Spatial and temporal synchronization of water and energy systems: Towards a single integrated optimization model for long-term resource planning

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Abstract

Feedback between the water and energy sectors exist across system life-cycles and link the resources both spatially and temporally. Tracking the impacts of policies made in one sector on the other can thus be complicated and several nexus methodologies have been developed to address these issues. However, the different physical, temporal and spatial characteristics of the water and energy systems present several hurdles including identifying which of the many links between the two systems to model, with what detail to represent each system and how to synchronize the temporal and spatial differences while simultaneously dealing with data scarcity and large uncertainties. This paper addresses some of these issues and presents a fully integrated hard-linked water-energy linear optimization model. Keeping in mind the varying needs of different stakeholders, the model is deliberately made flexible, allowing users to modify objective function sub-component weights as well as providing adjustable spatial and temporal scales. Additional system processes and end-user technologies can be added to the model while existing representations can be further refined depending on the detail required. The capabilities of the fully integrated model are investigated in an example case study for Spain. The performance of the model run in an integrated mode is compared to that of the model run in a non-integrated mode without any inter-sector links. An integrated approach is shown to have higher initial costs when planning for future scenarios as a result of the additional water-energy nexus constraints taken into consideration. However, the performance of an integrated plan is shown to have several benefits during simulations of future scenarios including lower total costs, better resource efficiency and improved robustness in the face of various sources of uncertainty.

Keywords: Water-energy nexus, integrated planning, optimization modeling

1. Introduction

In several regions of the world such as California, the Mediterranean region, China, India and the Middle East, concerns about future energy and water security are increasing due to various reasons including, growing populations, increasing pollution, overuse of non-renewable resources and the impacts of climate change. Inter-dependencies between the two sectors make the situation even more urgent and several international organizations have conducted various water-energy nexus studies [1, 2, 3, 4, 5, 6, 7] leading to a better understanding of the inter-relationships between the two sectors. Energy is used for water extraction, pumping, desalination, purification and distribution to end users while water is used in energy extraction and mining, hydro-power generation, power plant cooling and to irrigate bio-energy crops.

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Several energy production alternatives such as concentrated solar power (CSP), bio-fuels, hydraulic fracking for shale gas, coal-to-liquid plants, nuclear and carbon capture and storage (CCS) can be more water intensive than their traditional counterparts and will increase water stress if not planned for strategically [8]. Expansion of water infrastructure to ensure water security can also have important impacts on the energy sector. For example, a study from Texas [9] estimates desalination and long-haul transfer to be between nine to twenty three times more energy-intensive per unit of water than conventional treatment of local surface water, while in the Middle East, ignoring the additional feedback of electricity demand from future water system needs has been shown to lead to an almost 40% underestimation of future electricity needs for 2050 [10].

Such nexus impacts are becoming increasing concerns and call for more holistic, integrated assessments to better evaluate the robustness of different policies across both sectors. Taking the links between the sectors into consideration give rise to new questions that nexus models must answer: What will be the impacts of particular energy technologies on water resources and how will these impacts vary spatially? How will future water quality, quantity and temperature changes impact existing energy technology efficiencies? How much additional energy will be consumed by additional water extraction infrastructure and what alternatives are available? How will these impacts play out with seasonal changes in demands and resource availability? What role can demand side management play in cross-sectoral efficiency?

In response, many attempts have been made to incorporate elements of the water-energy nexus in several modeling efforts. A review of some of these studies, discussed in more detail in Section 2, reveals various hurdles that have prevented the development of the kind of tool that can reliably answer the nