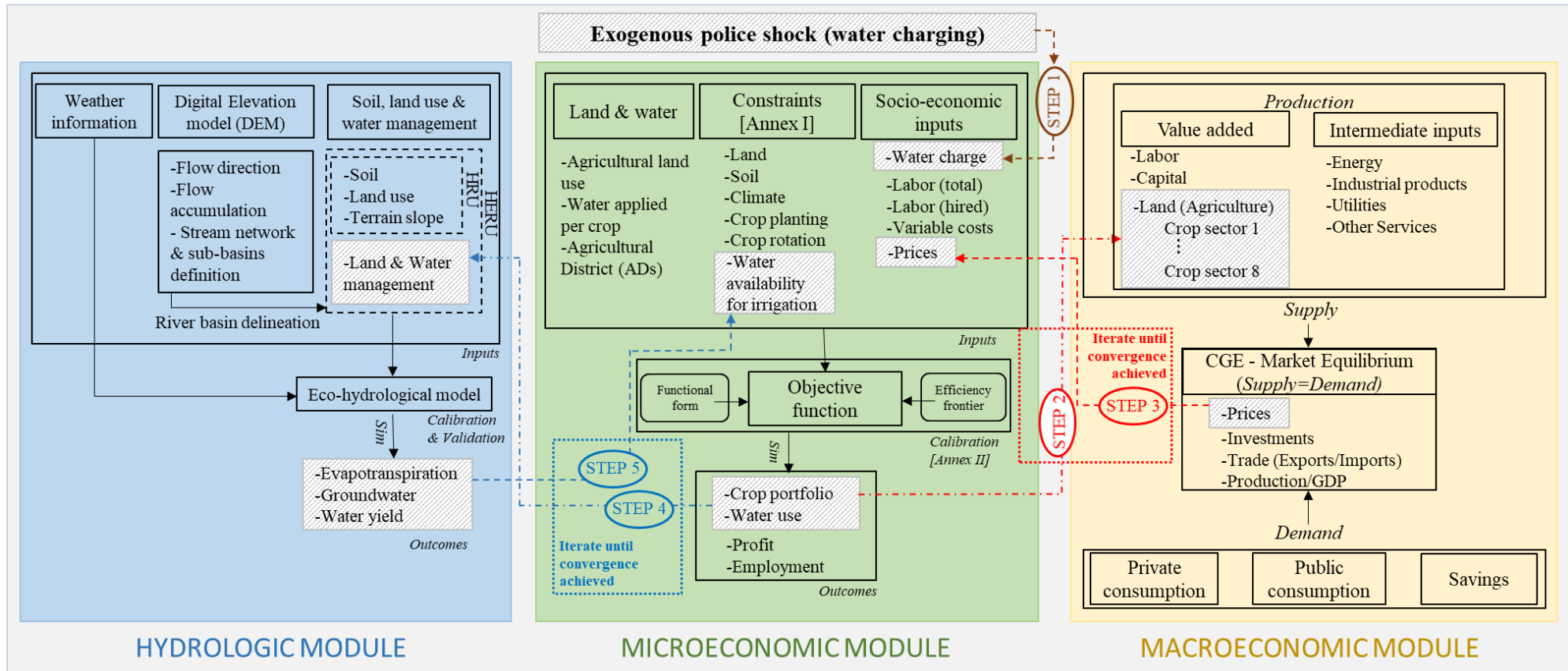


Figure 4. Conceptual representation of the coupled hydro-micro-macro-economic modeling framework under a time-invariant setting (taken from Pérez-Blanco et al., 2022). In step 1, a policy shock (in this illustrative example, water charging) is applied to the microeconomic model, whose solution provides reallocation of land among crops based on the preferences of economic agents; In step 2, land use changes and/or agricultural supply/quantities (depending on the detail offered by the macroeconomic model) as simulated by the microeconomic model in step 1 are aggregated and fed into the agricultural sector of the case study area's corresponding region in the macroeconomic model; a macroeconomic simulation is then performed with the new input information to find a new economic equilibrium and to provide a set of production quantities and

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commodity prices that are consistent with economy-wide effects; In step 3, changes in crop commodity prices in the relevant region are fed back into the microeconomic model, and economic agents in the case study area reassess their initial crop portfolio decision. Steps 1 to 3 occur iteratively until convergence is reached. Note that the coupling protocol between the micro- and macro-economic modules through land use and crop price changes yields a stable system (i.e. the micro- and macro-economic modules are in equilibrium simultaneously); In step 4, resulting land use choices and water use by economic agents are fed into the corresponding consolidated land areas of the hydrologic model (SWAT), which simulates the effects of the socioeconomic system on the water dynamics of the river basin; In step 5, relevant effects on the water system (i.e. water availability for irrigation) are passed as spatially-distributed information to the corresponding microeconomic agent. If the water availability constraint strengthens following the hydrologic simulation, forcing economic agents to adapt, the iterative process in step 1 to 3 is repeated until convergence is reached (i.e. models predictions are stable and consistent). Note that for climate-induced responses (e.g. climate change scenario analysis), simulations would run from the hydrologic (external climate forcing) to the microeconomic to the macroeconomic model (i.e. step 4 and 5 as first steps, followed by 1-3). The same rationale is valid for macro-economic induced responses, such as macroeconomic shocks due to COVID19, for instance. The overall simulation from steps 1 to 5 follows the rules established in the protocols' connection and is repeated in successive iterations until convergence of results provided by both water and human systems is reached. Convergence refers to a situation when information exchanged between models does not result in meaningful changes between two successive simulation iterations, and is assessed through a convergence test.

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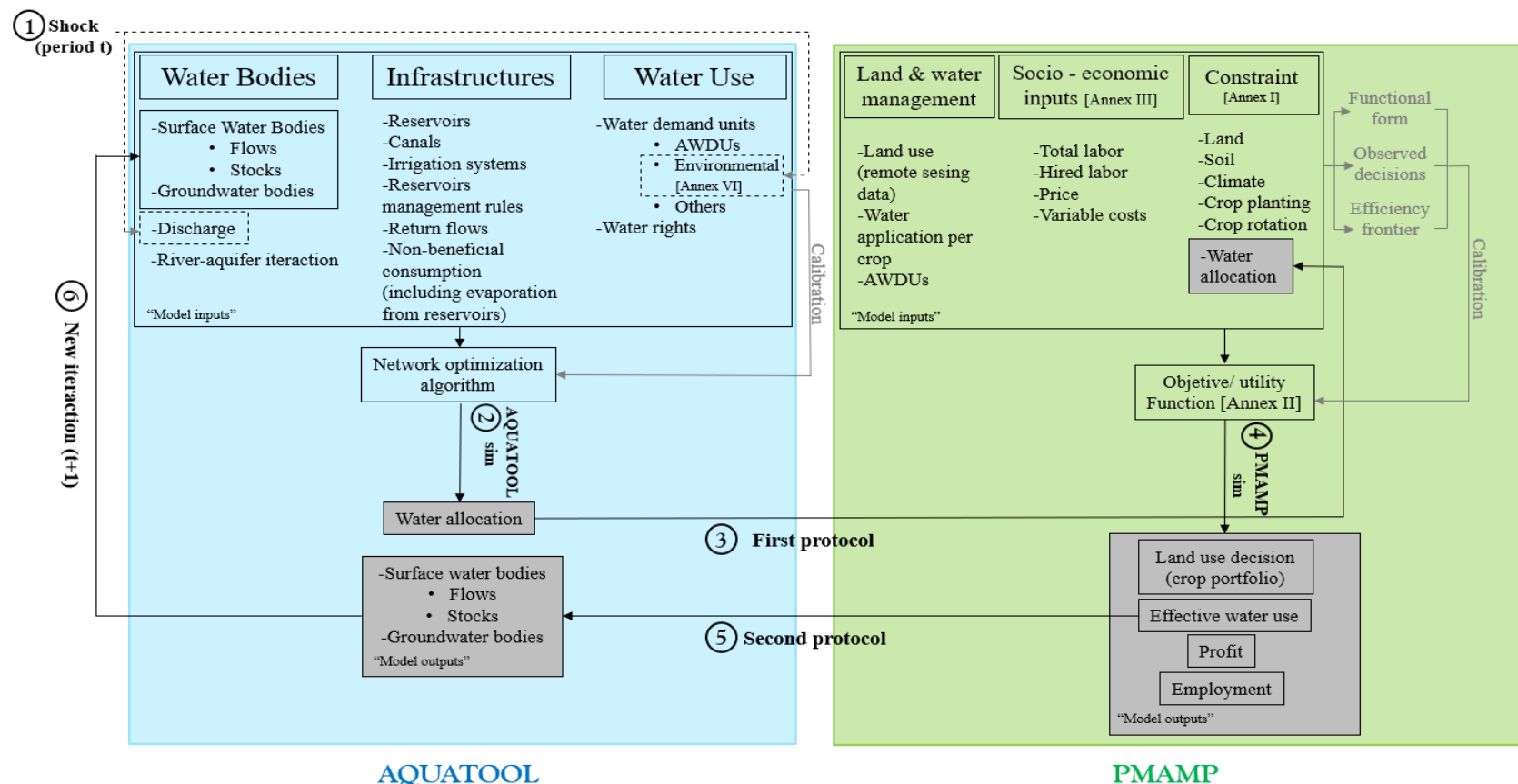


Figure 5. Conceptual design of the time-variant coupled human-water modeling framework (taken from Pérez-Blanco et al., 2021). Step 1 introduces a shock (new minimum environmental flows under climate change), which forces the AQUATOOL model and yields the new water allocations for each AWDU (Step 2). In Step 3, the new water allocation constraints are conveyed to each economic agent/AWDU in the microeconomic model (in this case, a PMAMP model has been chosen, but any other microeconomic model could be used) through the first protocol, and a simulation is run to determine land use and water application decisions (Step 4). In Step 5, information on effective water use is conveyed from the PMAMP to the AQUATOOL model through the second protocol, and this information is used to estimate the status of the water system

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(stock and flows of surface and groundwater bodies). Steps 1 to 5 occur over the same period t . Finally, in Step 6, the status of the water system in t is used as an input to start a new iteration by simulating a new period $t+1$.

4. Description of modeling suite for each living lab

The following subsections describe, for each lab: 1) the modules adopted with a list of the models used to populate them, and the protocols used to interconnect modules and models; 2) a Gantt chart describing key tasks and when they will take place; and 3) the key uncertainties identified, as well as sensitivity analysis tools proposed to quantify uncertainty.

In each lab this information was obtained through a questionnaire where the relevant modeling team was asked to address the following points.

Modules and protocols:

1. Provide a diagram showing the modules/systems planned, and their connections between modules/models.
2. Briefly describe each module.
3. Provide a description of the protocols that interconnect modules and models, accounting for: 1) the coupling variables, 2) the direction of the coupling, 3) the time setting (dynamic, static), and 4) the sequence of the coupling, where these are already defined.
4. Describe the already finished or pending tasks in terms of 1) data collection, 2) model calibration, and 3) simulation.

Gantt Chart: Please fill in the Gantt chart considering the following phases for each model: data, calibration, and simulation.

Key uncertainties and sensitivity analysis:

1. Identify and list key parameter, structural and input uncertainties.
2. Design and describe an uncertainty quantification plan for each lab, identifying the uncertainty and sensitivity analysis method(s) proposed for each lab.

Annex I presents an overview of the modules and models, which were described more in detail in D2.1 -*Blueprint for the modelling suite*. Data inputs for each model and setup are presented in Annex II.

4.1. Orontes River Basin

4.1.1. Modules and protocols

We will initiate our analysis by employing hydrologic modeling techniques to assess the impact of climate change and alterations in land use on water availability. Through the integration of multiple earth observation datasets, we aim to construct a comprehensive understanding of the basin's agro-hydrological dynamics. Finally, we will integrate agro-hydrological aspects with human systems by modeling the behavior of farmers, the main water users in the Orontes Basin, and their interactions with the physical system.

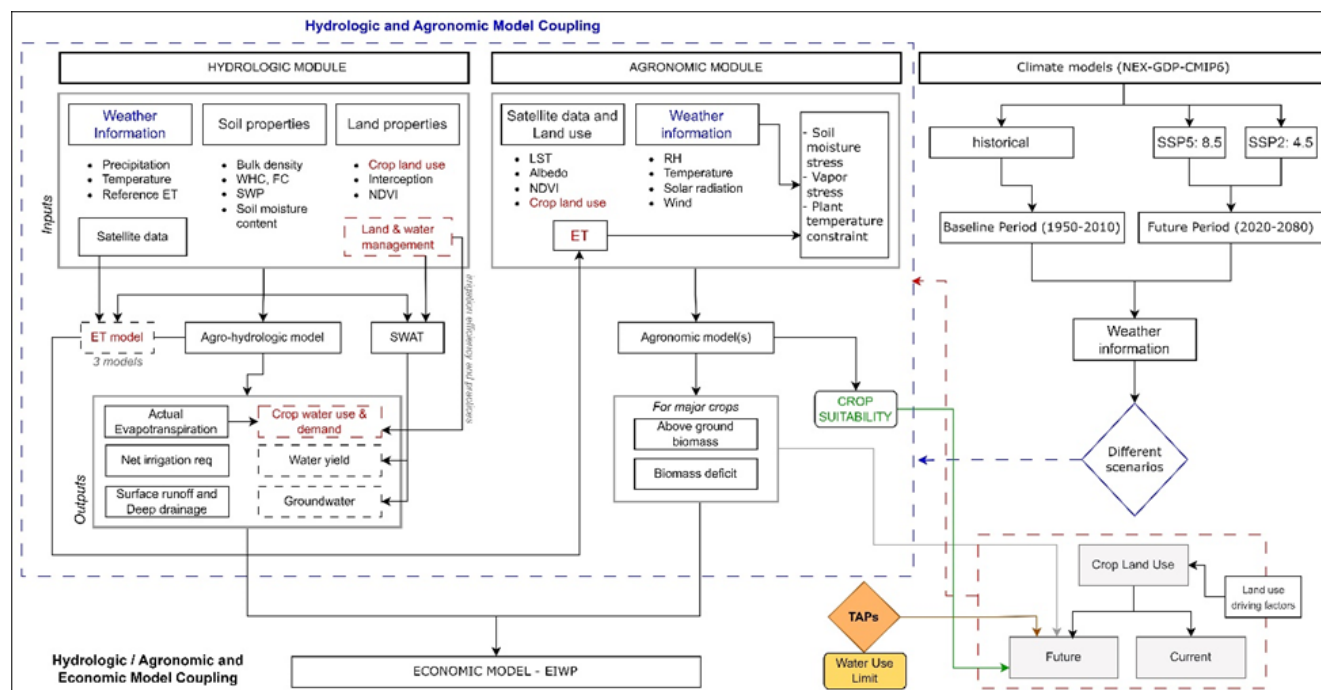


Figure 6. Orontes River Basin modules and protocols.

Hydrologic Module:

To delineate the runoff patterns within the basin, we will use both a simple water balance approach and a soil water balance model (agro-hydrologic), which accounts for variables such as snowpack accumulation. By incorporating future climate change projections, encompassing shifts in temperature and precipitation, we will forecast the basin's runoff under existing and potential land use change scenarios. This analysis will serve as a foundation for devising water allocation strategies that ensure sustainable utilization amidst evolving environmental conditions.

We will run a daily soil water balance model at the basin scale in the Lebanese part. We will use multiple data sources like precipitation, temperature, and vegetation indices, and calculate surface runoff and deep drainage. Evapotranspiration computations will consider both potential and actual rates, adjusting for soil moisture levels and vegetation cover (and crop map).

SWAT Model:

We will explore water allocation dynamics under various land use (based on suggested policies and future/projected crop land use vs. historic) and climate scenarios. We aim to understand the interactions between land use patterns and water availability within the basin. Other relevant outcomes from SWAT include water yield and groundwater.

Agronomic Module:

Using AUB's GYMEE model we will estimate biomass (above ground biomass and biomass deficit) associated with both current and future land use practices under different climate change scenarios. These estimations will provide insights for informed decision-making regarding potential land use adjustments aimed at mitigating the impact of climate change on water resources. The agronomic model will use ET output from the hydrologic model.

Economic Module:

We will incorporate a microeconomic model into our framework to explore the impacts of alternative policies including TAP on land and water use, as well as the impacts of changes of the water system on the human system, under alternative scenarios.

Interconnections between Models:

Output from microeconomic analysis, including agents' behavior on water and land use, will inform the land and water use in the agro-hydrologic model, allowing for an economic and physical assessment of agents' responses, thus enhancing understanding of the socioeconomic drivers of water usage and their impact on water balance dynamics.

In turn, output from the water balance analysis will constrain agents' decisions and drive the land use change analysis, providing insights into how changes in land use may impact runoff patterns and overall water availability.

Data from the water balance analysis, including soil moisture levels and effective runoff, will inform the Agronomic Analysis, aiding in biomass estimation by providing insights into soil moisture availability and potential water stress on vegetation.

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4.1.2. Gantt Chart

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Figure 7. Orontes River Basin Gantt Chart. Where data or calibration phases do not appear, this indicates that they have been already completed for those models.

4.1.3. Key uncertainties and sensitivity analysis

The agro-hydrologic model is subject to uncertainties stemming from input data and underlying assumptions, particularly given its uncalibrated nature. Potential errors may arise from inaccuracies in precipitation inputs and model parameterization.

Weather data uncertainty: In regions characterized by complex topography-plain interfaces, pixel-level data may not accurately reflect local conditions. This challenge could be mitigated by employing downscaling techniques using Machine Learning algorithms or lapse rate adjustments. We will consider alternative datasets for the calibration to account for the consequences of weather uncertainty in input data for the hydrological model SWAT. We will also quantify parameter uncertainties in SWAT model.

Satellite data (multispectral and thermal) uncertainty: The presence of clouds can lead to limited observations, introducing uncertainty, particularly during gap filling processes in scanline correction. Addressing this uncertainty necessitates robust strategies for handling cloud-induced data gaps.

Soil data uncertainty: In cases where soils exhibit significant heterogeneity at larger scales, the resolution of modeling data may not adequately capture field conditions. Discrepancies in soil composition, such as variations in percentage clay, sand, and silt, can result in differing estimates of soil moisture and water capacity, influencing model output. We will quantify uncertainties by using various models (HSEB, VIIRS SSEBOP) to estimate water use and various GCMs to be able to get a feel on how model choice affects policies.

Prices and costs uncertainty: economic prices and costs are typically obtained from surveys that are prone to experience biases leading to uncertainty in data inputs. We will conduct sensitivity analysis of relevant variables in the microeconomic models (yield prices, input costs) to quantify uncertainty and identify key vulnerabilities, their drivers, and potential tipping points.

4.2. Nitra River Basin

4.2.1. Modules and protocols

The diagram below shows the modeling framework for the Nitra River Basin, which focuses on the hydrology module. A comprehensive depiction that includes additional details and components of the models in the framework is available in D2.1.

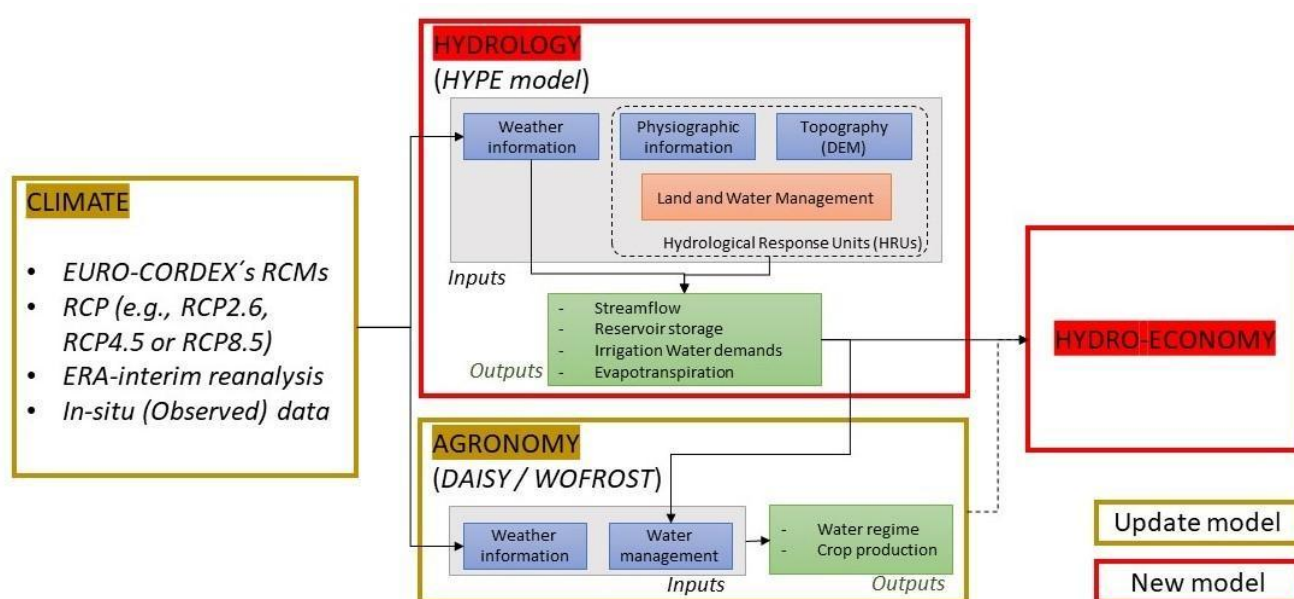


Figure 8. Nitra River Basin Diagram.

For the climate module, SHMÚ has been preparing climate scenarios for Slovakia, which are under development and not fully available for all parameters. SHMÚ uses five selected RCMs from the EURO-CORDEX initiative. Furthermore, climate change scenarios (e.g., RCP2.6, RCP4.5 or RCP8.5) are taken into consideration. In addition, other products are also available and considered within this module, such as CMIP6, ERA-interim reanalysis, CNRM_CM6, MPI. All of them provide information on climate variables used as forcing in hydrological and agronomic models, mainly.

For the hydrology module, water flows in the upper Nitra River Basin will be simulated using the Hydrological Predictions for the Environment (HYPE) model. It is a semi-distributed and process-based hydrological model, used for the assessment of water resources and water quality at small and large scales. This model is capable of simulating water balance and nutrient fluxes with a daily or sub-daily scale utilizing precipitation and temperature data as primary inputs, describing major water pathways and fluxes within a catchment. Catchments are segmented into sub-catchments, which are then subdivided into hydrological response units (HRU), defined as combinations of soil type and land use.

HYPE also incorporates simulations of water management practices. For instance, it can simulate regulated lakes or reservoirs with specific target release parameters. Moreover, the model includes the capability to simulate irrigation based on calculated crop water demands, which are determined by different methods integrated within the model's configuration.

The agronomy module includes two agronomic models (DAISY and WOFOST), both used to simulate agricultural production, water use and nutrient dynamics in agricultural soils. Climatological data are used as input for both models.

The economic module includes microeconomic (see Annex I) and potentially also macroeconomic models. The addition of the latter will depend on the magnitude of the local economic impacts identified using the microeconomic module.

For this living lab, development is currently underway for modules focused on water management, as well as (micro)economic modules. Particularly for the water management module, the HYPE model is expected to provide nuanced insights into water resource allocation, usage efficiency, and potential impacts of different management strategies. For the other modules under consideration, the selection of appropriate models is currently undergoing an evaluation process. The potential modelling frameworks to ensure that the most effective and relevant tools are chosen for the specific needs of the Nitra River Basin is under review.

The initial step is setting up the HYPE model using observed data, at daily or sub-daily timestep, for the key forcing variables (precipitation and temperature, mainly). This setup phase will be followed by a calibration and validation process, utilizing observed streamflow data to evaluate the performance of the model. Once calibrated and validated, the model will be used to incorporate input from different climate models. This will enable the assessment of the hydrological responses to a number of climate scenarios. A similar process might be adopted for the agronomic module, although with a distinct focus on assessing crop production. It is important to note that one key activity in the upper Nitra basin is coal mining, which has had a 100-yr-old history in the region. Yet, this is changing rapidly as coal mining has ended by the end of 2023 due to the commitment to phase out coal, which allows a transition from the coal-mining based economy to a potentially more sustainable and greener economy. Therefore, a microeconomic (and potentially a macroeconomic) model will be used to simulate the impacts of the region's transition on water balance, and vice versa, and inform thus water management in the affected part of the basin. To assess human-water system feedback we will link the output generated by the hydrological model, including simulated streamflows, with the hydroeconomic module. This integration will allow for a comprehensive assessment of the economic impacts of water resource management in the upper Nitra basin.

Data collection is still in progress. Data are not readily available due to legal reasons, and have to be purchased from the SHMÚ. As a first step, meteorological and hydrological stations in the basin have been defined and we are in a phase of acquiring datasets from the corresponding institutions. Once the information is available, the HYPE model will be setup.

4.2.2. Gantt Chart

Module	Model	Data/ Calib/ Sim	Month																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
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Figure 9. Nitra River Basin Gantt Chart. The data acquisition, calibration and simulation phases for the hydrologic module are tentative. For the agronomic, microeconomic and macroeconomic models data acquisition, calibration and simulation are still pending and conditional on data acquisition for the hydrological module. Where data or calibration phases do not appear, this indicates that they have been already completed for those models.

4.2.3. Key uncertainties and sensitivity analysis

1. Uncertainties in parameters that affect the streamflow simulation, including soil processes.
2. The choice of scale and division of the basin into sub-basins and hydrological response units, which can affect the sensitivity of the model to local variations.
3. The model's ability to accurately represent human interventions, such as the operation of dams.
4. Prices and costs uncertainty: economic prices and costs are typically obtained from surveys that are prone to experience biases leading to uncertainty in data inputs. We will conduct sensitivity analysis of relevant variables in the microeconomic models (yield prices, input costs) to quantify uncertainty and identify key vulnerabilities, their drivers, and potential tipping points.
5. Variability and errors in the input data, e.g. temperature, precipitation and streamflow data.
6. Uncertainties related to water use management data. This information is currently not available and constrain the calibration process.
7. Overall, data constraints are significant in this lab. Once this issue is overcome, a more thorough planning, including of uncertainty quantification, will be feasible.

4.3. Júcar River Basin

4.3.1. Modules and protocols

As summarized in the diagram presented in D2.1, the main improvement nodes for the Júcar River Basin (JRB) modelling analysis are: 1) hydro-economic models; 2) system dynamic model; 3) agronomic model; and 4) improved climate change projections. All models will be loosely coupled with no feedback loops, which means that all of them will be executed sequentially.

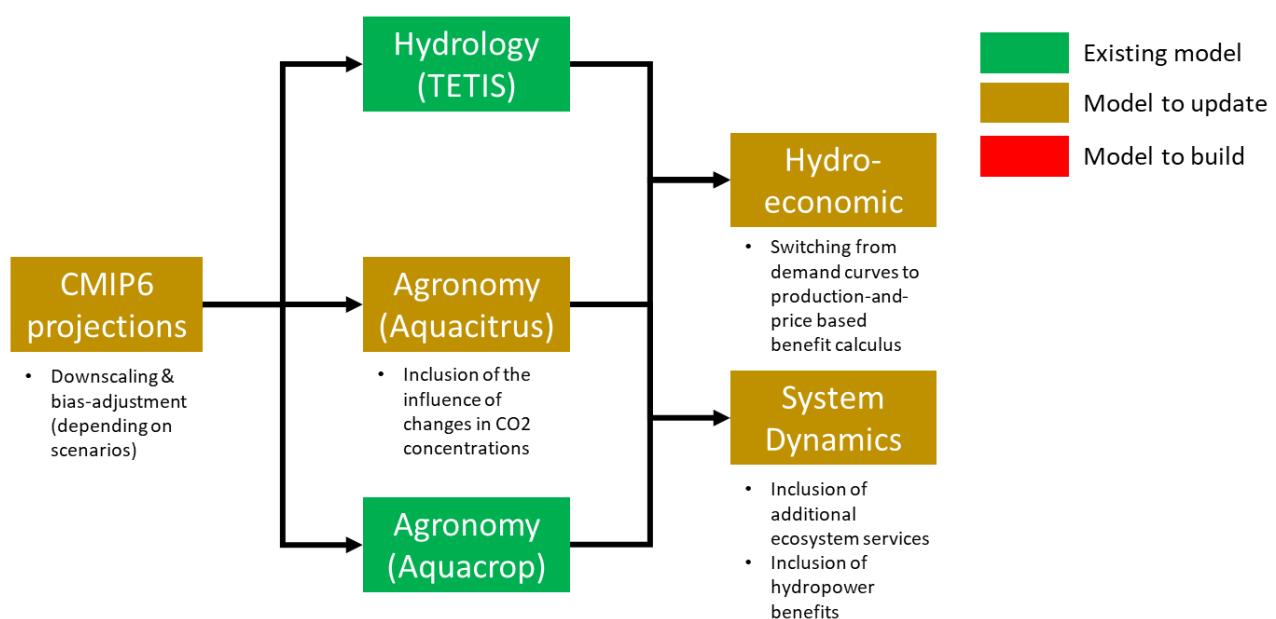


Figure 10. Júcar River Basin Diagram.

CMIP6 Scenarios specifically tailored for the Jucar River Basin through statistical downscaling are available, corresponding to those used by the ISIMIP project (5 climate models for SSP1_2.6, SSP3_7.0 and SSP5_8.5), downscaled against ERA5-Land (10 km resolution) using the ISIMIP BASD algorithm. Additional scenarios could be downscaled too by applying novel downscaling and bias correction methods, including artificial intelligence. The meteorological variables provided by these scenarios will be inputs for the hydrological and agronomic models.

The eco-hydrological model TETIS is a fully distributed model that estimates all the key stocks and flows of the hydrological cycle (e.g. surface runoff, infiltration, groundwater discharge, snowmelt and river routing) with a daily time step and a 250m pixel resolution. Its use in TRANSCEND will be the development of future hydrological scenarios in response to climate change projections. These scenarios will be used as inputs by the hydroeconomic and the system dynamics models.

Aquacitrus is an agronomic model designed for woody citrus crops. The model estimates the dynamics of citrus trees and can be used to estimate their irrigation needs in response to external factors such as climate variations, as well as expected crop yields in response to those needs. In TRANSCEND, this model will be used to infer future irrigation needs in response to climate change scenarios, which will be inputs for the hydroeconomic and the system dynamics models. Similarly, Aquacrop models for the herbaceous crops, which in the Jucar can be found in the Mancha Oriental area, will be used to estimate future irrigation needs to be introduced into the same models as described before.

The hydroeconomic model of the JRB estimates the physical (e.g. reservoir releases, storages, deliveries, pumping rates) and economic (e.g. demand benefits, costs, water values in reservoirs) variables associated with the current operation of the JRB at the monthly scale. The model is trained against historical records of the Jucar river basin (reservoir storages and releases, streamflows and demand deliveries). The physical features are computed using mass balance equations in system's nodes and arcs. The economic features are computed using two approaches: using economic demand functions (aka demand curves) and employing a variant of the FAO33 method that estimates the loss of agricultural production (with respect to the full-supply value provided by an agronomic model) in response to water deficits, and then obtains agricultural economic benefits multiplying the final production times the price of the crop associated with any demand. In demands with multiple crops, a crop mosaic is provided and the process described above is applied to all crops of the respective demand assuming an equitable water share across all the crops included. This model will be used in TRANSCEND to estimate how the performance of the system varies according to the changes in water availability and water demand.

The system dynamics model is being expanded to include additional ecosystem services and the dynamics land use based on long term dynamics within the model. This includes incorporating fish habitat curves in selected streams and accounting for hydropower production and its associated benefits. It is also foreseen to incorporate the economic features as they are computed by the

hydroeconomic model. Its use in TRANSCEND will be similar as the one of the hydroeconomic models, and depending on the degree of integration of the economic features both models might be unified into a single system dynamics hydroeconomic model.

These models and data collectively contribute to a more comprehensive understanding and management of the Jucar River Basin's water resources, agricultural productivity, and ecosystem services in the context of climate change and socio-economic developments. They are decision-making tools, helping predict outcomes and plan for sustainable resource use, thus reducing uncertainty associated with the policy relevance of future scenarios—given many of these scenarios are developed by decision makers themselves.

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4.3.2. Gantt Chart

[illegible]

Figure 11. Júcar River Basin Gantt Chart. Where data or calibration phases do not appear, this indicates that they have been already completed for those models.

4.3.3. Key uncertainties and sensitivity analysis

The key uncertainties identified in the Jucar river basin modelling suite refer to:

- Input uncertainties
 - From observations
 - From other models
- Model uncertainties
 - Parameter uncertainties
 - Structural uncertainties
- Future conditions uncertainties
 - Future climatology
 - Future socioeconomic drivers and projections

The evaluation of input uncertainties from observations is challenging because in most cases a single data source is employed (e.g. reservoir levels are provided only by the Jucar River Basin Agency). Consequently, no uncertainty analysis for observed input variables is proposed.

In order to address the rest of the uncertainties indicated above, the following uncertainty and sensitivity analyses are proposed:

- Inputs from other external models: the results from the uncertainty analyses performed for these models will be used as uncertainty estimators for this.
- Model parameter uncertainties: depending on the model, we will perform either sensitivity analyses based on the OAT method or the full factorial sampling, or uncertainty analysis using random sampling and/or Monte Carlo methods. The final choice of method will depend on the particular configuration of each model. For the case of TETIS, there has been a lot of research related to quantifying its uncertainty (e.g. Hernández López, 2012). For AQUACROP and AQUACITRUS, there is also literature on global sensitivity and uncertainty analyses (Xing et al., 2017; Guo et al., 2020). Uncertainty and sensitivity analyses to be performed will refer to key variables and parameters of each model in order to provide an adequate estimation with lean computing requirements.
- Model structural uncertainties: these uncertainties will be addressed by fitting error models to the selected variables, comparing model results with observations. This may lead to changes in the design of the model via parameters, and thus may be categorized as parameter uncertainty.
- Future climatology uncertainties: they will be addressed by adopting a scenario analysis strategy using CMIP6 projections. For each scenario, model outputs will be extracted and compared with other scenarios in order to find out how the results vary across them. Furthermore, for each scenario a multi-model ensemble will be adopted in order to quantify the uncertainties associated to the future projections of each particular scenario.
- Future socioeconomic drivers and projections uncertainties: they will be addressed similarly to the climatology uncertainties. In particular, CMIP6 scenarios are tailored to particular SSPs, for which socioeconomic and land use scenarios exist. Data on these projections per SSP will

either be collected from previous research projects or generated through the scenathons foreseen.

4.4. Reno River Basin

4.4.1. Modules

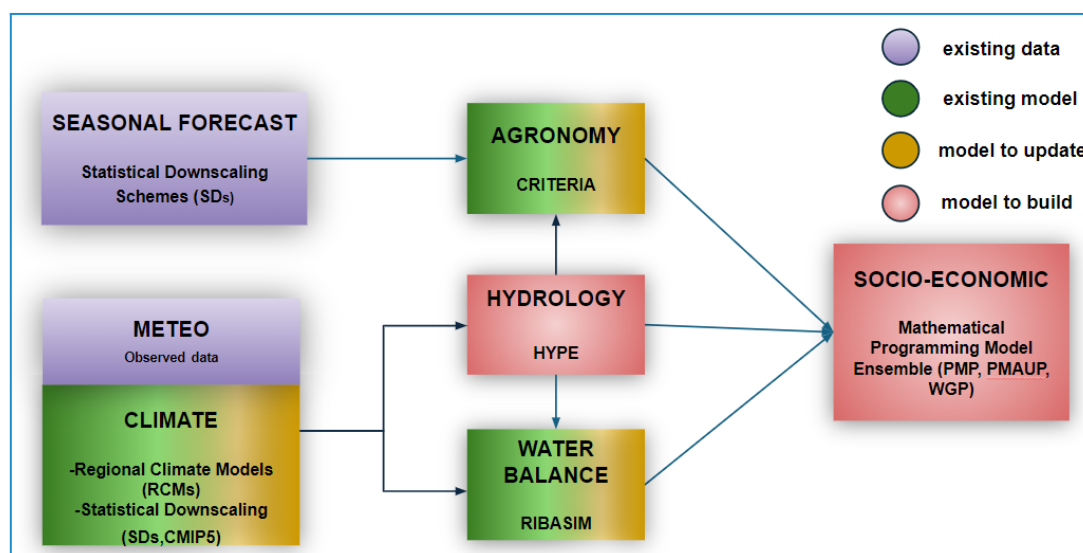


Figure 12. Reno River Basin Diagram.

As summarised in the above diagram the main modules involved in the modelling analysis over the upper Reno River Basin include **meteorological**, **climatological**, **agronomical**, **hydrological** and **socio-economic**. A brief description of each module is presented in the following.

Meteorological module

Statistical downscaling technique is implemented by Arpaie - Climate Observatory to provide operational calibrated probabilistic seasonal forecasts, using MOS approach, based on Copernicus Climate data (more details are available in D2.1 -*Blueprint for the modelling suite* - page 6). The seasonal forecasts produced over Reno basin are used as input in the "Agronomy module" to produce irrigation water demand for agricultural area, at meteorological time scale (seasonal).

Climate module

High-quality input climate data is requested by hydrologic models to accurately simulate runoff, infiltration, and groundwater recharge processes. Any inaccuracies in the input climate data can propagate through the modeling system, leading to significant errors in the prediction of water availability, flood and drought risk, and the overall water balance of a catchment or region and then further propagate into the socio-ecological systems models. To improve the spatial resolution and the

ability of the global climate models (GCMs) in representing small-scale features, dynamical and statistical downscaling methods are being developed and used as part of TRANSCEND for implementation over Reno River Basin, which we describe below.

Dynamical downscaling uses Regional Climate Models (RCMs) to zoom into a region of interest and simulate high-resolution climate (typically at scales of tens of kilometers or less) using GCM output as boundary conditions. This technique generally provides a more accurate representation of local climate compared to GCM simulations through higher resolution model physics, dynamics, and topographic and land cover data.

For the Reno Basin, precipitation and temperature products will be used from the European domain for the Coordinated Downscaling Experiment (EURO-CORDEX) initiative (EURO-CORDEX, 2022) (Gutowski et al., 2016). The output represents a large suite of RCM models using boundary conditions from a large suite of models taking part in Coupled Model Intercomparison Project Phase 5 (CMIP5) (Taylor et al., 2012). The historical simulations generally encompass the years 1948 to 2005. The climate change scenarios range from a low IPCC atmospheric greenhouse gas concentration scenario (RCP 2.6) to a very high IPCC concentration scenario (RCP8.5) from the year 2006 to 2100. In total, there are nearly 50 combinations of model and scenario simulations, which can provide a good indication of the uncertainties, including between the different scenarios and different models. The EURO-CORDEX simulations are performed at spatial resolutions of 0.44 degrees (EUR-44, ~50 km) and 0.11 degrees (EUR-11, ~12.5km). In cases necessitating daily input for HYPE, the standard EUR-11 output will be used. In cases where daily data are sufficient, the bias-adjusted output will be used (Menz Christoph, 2023, Casanueva et al., 2016).

An additional set of very high-resolution RCM simulations will be used specifically generated for the Italian peninsula and neighboring areas by CMCC (Raffa et al., 2023). These data are available at grid spacing approximately 2.2 km at hourly intervals for the period 1981 to 2070, under the IPCC scenarios RCP 4.5 and RCP 8.5.

Statistical downscaling applies empirical relationships between large-scale GCM-simulated climatic variables and observed local climate data to generate data at the local scale. This method has the advantage of being considerably less computationally demanding than dynamical downscaling.

Arpae-Climate Observatory produces future climate projections at local scale through statistical downscaling scheme, based on Perfect-Prog approach (CCAReg scheme, (Tomozeiu et al., 2007, 2018), details included in the Annex II. This technique will be applied to downscale seasonal temperature and precipitation over Reno Basin using multi-model approach, in the framework of RCP4.5 emission scenario and 2021-2050 period.

Another method using machine-learning approaches will also be investigated for downscaling in the basin.

Agronomic module

CRITERIA is the agronomic model developed at the premises of Arpae - Climate Observatory. It will be used to simulate agronomic values and crop yields in Reno River basin; its characteristics were already described in the D2.1 *Blueprint for the modelling suite* (pages 5).

Hydrological module

The hydrology module will be based on the Hydrological Predictions for the Environment (HYPE) model to simulate the dynamics of water flows in the Reno River Basin. For more details about the HYPE model, including its methodologies and open-access code, please refer to (Lindström et al., 2010) and/or visit <https://hypeweb.smhi.se/model-water/> (last access: 30 April 2024).

The Reno River basin closed at Casalecchio, near Bologna, has a catchment around 1050 km². The elevation ranges from 1900 m to 63 m, with most precipitation from October to April, peaking in November, which significantly influences the runoff and flood patterns. Notably, the discharge for a 10-year return period is estimated at around 1100 m³/s, based on 70 observed annual maxima (Montanari and Toth, 2007).

HYPE is a semi-distributed and process-based hydrological model, used for the assessment of water resources and water quality at small and large scales. This model is capable of simulating water balance and nutrient fluxes with a daily or sub-daily scale utilizing precipitation and temperature data as primary inputs. Catchments can be segmented into sub-catchments, which are then subdivided into hydrological response units (HRU), which are defined with specific combinations of soil type and land use.

HYPE also incorporates simulations of water management practices. For instance, it can simulate regulated lakes or reservoirs with specific target release parameters. Moreover, the model includes the capability to simulate irrigation based on calculated crop water demands, which are determined by different methods integrated within the model's configuration.

Water Balance module

To evaluate the water balance at the basin scale, the RIBASIM water balance model will be used (<https://oss.deltares.nl/web/ribasim/ribasim>). This model is already operative and calibrated for the Reno by Arpae - Hydrology Area.

RIBASIM is a generic model package for simulation of the behaviour of river basins during varying hydrologic conditions. The model is a comprehensive and flexible tool to link the hydrologic inputs of water at various locations to the various water-using activities in the basin and to evaluate a variety of measures related to infrastructure and operational management. It provides an efficient handling and structured analysis of the large amounts of data commonly associated with (complex) water resources systems.

The types of analysis addressed by the model are the following:

- evaluation of the limits on resources and/or the potential for development in a basin. Given the available water resources and their natural variations, to what extent can a river basin be developed in terms of reservoirs, irrigation schemes, water supply systems, while avoiding unacceptable shortages for users? When and where will conflicts between water users occur? Which combination of infrastructure and operational management will provide an optimum use of the available resources?
- evaluation of measures to improve the water supply situation: measures concern changes in the infrastructure, operational management and demand management; evaluation of the origin of water for every location in the river basin as a first step towards an actual water quality analysis without the necessity of having available information with regard to waste loads, waste water discharges and water quality of (upstream) sources the effect of measures on the distribution of water from the various sources in the basin is calculated (influence area of a source of water);
- simulation of the water balance of the region/basin forms the basis for such analyses. RIBASIM provides the means to prepare such balance with sufficient detail, e.g. taking into account reuse of water, and with facilities to vary the simulated configuration and to process results.

Water allocation simulation

To perform river basin simulations with RIBASIM, a model schematization of the study area is prepared in the form of a network, consisting of nodes connected by links. Such a network represents all the features of the basin that play a role in its water balance. Four main groups of schematization elements are differentiated in the model:

1. Infrastructure, both natural and manmade (reservoirs, lakes, rivers, canals, surface water, aquifers and pumping stations, pipelines);
2. Water users, or in a wider sense: water related activities (domestic, municipal and industrial water supply, agriculture, hydropower, aquaculture, navigation, recreation, nature);
3. Management of the water resources system (operation rules for surface water reservoirs and diversions, aquifers, priorities and proportional water allocation, minimum flows in certain river stretches for sanitary or ecological reasons);
4. Hydrology (inflows to the system, inter-basin flows, precipitation, evaporation), geo-hydrology (groundwater), and hydraulic behavior (e.g. flow level relationship);

Model schematization

Even though the model is conceived for steady-state calculations, an incorporated Muskingum-Cunge scheme allows for simple channel routing within the system, where water travel times need to be evaluated.

To fully describe the basin, it is necessary to prepare a schematization of the hydrographic basin, in which the following elements are explicitly modelled:

- irrigation areas: computation of water demand on the network considering crop characteristics, irrigation practice parameters and actual rainfall; conjunctive use of groundwater and surface water

for various water users like irrigation and public water supply in cities; water balance of aquifers; pumping capacity and maximum groundwater depth for abstraction from an aquifer; minimum flow requirements for sanitation, navigation or ecology; loss flow from river stretches to groundwater; run-of-river; power plants; hydropower production requirements at surface water reservoirs in the Alps: firm (guaranteed) and secondary energy, scheduling; return flows from users (agriculture, aquaculture, public and industrial water supplies); additional (backwater) abstractions from surface water reservoir for various water users; surface water reservoir operation rules (firm storage, target storage e.g. for average maximum energy generation, flood control storage); sub-catchments (water districts) which form a hydrological unit from the viewpoint of water supply and demand; hydraulic description of (part of) river stretches and partitions of surface water reservoir; various hydrologic flow routing methods (2-layered Muskingum, Puls method, Manning, Flow-water level relation); routing of flow salinity and computation of flow composition.

Input for RIBASIM covers the following information and data:

- river basin network schematization: location of surface water reservoirs, aquifers (groundwater reservoirs), irrigation areas, diversion weirs, (river) channels, sub-catchments comprising a system of nodes and links; model data characterising each node and link in the schematization; preferred sources of water for the identified water users in the basin; water allocation rules and operation rules for surface water reservoirs, aquifers and diversions; hydrologic data (time series of available flow at the system boundaries e.g. from inter-basin transfers, open water evaporation, rainfall, general district water demand and discharges, water district runoff); salinity data (lookup tables for the Adriatic Sea boundary).

By implementing the model in the DELFT-FEWS system it is possible to update the inputs in real time, allowing the development of early warning scenarios for scarcity events.

The output of RIBASIM covers the following information and data:

- simulation results can be processed with a variety of standard postprocessors into graphs, spreadsheets, maps and tables. By implementing the model in the DELFT-FEWS system it will serve as a graphical user interface; for a quick visual interpretation of results a number of graphs can be produced on screen (e.g. during calibration testing) via the DELFT-FEWS time series visualization tools. The form of the graphs can be adapted according to the user requirements. Graphs show e.g. the applied cropping pattern, the water allocation, the shortages per user, the actual surface or groundwater reservoir storage, the overall water balance of the basin and the energy production; tables range from summaries of the main results (success rate, allocated amounts of water, water shortages, water utilisation rate, failure year percentage and energy production) to user-defined tables with detailed results per time step for specific variables per node or link.

Socio-economic module

The Socio-economic Module will make use of an ensemble of models to understand human behavior and anticipate their responses. The multi-model ensemble consists of five different programming models, namely: 2 Positive Mathematical Programming Models (PMPs), 2 Positive Multi-attribute Utility Programming models (PMAUP) and 1 Linear Programming Mode (LP). These economic models have been frequently used in the literature of agricultural and water management. The objective of this ensemble is to elicit farmers' behavior and their optimal crop portfolio to maximize the utility, subject to a set of constraints (Graveline, 2016a). The reader can refer to Annex I for more details on the different models used. The microeconomic module will receive input from the other modules in terms of water availability for the economic agent and yields under climate change, as well as other relevant constraints/data inputs, and produce the new crop portfolio responses and related profit, employment, Gross Value Added and other relevant aspects.

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4.4.2. Gantt Chart

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Figure 13. Reno River Basin Gantt Chart. Where data or calibration phases do not appear, this indicates that they have been already completed for those models.

4.4.3. Key uncertainties and sensitivity analysis

List of key parameters of uncertainties in modelling (and related monitoring):

1) *Input uncertainty*

-quality, spatial and temporal resolution of observed climatological data over the Reno Basin used in the calibration and validation of SDs. To reduce the uncertainties related to these, the calibration and validation of SDs is done using temperature and precipitation data derived from Eraclito gridded data base (<https://dati.arpae.it/dataset/erg5-eraclito>). This is obtained based on controlled and homogenized station data from Emilia Romagna, over 1961-2010 period. In addition, the climatological data over Reno Basin and large-scale data derived from ECMWF reanalysis are filtered before used in the calibration of the SDs.

Furthermore, hydrological and agrometeorological observed data accuracy is also affected by instrumental sensitivity and accuracy. This is overcome by a daily quality control for agrometeorological data and a yearly quality control for hydrological data. This reduces uncertainty, but does not remove it.

For the economic model, we will conduct global sensitivity analysis of relevant variables in the microeconomic models (yield prices, input costs) to quantify uncertainty and identify key vulnerabilities, their drivers, and potential tipping points.

2) *Parameter uncertainty*

Parameter uncertainty will be assessed in the calibration process using info about data uncertainty (for example the discharge which has already uncertainty due to e.g. the rating curve that converts water level into discharge). Global sensitivity analysis will be conducted to the extent allowed by the computational cost for HYPE and the microeconomic ensemble.

3) *Structural uncertainty*

The statistical downscaling (CCReg) implemented to project future amounts of precipitation and temperature over Reno basin assumes that the relationships between local (predictand) and large scale (predictors) identified over present period is kept also over the future. To reduce the uncertainty based on this assumption, the link predictor-predictand is tested and quantified over different time periods. This is done by applying canonical correlation analysis (CCA), that identifies strong and physically meaningful relationships predictor-predictions, over different periods. In this work, the calibration and validation periods are inverted. Also, the input data are filtered before the CCA such as to separate the signal by the noise. Another source of uncertainty in the CCAReg is represented by the skill of GCMs, namely how well they can reproduce the atmospheric patterns (predictors). The range of uncertainty due to GCMs, formulation in general, and parameterizations, is assessed and reduced using a multi-model approach. In this work up to six GCMs from Cmp5 will be used to feed the seasonal CCAReg scheme. To have greater statistical robustness of climatological projections, the

changes obtained through the statistical downscaling applied to vary GMCs- Cmp5 are combined with the Ensemble Mean technique.

The uncertainties quantification and sensitivity analysis in climatological modules will be assessed using outputs provided by different RCMs and SDs (feed by different GCMs), constructed also in the framework of different emission scenarios (RCMs case). Bias adjustment of future changes, construction of Probability density functions (Pdfs) and box plots of projections will be the main tools used to solve and to quantify the key parameters of uncertainties in statistical downscaling, over 2021-2050 (RCP4.5).

For the hydrological modelling of the Reno basin, the main source of uncertainty is associated to parameters that affect the streamflow simulation and also the soil moisture and soil processes, e.g. within the HYPE model 11 parameters should be calibrated. Also, the choice of scale and division of the basin into sub-basins and hydrological response units, which can affect the sensitivity of the model to local variations.

Structural uncertainty will be also explored in the microeconomic model via a multi-model ensemble (see previous subsection).

4.5. Titicaca – Desaguadero - Poopo

4.5.1. Modules

The representation of the basins of Lake Titicaca, Desaguadero River and Lake Poopo relies on a sequence of models that build on top of a WEAP model previously developed in Peru and Bolivia. The following figure describes the different components (to be) developed for the modelling. Importantly, the study area for which this analysis is being developed has been modified from the original basin scheme at the request of the Ministry of Foreign Affairs of Peru, with the focus of the study being the basins of Titicaca, Desaguadero and Poopo.

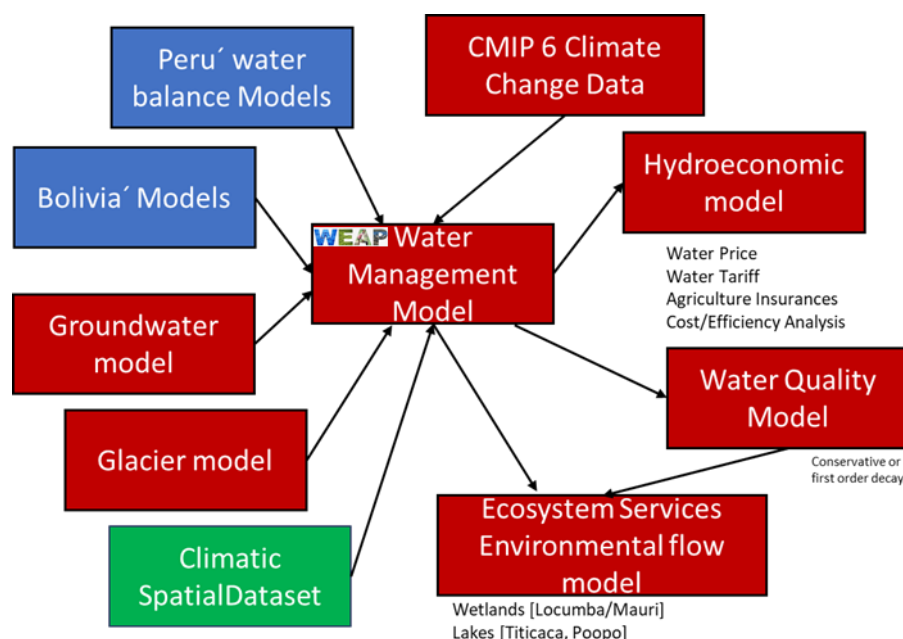


Figure 14. Caplina-Mauri-Desaguadero System Diagram.

The water modelling components to describe surface soil water transport processes will be covered through the soil moisture method available in WEAP as described in Yates et al., (2005) . The reference surface evapotranspiration component will be addressed through the Penman Monteith method as recommended and described in Pereira et al., (2015). The glacial component will be developed through simplified procedures based on degree/month factor methods that take into consideration a simple mass balance as described in Condom et al., (2011).

SEI developed a supply and demand model [WEAP platform] for the basin system of Lake Titicaca, Desaguadero, Mauri, and Lake Poopo (Lima-Quispe et al., 2021), to evaluate the effects of increasing agriculture irrigation and the influence of climate variability. According to the analysis of Lima N., et al., (2021), 80% of the changes in the volume of Lake Titicaca (the largest lake in South America) are related to climatic variability and the remaining 20% related to regulation and consumption for agricultural production. In the case of Lake Poopo 65% is attributed to climate variability while 35% has its source in the regulation of productive systems in the Lake's contribution areas. In this case, the model allowed establishing representation of water use, as well as the fluctuation in the supply of both the water system, as well as the two lakes of the system. This is the starting point of the hydrological model for the living lab.

Climatic module

Future climate conditions are a relevant uncertainty factor for water resource management; furthermore, how the climate will evolve and how it will affect future water availability are important unknowns to consider. To analyse these uncertainties, the results presented in the sixth Assessment Report (AR6) of the Intergovernmental Panel on Climate Change (IPCC) will be used. This data is

described in O'Neill, et al., (2016). For the Living-Lab climate modelling, 20 General Circulation Models (GCM) and the 4 Shared Socio-economic Trajectories scenarios prioritized in the AR6-IPCC (SSP) will be evaluated. The selection of the GCMs will be based both on the availability of information necessary for the WEAP model (precipitation, average temperature, and extreme monthly temperatures) and on whether they have been evaluated in the 4 SSP scenarios.

Agricultural module and monitoring

Agricultural information is relevant in the Living-Lab due to the scale of water use, as well as its economic impact on local markets in different municipalities in Peru and Bolivia. There are official databases on the agricultural area in the basins, and the official records and licenses provided to local agricultural systems are also available. Building on monitoring activities in WP4, we will provide a complete assessment of all agricultural production through remote sensing, identifying and classifying agricultural areas in terms of the most important productive systems focused on plantations of quinoa, alfalfa, corn, barley, potatoes, among others. We will use classification methodologies informed by field sampling produced in official surveys and censuses developed by Peru and Bolivia for official reports (2018 and 2013 respectively), as well as remote sensing and other activities to be developed in the project. Likewise, the agricultural production patterns and water use, at the start of sowing, growth and harvest is not completely understood for the region, a gap that we will address via monitoring of the phenological processes through remote sensors and vegetation indices that allow us to know the production dynamics for the different economically and socially most relevant crops. To this end, we will use methods such as those described in Bellon et al., (2017), Gurgel and Ferreira (2003), Hall-Beyer, M. (2003).

For modelling of agricultural water needs, and the impacts on production outcomes of meeting or not meeting these demands, WEAP includes an in-built crop model (MABIA) that is based on the FAO56 modelling approaches. Key weaknesses of the FAO56 approach is that crop development is fixed and assumed to not be impacted by water stress. FAO56 also does not account for non-water related causes of crop stress such as high or low temperatures, or the impacts of changing CO₂ concentrations on crop water productivity (Steduto et al., 2009). To address these limitations, as part of the work in TDP Living Lab we will develop approaches to couple WEAP with AquaCrop-OS: an open-source crop-water simulation model developed by the UoM team within the TRANSCEND consortium (Foster et al., 2017; Kelly and Foster, 2021). Coupling will be achieved through crop-water production functions, externally generated in AquaCrop-OS following the broad approaches set out by Foster and Brozović (2018). Functionality will be developed to enable crop-water production functions to be used as inputs to both WEAP and the microeconomic module. In the microeconomic model, crop-water production functions will be used as the basis for mathematical optimization of crop and irrigation portfolios. In WEAP, crop-water production functions will enable quantification of agricultural water demands and associated production outcomes under stochastic climate variability and climate change scenarios.

Hydro economic module

The hydroeconomic module consists of a coupling between WEAP and an ensemble of microeconomic mathematical programming models that represent the behavior of agricultural water users (described in Annex I). The ensemble of microeconomic models will be pre-run for all relevant TAPs, scenarios and water use, yields, and other relevant inputs (which should be consistent with those used in the WEAP model). Subsequently, the resultant land use portfolios simulated with the microeconomic ensemble will be integrated into the WEAP architecture as plausible land use files. In this way, each simulation run in WEAP will lead to a land allocation consistent with those predicted by the microeconomic ensemble, which will in turn lead to impacts on the water system as modeled by WEAP.

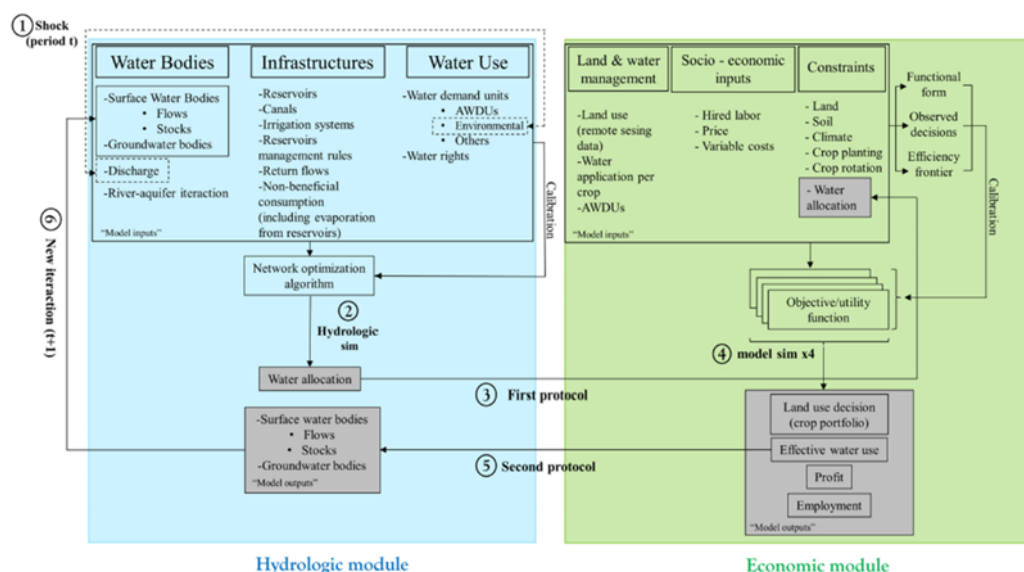


Figure 15. Hydro-economic coupling implementation in the Caplina-Mauri-Desaguadero System.

Deliverable 3.2 – Modeling suite prototype and sourcebook

4.5.2. Gantt Chart

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Deliverable 3.2 – Modeling suite prototype and sourcebook

Figure 16. Caplina-Mauri-Desaguadero System Gantt Chart. Where data or calibration phases do not appear, this indicates that they have been already completed for those models.

4.5.3. Key uncertainties and sensitivity analysis

Visualization and comprehension of uncertainty is difficult to understand for stakeholders. A key objective of the modeling work in this lab is to ensure our modeling outputs are useful for practical applications in daily activities such as development of projects and actions related to water infrastructure and regulation for water related issues in both Peru and Bolivia. Our modeling outputs will be dependent on factors such as changes in precipitation, temperature and other climatic factors that will modify water availability and other key aspects conditioning TAP performance. Likewise, scenarios of changes in demographic, productive, as well as economic aspects will generate changes in water use. The following figure shows a simple approach to assess the degree of uncertainty of the different variables that are going to be explored for the lab, in which a plausible range is defined that has the influence of all the results generated while reflecting an interval on which measures to adopt strategies can be worked on. The “Reliability Ensemble Averaging” (REA) method will allow us to calculate the average, the range of uncertainty and a measure of reliability of TAP under multiple regional climate changes from sets of experiments with different coupled atmosphere-ocean general circulation models (which in our case will come from CMIP6 models) (Giorgi and Mearns, 2002) (Figure 17).

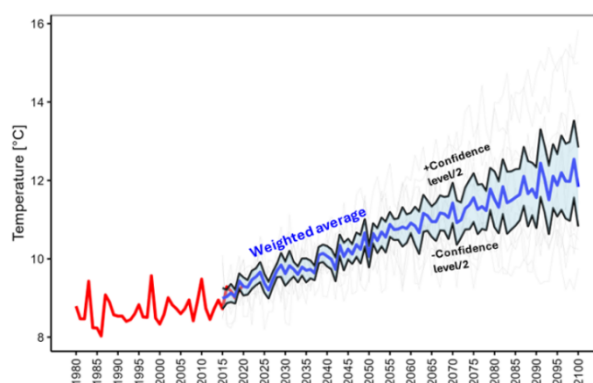


Figure 17. Projected climate variable (temperature) under CMIP6 models and REA average and range scheme.

4.6. Mahanadi River Basin

4.6.1. Modules

The modelling framework for the Mahanadi basin integrates hydrological, and microeconomic models to comprehensively assess the interactions between water resources, agricultural practices, and economic policies.

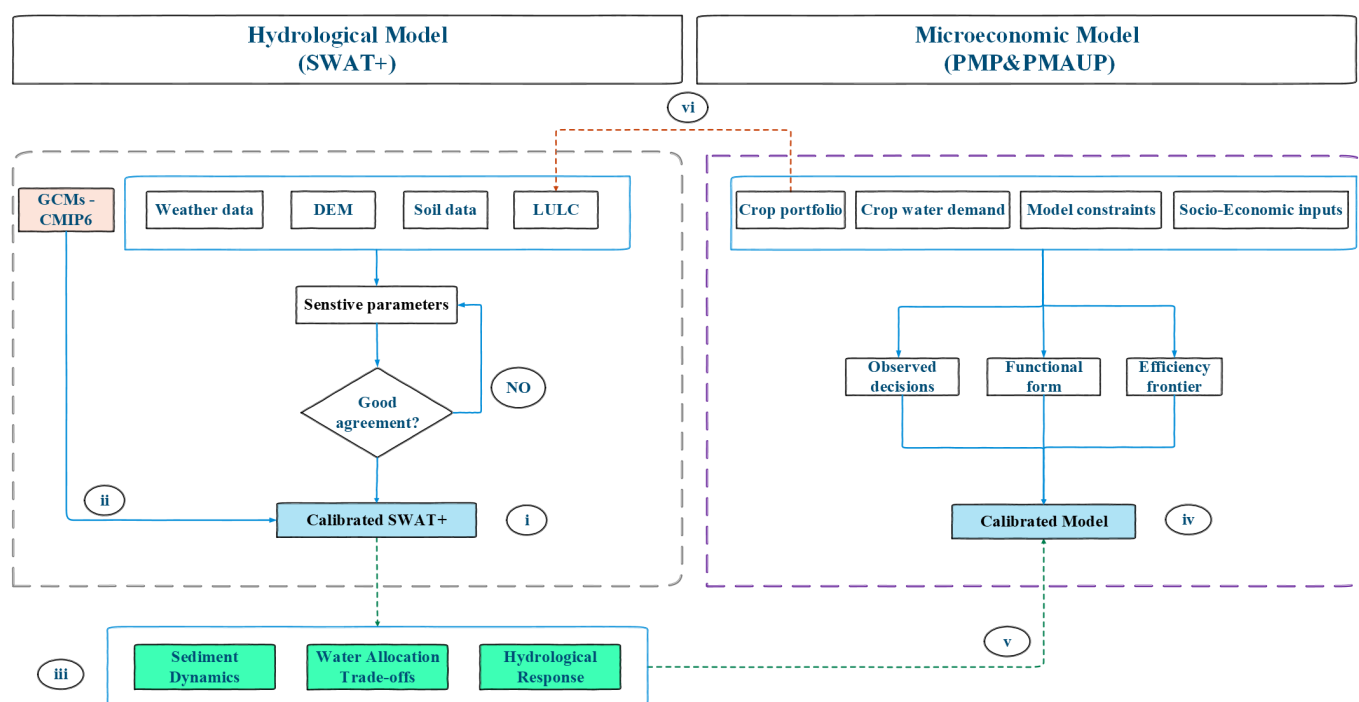


Figure 18. Mahanadi River Basin Diagram.

Hydrological Module: SWAT+ model

The Soil and Water Assessment Tool (SWAT+) will be employed to simulate the hydrological cycle. This model integrates various hydrological processes, such as surface runoff, evapotranspiration, and groundwater flow, to predict the impact of different land management practices on water resources. Furthermore, the model will integrate climate change scenarios from the CMIP6 dataset, providing a comprehensive view of the future basin's hydrology under various climate conditions.

A significant issue in the basin is the accumulation of sediment in reservoirs, which reduces their capacity and affects water storage and management. We will also investigate the sediment dynamics and deposition within the basin, enabling the assessment of sediment management strategies and their impacts on reservoir capacity and water availability.

Furthermore, the basin is facing substantial water allocation challenges that impact agricultural, industrial, and domestic water consumption. These difficulties are exacerbated by the consequences of climate change, rapid industrialization, and increasing agricultural demands. We will evaluate the trade-offs in water allocation across agricultural, industrial, and hydropower sectors to develop effective strategies for sustainable water management.

Microeconomic Module: PMP&PMAUP ensemble of models

The microeconomic module will utilize Positive Mathematical Programming (PMP) and Positive Multi-Attribute Utility Programming (PMAUP) models to simulate agents' responses to water and land use policies. This ensemble of models considers socio-economic inputs, constraints, and water requirements to determine the optimal crop portfolio for each agent. By calibrating the model against

available data for each agent, it can simulate responses to different levels of water availability, from full supply to complete restriction, as well as employing management policies (e.g., water pricing).

Coupling Protocols:

Coupling Between Microeconomic and Hydrological Models:

- ⊙ Coupling Variables: Land use (Crop portfolio)
- ⊙ Direction: Microeconomic Model (PMP& PMAUP) ↔ Hydrological Model (SWAT+)
- ⊙ Time Setting: Dynamic (annual or interannual updates)
- ⊙ Sequence:
 - Start with the baseline crop portfolio from PMP& PMAUP.
 - Set up SWAT+ with the initial land use classes and baseline crop portfolio.
 - Run SWAT+ to simulate the hydrological cycle and assess water availability at the specified timestep.
 - Update the land use in SWAT+ based on agents' response to water availability.
 - Rerun SWAT+ and continue the process until the end of the simulation period.

Deliverable 3.2 – Modeling suite prototype and sourcebook

4.6.2. Gantt Chart

[illegible]

Deliverable 3.2 – Modeling suite prototype and sourcebook

Figure 19. Mahanadi River Basin Gantt Chart. Where data or calibration phases do not appear, this indicates that they have been already completed for those models.

4.6.3. Key uncertainties and sensitivity analysis

Hydrological Model: SWAT+

Parameter uncertainties in the SWAT+ hydrological model primarily involve soil properties that influence infiltration rates, runoff generation, and soil moisture dynamics. Additionally, uncertainties in hydrological parameters, such as the runoff curve number (CN.mgt) and base flow recession constant, are significant due to their dependence on land use, topography, and climatic conditions. Input uncertainties are introduced by climate projections from the CMIP6 dataset, which, despite providing a range of future scenarios, are inherently uncertain due to the complexity of climate systems and modeling assumptions. These uncertainties necessitate careful calibration and validation against observed data to ensure the model's reliability in predicting the hydrological cycle and water availability in the basin.

Uncertainty also arises in reservoir simulations, particularly under future climate change scenarios. Reservoir operations, including storage, release schedules, and water allocation, are critical for managing water resources. Climate change can alter precipitation patterns, inflow volumes, and evaporation rates, impacting reservoir levels and management strategies. Predicting these changes involves considerable uncertainty due to the interplay between climatic variables and human management decisions.

Microeconomic Model: PMP& PMAUP

Structural uncertainties related to the assumptions about agents' decision-making processes and economic behaviours. These assumptions may not fully reflect the diversity and complexity of actual agents' behaviours. To address these structural uncertainties, we will employ multiple economic models, such as PMP and PMAUP, to simulate agents' responses to water and land use policies. Using different models allows us to compare outcomes and better understand the range of possible responses. Input uncertainties can be also relevant and include variations in key socio-economic inputs such as crop yield and prices. The latter are exogenous to the Mahanadi lab model and will be simulated using global sensitivity analysis that correlate the endogenous changes in yield (agronomic model) and land use (economic model) with changes in prices, where decreasing supply/quantities leads to higher prices, and vice versa.

4.7. Tympaki River Basin

4.7.1. Modules

The modeling framework flowchart for the Tympaki basin is presented below.

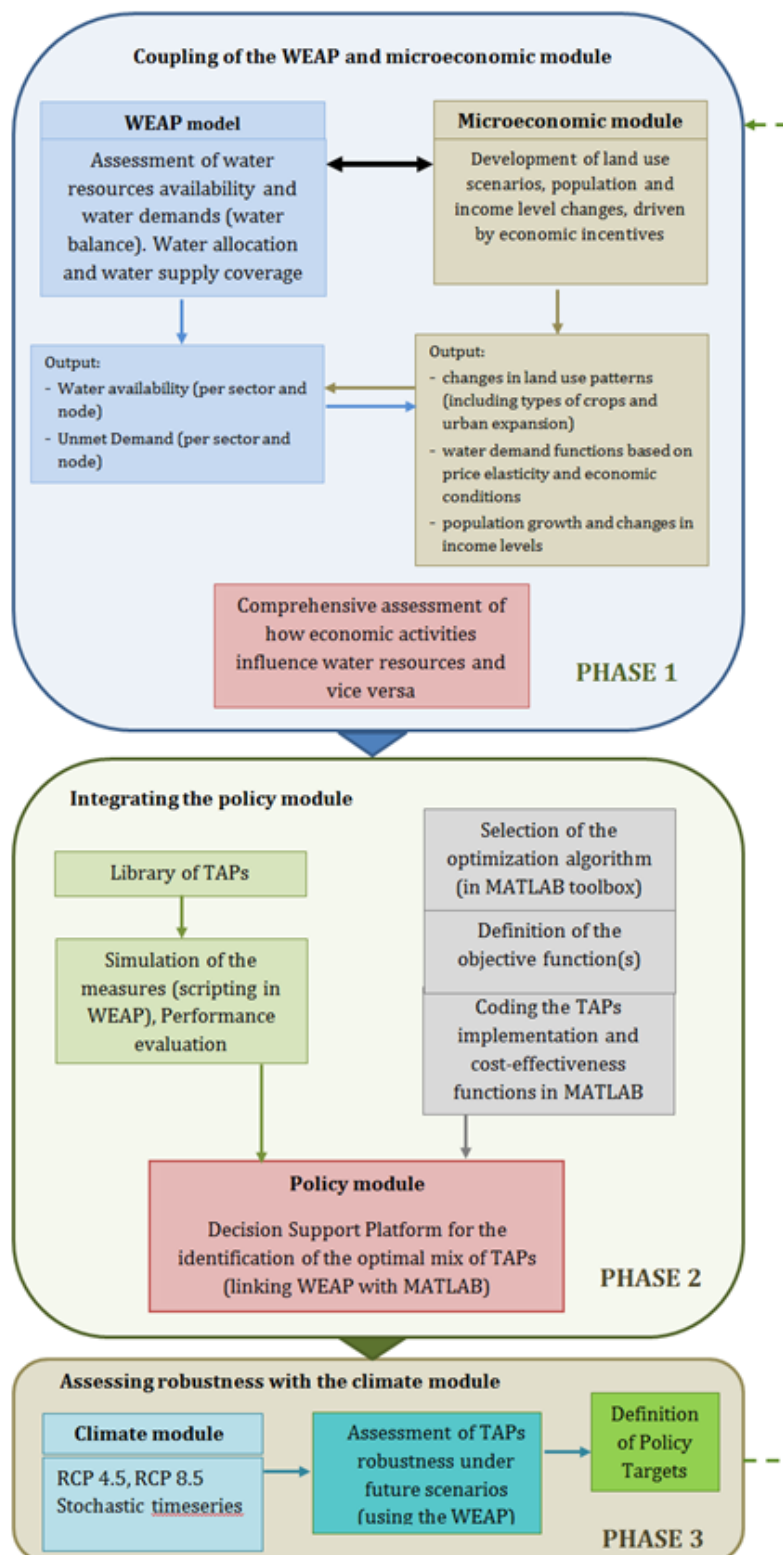


Figure 20. Tympaki River Basin Diagram.

The main modelling environment will be developed in WEAP (**Water Balance module**). A detailed water resources management model will be developed for the Tympaki basin, at monthly scale and sub-catchment level, which will represent the water balance in the basin using physical-based hydrological modelling in WEAP. The baseline (current account in WEAP) will opt to cover at last 10 years of the most recent period, e.g. 2013-2023.

Different climate scenarios will be fed into the calibrated WEAP model, based on the RCP4.5, RCP8.5 and stochastic timeseries, to assess water resources in the future (**Climate module**). The key variables feeding WEAP will be timeseries of precipitation and ET as derived from the future climate simulations/ scenarios. The response of the WEAP model to these forcing parameters will be evaluated in terms of changes in the hydrological and water balance components (i.e. unmet demand, water supply coverage and reliability) for the target year 2040 against the business-as-usual baseline (current account). We will use outputs from CMIP6 and AgMIP to assess impacts on crop yields and productivity as part of our **agronomic module**.

The WEAP will be further coupled with a **Microeconomic module** for integrating the water resource management capabilities of WEAP with the economic analysis of the microeconomic model. This integration will allow for a comprehensive assessment of how economic activities influence water resources and vice versa. The primary goal of the coupling will be to assess the effect of economic growth on water demand, more specifically the effect of different land use scenarios as outputted from the microeconomic model on water demand, and consequently the resulting unmet demand and water allocation. The key interconnections between WEAP and the microeconomic model are the following:

- From the Microeconomic Model to WEAP:
 - Land Use Changes: Outputs from the microeconomic model, such as changes in land use patterns (including existing and new crop varieties/management practices) due to economic incentives or policy changes, feed into WEAP to update land cover and land use data.
 - Crop Types and Yields: Information on crop types and their respective yields can be used in WEAP to estimate irrigation demands and agricultural water use.
- From WEAP to the Microeconomic Model:
 - Water Availability for Irrigation: WEAP will provide data on the availability of water for irrigation, which affects agricultural productivity and economic outputs in the microeconomic model.

The microeconomic model will focus on the agricultural sector. Other water uses such as urban water use will be assessed based on projections consistent with RCP climate scenarios (SSP). This information will allow us to define population growth and income levels, projections of population growth and changes in income levels, and how they affect on household demand based on estimations of future urban water use, which will be inputted into WEAP.

The coupling between the WEAP and the microeconomic module is bidirectional and resembles that developed for the Desaguadero-Titicaca-Poopo. There is an iterative exchange of data between WEAP and the microeconomic modules, ensuring that feedback loops are accounted for and that both models influence each other's outputs. The setup will be designed to be dynamic in principle, although for certain land use scenarios a single-time-step exchange might be used, especially for scenarios where long-term equilibrium states are of interest rather than short-term dynamics. Regarding the sequence of the coupling the following steps are identified:

1. Prepare Baseline Data: Ensure both models have consistent and harmonized baseline data.
2. Run Microeconomic Module: Generate initial projections of land use and land use changes, economic outcomes, and water demand, for multiple alternative TAPs. These pre-run simulation outputs will be incorporated into WEAP as land use files. Output variables: Land use data, and related water use data and economic activity data (employment, profit, Gross Value Added).
3. Update WEAP Inputs: Input microeconomic outputs into WEAP. This includes updating land use files in WEAP with those produced in the microeconomic model for multiple plausible futures accounting for alternative microeconomic models (ensemble), climate scenarios (which affect yield inputs), and input and crop prices (sensitivity analysis). We will also define population growth, income growth and water use growth projections for urban uses.
4. Run the coupled WEAP and microeconomic model: Simulate water resources availability and allocation, and the repercussions in terms of actual land and water use by irrigators using the updated input (land use data and related water use data) from microeconomic model and urban water use projections. Output variables: Water availability data, and water allocation data, and the corresponding land use data, effective water use, and economic activity data.
5. Iterate: Continue the iterative process for dynamic coupling or finalize analysis for static coupling. This iterative process continues for the desired time horizon, e.g., 2040.
6. Analyze Results: Evaluate the integrated outputs to inform water resource management and economic policies.

Data exchange between the WEAP and the economic module will be done either via direct data import/export files or through API and scripting (custom scripts to automate data exchange between the models).

Finally, a **Policy module** will be developed. A portfolio of TAPs will be collected jointly with the stakeholders. Indicative TAPs include: water allocation reform, adjustment of water rights, water abstraction enforcement and control, drought insurance, transformative subsidies, alternative crops, improved monitoring, etc. The policy module will feed the coupled WEAP and microeconomic model, where different TAPs will force the relevant component of the coupled model. For example, water pricing will impact the microeconomic component and cascade to the hydrological model afterwards in an iterative way; while quotas will impact the hydrological model, and cascade to the microeconomic model afterwards. The policy module will most likely be developed in Matlab, linked

to WEAP through an API, and will be able to select the optimal mix of TAPs under specific policy objectives set by the user.

Task planning: data collection is ongoing, as well as the schematization of the water resources model. Once finalized, this schematic representation will be modeled and parametrised within WEAP, followed by model calibration. In parallel the development of the microeconomic module will take place. These are the Phase 1 activities. Phase 2 concerns the development and integration of the policy module, and Phase 3 the assessment of the robustness of the selected TAPs under future scenarios (as outputted from the climate module). A detailed timeplan is presented in the Gantt Chart below.

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4.7.2. Gantt Chart

[illegible]

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[illegible]

Figure 21. Tympaki River Basin Gantt Chart. Where data or calibration phases do not appear, this indicates that they have been already completed for those models.

4.7.3. Key uncertainties and sensitivity analysis

1. Input uncertainty refers to the uncertainties associated with baseline data inputs and external driving forces that influence the model. This includes:

Baseline Data Inputs:

- **Hydrological Data:** uncertainty in observed hydrological data, mainly streamflow data which are often derived from water level data, groundwater levels, soil moisture data.
- **Water Use Data:** uncertainty in current (and projected) water use volumes and patterns across different sectors (agriculture, industrial, municipal).
- **Water Abstraction Volumes:** uncertainty in current water abstraction volumes due to the numerous private unmetered wells
- **Land Use Data:** inaccuracies in land use patterns that affect runoff, infiltration, and water demand.
- **Socio-economic Data:** variability in socio-economic factors such as prices, costs, yields, water use, and technological advancements that influence water demand and crop production.

External Driving Forces:

- **Climate Change Scenarios:** uncertainty in future climate projections and scenarios, including variations in temperature, precipitation, and extreme weather events.
- **Policy Designs:** variability in potential future policies regarding water allocation, conservation measures, and infrastructure investments.

2. Parameter uncertainty refers to uncertainties associated with the model parameters that are used to calibrate the model. This includes:

Calibration Parameters:

- **Runoff Coefficients:** uncertainty in parameters and methodology that determine how much precipitation contributes to surface runoff versus infiltration.
- **Evapotranspiration Rates:** variability in the rates at which water is evaporated and transpired from different land cover types.
- **Soil Moisture Characteristics:** uncertainty in parameters describing soil properties that affect water retention and percolation.
- **Demand Elasticities:** parameters that determine how sensitive water demand is to changes in price, population, or economic conditions.

Fixed Parameters:

- Parameters such as water use efficiency rates, utility function parameters, or crop coefficients may need to be estimated or calibrated, introducing uncertainty.

Calibration Methods:

- The methods used to calibrate these parameters by comparing model outcomes to observed data can also introduce uncertainty. For example, different optimization techniques or historical data sets might yield different calibrated values. Also, different calibration methods for microeconomic models, even within the same modeling family, can yield different results.

3. Structural uncertainty refers to uncertainties stemming from an insufficient understanding of the relationships within the model. This includes:

- **System Boundary Definition:** incorrect or simplified boundaries of the water resources system being modeled, which might exclude important processes or interactions.
- **Functional Forms:** simplified or incorrect mathematical representations of hydrological processes, such as the equations governing surface water-groundwater interactions
- **Parameterization:** the choice and definition of variables and parameters, which might oversimplify complex processes (e.g., lumping diverse land uses into broad categories).
- **Model Equations:** the specific equations and algorithms used to simulate water flow, demand, and allocation might not fully capture the complexities of the real-world system. For example, linear approximations of nonlinear processes can introduce errors.
- **Assumptions and Algorithms:** assumptions about future technological developments, economic growth, or policy effectiveness can introduce structural uncertainties. For example, assuming constant technological efficiency improvements might not be realistic.
- **Coupling Design:** when integrating WEAP with microeconomic and other models (e.g., climate models), uncertainties can arise from how these models are coupled and how well they communicate with each other.

Techniques like multi-model ensembles, sensitivity analysis, scenario analysis, and probabilistic approaches can help quantify and mitigate the above-mentioned uncertainties. The following methods are suggested:

- For the input uncertainty analysis a Monte Carlo simulation can be performed to generate probabilistic distributions for uncertain input variables and propagate these through the model. A scenarios analysis is also planned, developing and analyzing multiple scenarios representing a range of possible futures for climate change, socio-economic conditions and policy options/ TAPs.
- For the parameter uncertainty a local and a global sensitivity analysis will be performed. For the local sensitivity analysis we will vary one parameter at a time (OAT) while keeping others constant to identify which parameters have the most significant impact on model outputs. For the global sensitivity analysis it is suggested to use methods like the Sobol' indices to assess the contribution of each parameter to the overall output variance, considering interactions between parameters. For the calibration uncertainty Bayesian methods will be used to update parameter estimates based on observed data, providing a probabilistic framework for parameter uncertainty.
- For the structural uncertainty we will perform a structural sensitivity analysis to assess how changes in model structure (e.g. different formulations of hydrological processes, different evapotranspiration models, different representations of groundwater-surface water interactions, different soil moisture methods) impact the results (test different model structures by altering key assumptions and formulations and compare results to assess the impact of structural choices on model outputs). For example, we will explore the use of an ensemble of microeconomic models with two PMP and two PMAUP models to check how different microeconomic modeling structures impact simulations outcomes.

4.8. Summary

Table 1 summarizes the modules adopted in the labs, and the models used to populate them, in each of the labs; while Table 2 summarizes the protocols and coupling approach, and uncertainty quantification techniques adopted, also per lab. Regarding the modules adopted, all labs will model endogenously (i.e., with an explicit model that is part of the modeling framework) the hydrologic and economic systems. All labs will model the climate system, albeit only one endogenously (the Reno, using ad-hoc statistical and dynamical downscaling) and the remaining exogenously by incorporating existing outputs from modeling and downscaling experiments such as CMIP6 and Cordex. 6 out of 7 labs will model the agricultural system endogenously (Orontes, Nitra, Húcar, Reno, Titicaca-Desaguadero-Poopo, Mahanadi), and one exogenously (Tympaki). One lab (Reno) will model the meteorological system, endogenously.

Selected models for the hydrological module include SWAT+ (Orontes, Mahanadi), HYPE (Nitra, Reno), Ribasim (Reno, as water balance model linked to HYPE), WEAP (Tympaki, Titicaca-Desaguadero-Poopo), and TETIS (Júcar); for the economic module, PMP and PMAUP (Orontes, Nitra, Reno, Titicaca-Desaguadero-Poopo, Tympaki, Mahandi) and linear models (Júcar, Mahanadi); for the agronomic module, GYMEE (Orontes), DAISY, WOFOST (Nitra), Aquacitrus (Júcar), CRITERIA (Reno), AquaCrop (Titicaca-Desaguadero-Poopo), SWAT+ tool (Mahanadi) and CMIP6 and AgMIP (Tympaki); for the climatic module, CMIP6 (Orontes, Júcar, Nitra, Titicaca-Desaguadero-Poopo, Mahanadi and Tympaki) and ad-hoc statistical and dynamical downscaling experiments (Reno); and for the meteorological module, the ARPAE-CO model (see D2.1 for a detailed description of these models).

Regarding the protocols and coupling approach adopted, the Orontes, Reno, Titicaca-Desaguadero-Poopo and Tympaki labs have opted for a combination of bidirectional and sequential coupling protocols, where bidirectional protocols are adopted for the coupling between the hydrological and economic module, and sequential protocols adopted for the couplings climate→hydrological, agricultural→economic, agricultural→hydrological, and meteorological→agricultural (i.e., climate and agronomic modules provide inputs to the economic and hydrological modules, which are then run iteratively). The Júcar lab has adopted an entirely sequential approach, while for the Nitra the conceptual design of the coupling has been delayed until the availability of data for the calibration and setup of the proposed models is confirmed.

Regarding uncertainty quantification (with the exception of the Nitra for which the definition of uncertainty quantification methods has been delayed until the availability of data for the calibration and setup of the proposed models is confirmed), all labs quantify (at least to some extent) input, parameter, and structural uncertainties. Input uncertainty is quantified using scenario-based approaches for all labs (excluding Nitra) and most systems, typically relying on outcomes from selected RCP and SSP scenarios; while global sensitivity analysis methods are proposed for the economic module in the Orontes, Reno, Titicaca-Desaguadero-Poopo, Mahanadi and Tympaki; and

for the hydrologic module in the Orontes and Mahanadi leveraging on SWAT+ tools. Parameter uncertainty is quantified using local sensitivity analysis for the Júcar (economic and/or agricultural modules), and using global sensitivity analysis in the Orontes (economic), Júcar (economic and/or agriculture), Reno (hydrologic, economic), Titicaca-Desaguadero-Poopo (hydrologic, economic), Mahanadi (hydrologic, economic), and Tympaki (hydrologic, economic). Finally, structural uncertainty is quantified using multi-model ensemble experiments in the Orontes (economic and climate modules, as well as water use data inputs), Nitra (climate), Júcar (climate), Reno (climate, economic), Titicaca-Desaguadero-Poopo (climate, economic), Mahanadi (climate, economic), and Tympaki (climate, economic).

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Table 1. Summary of the modules adopted in the labs, and the models used to populate them, per lab.

Module and features		Hydrologic		Economic		Agronomic		Climatic		Meteorological	
		Endogenous?	Name	Endogenous?	Name	Endogenous?	Name	Endogenous?	Name	Endogenous?	Name
Laboratory	Orontes	Yes	SWAT+	Yes	PMP, PMAUP	Yes	GYMEE	No	CMIP6	NA	NA
	Nitra	Yes	HYPE	Yes	PMP, PMAUP	Yes	DAISY, WOFOST	No	CMIP6	NA	NA
	Júcar	Yes	TETIS	Yes	Linear, integrated in TETIS	Yes	Aquacitrus	No	CMIP6	NA	NA
	Reno	Yes	HYPE & RIBASIM	Yes	PMP, PMAUP	Yes	CRITERIA	Yes	Statistical and Dynamical downscaling	Yes	ARPA E-CO
	Titicaca-Desaguadero-Poopo	Yes	WEAP	Yes	PMP, PMAUP	Yes	AquaCrop	No	CMIP6	NA	NA
	Mahanadi	Yes	SWAT+	Yes	Linear, PMP and/or PMAUP	Yes (as part of SWAT)	SWAT+ tool	No	CMIP6	NA	NA
	Tympaki	Yes	WEAP	Yes	PMP, PMAUP	No	CMIP6, AgMIP	No	CMIP6	NA	NA

Table 2. Summary of the protocols and coupling approach, and uncertainty quantification techniques adopted, per lab.

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Coupling/uncertainty approach		Coupling	Uncertainty		
			Input uncertainty	Parameter uncertainty	Structural uncertainty
Lab	Orontes	Bidirectional (econ-hydro) & sequential (agro-hydro, agro-econ, clima-hydro)	Scenario based (hydro, agro, clim, econ), sensitivity analysis (factorial, hydro and econ)	Sensitivity analysis (factorial, econ)	Ensemble (econ, clim; and water use data inputs)
	Nitra	NA	NA	NA	Ensemble (clim)
	Júcar	Sequential	Scenario based	Sensitivity analysis (OAT and Monte Carlo, econ, agro)	Ensemble (clim)
	Reno	Bidirectional (econ-hydro) & sequential (meteo-agro, agro-hydro, agro-econ, clima-hydro)	Scenario based (hydro, agro, clim, econ), sensitivity analysis (econ, hydro)	Sensitivity analysis (factorial, hydro, econ)	Ensemble (clim, econ)
	Titicaca-Desaguadero-Poopo	Bidirectional (econ-hydro) & sequential (agro-hydro, agro-econ, clima-hydro)	Scenario based (hydro, agro, clim, econ), sensitivity analysis (global, econ)	Sensitivity analysis (factorial, hydro, econ)	Ensemble (clim, econ)
	Mahanadi	Bidirectional (econ-hydro)	Scenario based (hydro, clim, econ), sensitivity analysis (global, hydro and econ)	Sensitivity analysis (global, hydro, econ)	Ensemble (clim, econ)
	Tympaki	Bidirectional (econ-hydro) & sequential (clima-hydro, agro-hydro, agro-econ)	Scenario based (hydro, clim, econ, agro), sensitivity analysis (global, econ)	Sensitivity analysis (global, hydro, econ)	Ensemble (clim, econ, agro)

5. Contribution to KPIs, outcomes (5-6 years) and impact (7-10 years)

Table 3 maps the contribution of the present deliverable to KPIs, outcomes and impact included in the GA and further developed in the Annex II of D6.1.

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Table 3. Contribution to KPIs, outcomes (5-6 years) and impact (7-10 years)

KPI/O/I	Category	Description	Contribution of this deliverable
KPI1	Transformation KPIs	-Adopt 7 robust TAP -Develop multi-sector and multi-stakeholder partnerships that create and operationalize novel financing mechanisms in 5+ labs. -Demonstrate feasibility and performance of TAP in 7 labs	This deliverable will contribute to the present one by providing outputs to demonstrate the adoption of robust TAPs.
KPI2	Legacy KPIs	-Validate ecosystem of innovation in 7 labs, including 3 transboundary labs. -Initiate ecosystem of innovation in 8+ inspiration labs, including 5+ transboundary labs -Secure 50 000+ EUR/year/lab, for 3+ years and in 4+ labs & 4+ inspiration labs, by the last year of the project	This deliverable will contribute to the present one by providing outputs to demonstrate the adoption of robust TAPs.
KPI3	Monitoring KPIs	-Water accounting and monitoring toolbox using in-situ/satellite data adopted in 7 labs.	NA
KPI4	Engagement KPIs	-Develop 7 local knowledge networks and 1 international knowledge network. -Adopt Talanoa Dialogue in 7 labs. -Engage 200+ stakeholders. -Train 70+ stakeholders in labs -Train 20+ stakeholders outside labs -Train 70+ young scientists	12 young scientists
KPI5	European Green Deal KPIs	-Mainstream project methods and results into 3+ EGD strategies (including Climate Adaptation, Biodiversity, and Farm to Fork strategies)	NA
O1	Outcome 1	Adopt robust TAP in 15+ labs, including 5 large-scale demonstrators in regions enrolled in the Mission on climate adaptation.	NA
O2	Outcome 2	-Validate ecosystem of innovation in 15+ labs. -Monitor TAP performance using digital technologies in 15+ labs. -Adopt TAP including climate & irrigation services in 10+ labs.	
O3	Outcome 3	-Adopt and validate the ecosystem of innovation in 8+ transboundary labs. -Develop an internationally accepted and standardized mechanism for the allocation of water in transboundary river basins.	The current model ecosystem of innovation is being experimented in the Murray-Darling Basin. The suite are being adopted in Comporta (Portugal) complemented with novel models.
O4-5	Outcome 4-5	-Adopt impact assessment & water accounting monitoring toolbox in 15+ labs -Disseminate and promote toolbox adoption in regions enrolled in EU	NA

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		Mission on Climate Adaptation -Increase efficiency by 50%+ and reduce WEI+ by >5% in labs by 2030.	
O6	Outcome 6	-Multi-sector and multi-stakeholder partnerships that create and operationalize financing mechanisms in 12+ labs.	NA
O7	Outcome 7	-Develop 15+ local knowledge networks and expand the international knowledge network. -Engage 500+ stakeholders. -Adopt Talanoa Dialogue in 15+ labs. -Train 150+ stakeholders & 150+ young scientists.	NA
O8a	Outcome 8a	-Mainstream uncertainty assessment and robust decision making in all EGD strategies. -Work with all regions in the Mission climate adaptation.	The current model has been designed to complement existing labs.
O8b	Outcome 8b	-Increase water efficiency by 50% in labs (SDG6.4.1). -Reduce WEI+ by >5% in labs (SDG6.4.2). -Increase IWRM by 10+ points in labs (SDG6.5.1). -Establish 8+ transboundary arrangements (SDG6.5.2). -Enhance growth and welfare in 8+ labs in developing countries (contribution to SDG6.1) -Support and strengthen the participation of 15+ local communities in knowledge networks (SDG6.B)	NA
I1	Impact 1	-Reach out & inform 10 000+ stakeholders. -Promote the adoption of our groundbreaking ecosystem of innovation in 200+ basins	NA
I2	Impact 2	-Train 1000+ stakeholders & engage 500+ scientists. -Foster adoption of robust TAP in 200+ basins (100+ by 2030).	NA
I3	Impact 3	-Foster adoption of an impact assessment and water accounting monitoring toolbox in 250+ basins. -Stimulate adoption of modeling suite in 250+ basins.	The current model ecosystem of innovation is being experimented in the Murray-Darling Basin. The modeling suite are being adopted in Comporta (Portugal) and complemented with existing models and novel models.
I4	Impact 4	-Foster adoption of TAP that unleash the potential of LULUC for carbon sequestration in 100+ basins. -Promote the adoption of TAP that store water and carbon through natural water retention measures in 75+ basins.	NA
I5	Impact 5	-Adopt TAP that enhance adaptive capacity and resilience of water and soil systems through nature-based solutions and resilience instruments in 100+ basins.	NA
I6	Impact 6	-Foster uncertainty assessment in EC's Strategic Foresight reports and all EU environmental policies & strategies, to achieve robust management of scarce resources. -Foster the adoption of our groundbreaking ecosystem of innovation to accelerate societal transformations in the 150+ European regions and communities supported by the Mission on climate adaptation; and deliver systemic transformations on the ground in 75+ large-scale demonstrators by 2030.	NA

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Annex I: Modules of TRANSCEND modeling suite

1.1.1. Microeconomic module

TRANSCEND focuses largely on agricultural basins. Accordingly, this module focuses mainly on the behavior and responses of agricultural water users (as well as rainfed farmers to account for potential transitions to and from irrigated agriculture) through microeconomic modelling. In microeconomic agricultural models, the agent (i.e. a farmer or a representative group of farmers) decides on the crop portfolio (yearly or plantation decisions for multiple years) and timing, water withdrawals and capital investment, so to maximize its utility in accordance to one (single-attribute) or multiple (multi-attribute) utility-relevant attributes and a number of constraints defining a domain. Literature typically simplifies this decision-making process by representing each possible combination of crops, timing, water application (if production functions are incorporated to the decision making problem, then water application is an input rather than a separate crop) and capital as a separate crop with unique characteristics, so that the utility maximization problem is reduced to a decision on the crop portfolio x within a domain $F(x)$ (Graveline, 2016b):

$$\text{Max } U(x) \quad x = U(z_1(x); z_2(x); z_3(x) \dots z_m(x)) \quad [1]$$

$$\text{s.t.: } 0 \leq x_i \leq 1 \quad [2]$$

$$\sum_{i=1}^n x_i = 1 \quad [3]$$

$$x \in F(x) \quad [4]$$

$$z = z(x) \in R^m \quad [5]$$

where $x \in R^n$ is the crop portfolio or decision variable, which is represented by a vector containing the land share devoted to each individual crop x_i ($i = 1, \dots, n$). Note that each crop i has a unique combination of utility-relevant attributes $z(x)$ attached (notably profit, but also risk or management complexity aversion). Attributes are quantities of dimension one, obtained dividing their observed values by the maximum value they can possibly attain in the model (accounting for the domain). Increasing the provision of any given attribute improves agent's utility, provided the provision of the remaining attributes is kept constant ("more is better"). Convexity holds, i.e. increasing the provision of a utility-relevant attribute will reduce the provision of another utility-relevant attribute; otherwise there is no tradeoff and the choice between the two attributes becomes irrelevant, meaning one of them is not utility-relevant and can be discarded. The domain $F(x)$ is defined by a set of quantifiable constraints, including agronomic (e.g. crop rotation), policy (e.g. Common Agricultural Policy rules), information (e.g. know how), land (i.e. agricultural and irrigable area) and water availability constraints.

The attributes in the utility function and their parameter values can be elicited using normative methods based on value judgments by experts (e.g., the agent aims to maximize total profit); or positive methods that use mathematical programming models to identify the utility-relevant attributes and *calibrate* the parameters that more accurately reproduce observed decisions. Positive methods are typically preferred by researchers due to their ability to more accurately reproduce observed behavior (Graveline, 2016b). Most frequently used positive models include Linear Programming (both single- and multi-attribute), Positive Mathematical Programming – PMP (single-attribute), and Positive Multi-Attribute Programming – PMAP (multi-attribute).

LP models including WGP can be calibrated in two ways: one method specifies all the constraints related to technical processes, and differentiates between technologies or soil-climate conditions to multiply the number of activities (Galko and Jayet, 2011); the other increases the degrees of freedom of the model (Bartolini et al., 2007). LP calibration methods impose several constraints that often lead to corner solutions: the agent chooses the crop that maximizes utility until a constraint becomes binding and prevents further specialization. The “historical crop mixes” approach developed by McCarl (1982) avoids extreme specialization, but introduces additional rules to the model, which becomes “overly constrained” (Graveline, 2016b). An additional limitation of LP is that inputs are used in fixed proportion, making this approach inadequate to simulate some adaptation options (e.g., deficit irrigation). Some have criticized the inability of LP to “approximate, even roughly, realized farm production plans and, therefore, to become a useful methodology for policy analysis” (Paris, 2011). Yet, despite these limitations and criticism, LP remains to date one of the most frequently used models to assess agent’s responses to water and other agricultural policies (Graveline, 2016b). The microeconomic module ensemble will explore several LP models, including the weighted goals programming calibration method developed by Sumpsi et al. (1997) (termed WGP), which relies on the degrees of freedom approach.

PMP is the most widely used mathematical programming method (Graveline, 2016b). PMP models are calibrated using “information contained in dual variables of calibration constraints, which bound the solution of the original LP problem to observed activity levels” to “specify a non-linear objective function such that observed activity levels are reproduced by the optimal solution of the new programming problem without bounds” (Heckelei and Britz, 2005). To this end, a calibration in three steps is proposed. First, a land use constraint is introduced in the domain $F(x)$ to bound the simulated crop portfolio to observed choices, and the dual values associated to such constraint are obtained for each crop i in the portfolio. Second, dual values are used to introduce a non-linear shadow cost to the objective function, usually through a quadratic function. Third, the resultant non-linear objective function obtained in the second step is maximized subject to the same domain that was used in the first step, which perfectly represents observed irrigators’ choices. PMP has several advantages: it guarantees increasing (decreasing) marginal cost (yield), and can be readily used even when relevant primary data is not available (Graveline, 2016b). In addition, although PMP models are single-attribute and use expected profit as the sole utility-relevant attribute, the non-linear term in the objective function can implicitly capture other factors (missing attributes, constraints) driving the behavior and crop portfolio choices of farmers (Heckelei and Britz, 2005). On the other hand, the most common criticism to PMP refers to the economic/technological rationale (or lack thereof) behind the non-linear terms in the objective function, which makes necessary the use of ad-hoc arguments to explain the outcomes of the model after a policy shock (Heckelei and Britz, 2005). The microeconomic

module ensemble will explore several PMP models, including the original dual cost variable approach developed by Howitt (1995) and the approach developed by Cortignani and Severini (2009).

PMAP models elicit the parameters of a multi-attribute objective function by means of equalizing the slope of the indifference curve, or marginal rate of substitution, to the tangency point along the efficiency frontier, or marginal rate of transformation (Essenfelder et al., 2018). This yields as many candidate objective functions as possible combinations of utility-relevant attributes are explored, which are subsequently ranked according to their performance/calibration residual metrics in order to determine the most accurate representation of the objective function. While all the PMAP calibration techniques available in the literature share the calibration process described above, they differ in the method used to approximate the efficiency frontier (Gómez-Limón et al., 2016; Gutierrez-Martin and Gomez, 2011). PMAP models offer the advantage of smooth and realistic calibration results while avoiding the use of ad-hoc dual variables in the objective function. On the other hand, since PMAP models use a limited number of assumptions (no dual variables, no fixed proportions, no limitation in the number of utility-relevant attributes), in those cases where there is a large number of choices within the portfolio and cross-sectional variation is low (time-series variation might be confounded with other trends), the calibration may be unstable and challenging to rationalize (e.g., “jumpy behavior” in parameter values when additional attributes are considered); and occasionally unfeasible (Gutierrez-Martin and Gomez, 2011).

1.1.2. Macroeconomic module

Macroeconomic modelling examines dynamics of aggregate quantities such as goods and services produced, income, capital employment, and prices at the regional (Carrera et al., 2015; Dixon et al., 2011), national (Bosello et al., 2012b; Ciscar et al., 2011) and global levels (Hertel, 1997; Lenzen et al., 2013). The two most used models for assessing the broad economic impacts of environmental changes are Computable General Equilibrium (CGE) and Input-Output (IO) models.

IO models reflect the economic interdependencies between sectors and regions within an economy, through intermediate supply and final demand, based on linear relations (Koks et al., 2015). Linear IO models applied to water typically combine input-output matrices and water accounts and apply a structural decomposition analysis that disaggregates the effects of a given shock on economic outputs and water use at different levels, from urban (Wang et al., 2009) to multi-regional (Wan et al., 2016). Because of their descriptive nature, researchers have frequently resorted to IO models to determine which sectors consume more water (directly and indirectly) (Bogra et al., 2016), estimate their productivity (apparent and induced) (Duarte et al., 2002), assess their exposure and vulnerability to shortages (Zhao et al., 2015), and support the design of water and agricultural policy (González, 2011; Llop, 2008). Despite much progress, linear IO models still tackle two major issues insufficiently: (i) disruptions, such as droughts, are most often a disruption in the supply-side of the production chain; and (ii) modelling the substitution capabilities of other regions and/or other industries. Non-linear optimization has been combined with IO modelling techniques to overcome these issues, thus providing the simplicity of IO modelling (i.e. Leontief production function) while allowing for some

more flexibility (Baghersad and Zobel, 2015; Oosterhaven and Bouwmeester, 2016). One such approach can be found in the MultiRegional Impact Assessment (MRIA) model (Koks and Thissen, 2016). With the use of the MRIA model, the first aforementioned issue is tackled by using optimization techniques to solve the model, which allows for taking endogenous import and supply constraints into account in an essentially demand-determined model. This overcomes two potential concerns: (i) the need for translating the supply-side shock into a demand-side shock and (ii) the need for using a supply-driven IO model. The second issue is tackled by introducing (multiregional) substitution possibilities, i.e., allowing products to be produced by different industries in the same or other regions. This approach allows for an endogenously determined new post-disaster optimum with shifts between main suppliers within the boundaries of the existing (trade and) production structure of the (regional) economy.

In **CGE models**, agent behavior is calibrated from observed economic flows registered in Social Accounting Matrices (SAM). The main features of these models are based on a neo-classical formulation assuming perfect competition, full employment of production factors, and savings-driven investments. The economy is modeled through representative agents that minimize private expenditure to attain a given utility level. Markets are always in equilibrium meaning the demand equals supply and are cleared by adjustments in prices. Changes in prices provide a signal for all markets highlighting the intertwined nature of the underlying SAM data. Depending on the calibration data (SAM) CGE models are usually available at the national and multi-regional level with some extensions at the subnational level. Moreover, these models have been also used for water related research in different contexts. Water use in CGE models can be represented either implicitly (irrigated land, which itself embodies water) or explicitly. The latter approach is used, e.g. by Darwin et al. (1995) for the US, although replication of this approach elsewhere can be challenging due to limited information on water use, value and prices. On top of that, the shadow price of water may not meet the gap between irrigated and rain-fed production to pay for the returns to water. Accordingly, in Berritella et al. (2007), irrigated land production is represented by using a nested Constant Elasticity of Substitution (CES) function in which water and other inputs enter in a fixed proportion. Water demand responds to a water rent, which in turn derives from supply constraints. Calzadilla et al. (2011) use a more flexible three-level CES production function, which allows for different degrees of substitutability between inputs at each level and permits two ways of reallocating water: substituting other inputs for water and reducing demand for water intensive products. Yet, since rain-fed and irrigated production appear as part of the same aggregate national production function, it is not possible to stop irrigating an area in favor of rain-fed agriculture –a major weakness that complicates policy assessment (e.g. irrigation restrictions). Finally, Parrado et al. (2020, 2019) couple a version of the ICES CGE model where water is modeled implicitly and land explicitly with a microeconomic model where land and water are both modeled explicitly. Thus, the microeconomic model provides information on water and land use decisions, the latter of which are fed to the CGE to model to assess impacts on input and output price dynamics, which in turn again condition microeconomic decisions. The **ICES CGE model**, developed by CMCC, has been extended at the subnational level (NUTS2) to support more granular research analysis and **is the default model used in the macroeconomic module**.

1.1.3. Climate module

The climate module will be populated with conventional multi-model ensembles developed in the context of major ensemble experiments, namely CMIP6 (2022), EURO-CORDEX (2022) and ISIMIP (2022). TRANSCEND will not conduct any additional simulations using climate models. All data imported from climate modeling will force relevant modules (e.g., agronomic, hydrologic) following a one-way protocol. Human system modules will adopt Shared Socio-Economic Pathways coherent with the RCP scenarios used in the climate module.

As regards the statistical downscaling scheme (CCAReg), implemented by Arpae, this is a multivariate regression based on canonical correlation analysis (Tomozeiu et al 2018). The model is a Perfect Prog approach, implemented at seasonal level. The calibration and validation of the statistical scheme is carried out using observed atmospheric large scale fields (predictors) derived from Ecmwf reanalyses (<http://www.ecmwf.int/products/>) and observed temperature and precipitation seasonal indices (predictands), over Reno basin (<https://dati.arpae.it/dataset/erg5-eraclito>), 1961-2010 period. To obtain future climate projections, CCAReg implemented as previously described, is feed with the atmospheric large scale fields simulated by different global climate models from the Coupled Model Intercomparison Project (Cmip5, <https://esgf-node.llnl.gov/projects/cmip5/> over 2021-2050 period. Climate projections of seasonal minimum, maximum temperature and precipitation over Reno basin are constructed in the framework of RCP.4.5.

1.1.4. Hydrologic module

Hydrological models are simplified representations of real-world water systems (e.g., surface water, soil water, wetland, groundwater, estuary) that aid in understanding, predicting, and managing water resources. TRANSCEND puts focus on the study of flow quantity, albeit quality of water will be also reported.

A large pool of *hydrologic* models is available from the literature to populate the hydrologic module (see e.g. <http://hydrologicmodels.tamu.edu/models.htm>). Two key families of hydrological models can be distinguished: 1) global hydrological models used to characterize global water and energy fluxes and stores and to model their future trajectories; and 2) regional hydrological models used for individual river basins, which require more detailed input data, have higher spatial resolution to represent the modelled processes, and are tuned specifically to represent the observed hydrological processes and discharge dynamics (Harou et al., 2009). The literature shows that global models typically have a less satisfactory performance in terms of reproducing monthly and annual runoff values, with the regional models outperforming them—albeit it is noted that both global and regional models can generally reproduce the observed seasonal and interannual runoff variability. Thus, “while the land surface and global hydrological models cannot adequately simulate the actual runoff

time series and long-term average volumes, they can reasonably simulate the monthly and interannual runoff variability and trends and can therefore be reliably used for broadscale or comparative regional and global water and energy balance assessments and simulations of future trajectories” (Zhang et al., 2016). A key advantage of global models is that the use of an ensemble of hydrological models is less costly and therefore more frequently used, mainly due to the large effort needed to setup and calibrate regional models. TRANSCEND aims to setup an ensemble of hydrological models to assess the impacts of TAP. To this end we will use regional models.

To be compatible with the protocol-based modular framework in TRANSCEND, hydrologic models must meet some criteria, namely:

- 1) be regional hydrologic models –i.e. working at a watershed or catchment scale;
- 2) be spatially distributed –i.e. fully or semi-distributed models, to be capable of representing responses from economic agents; and
- 3) have a land management module –i.e. be capable of connecting land management actions taken by the different economic agents and hydrological responses (Essenfelder et al., 2018).

Models complying with these criteria include SWAT or TETIS, i.a..

1.1.5. Water allocation (management) module

Climate and hydrology models will estimate current water resources and their future trends. Yet microeconomic and agronomic modeling will require an estimate of the water availability for each crop, in a specific climate condition and soil type, to provide an accurate estimation of crop yield, land allocation and market value. To this end, there is a need of a water management module that resolves the water balance equations at river basin scale and for medium to long term horizon and allocates resources, while accounting for key infrastructures along the basin and their operation. A large set of water management tools are developed and made available for water managers to assist the identification of acceptable allocation solutions. Some of these tools, which comply with the criteria identified in the previous section and can be directly coupled to microeconomic models, are listed below:

- RIBASIM <http://www.wldelft.nl/soft/ribasim/int/index.html> : River Basin Simulation Model is a generic model package for analyzing the behavior of river basins under various hydrological conditions.
- WEAP <http://www.weap21.org/> : Water Evaluation And Planning" takes an integrated approach to water resources planning. It is a microcomputer tool for integrated water resources planning. It provides a comprehensive, flexible and user-friendly framework for planning and policy analysis.
- MIKE BASIN <http://www.dhisoftware.com/mikebasin/Description/>: Addresses water allocation, conjunctive use, reservoir operation, or water quality issues. It couples ArcGIS with hydrologic modeling to provide basin-scale solutions.

- AQUATOOL <https://aquatool.webs.upv.es/aqt/en/home/>: AQUATOOL is a development environment for Decision Support Systems (DSS) for watershed planning and management or water resource systems that provides resources to help the analysis of various problems related to the water management. It is the main DSS for river basin planning in Spain.

1.1.6. Agronomic module

The agronomic module will provide valuable information e.g. on water-yield production functions via models such as AQUACROP. All data imported from agronomic modeling will force the microeconomic system (yield) and hydrological system (where key variables such as evapotranspiration are relevant) following specific protocols. Outputs from the agronomic ensemble will be imported into the modeling framework observing coherence among climate and other key scenarios (e.g., the RCP forcing the agronomic module is compatible with the SSP forcing the macroeconomic module).

Annex II: Data inputs

The data inputs used to populate the models listed in this deliverable are available in Annex II – Metadata. This metadata file is a living document that will be uploaded periodically by all partners to reflect any updates that are done to the modeling inputs. Annex II – Metadata can be found at the following link:

[Link to Annex II - Metadata](#)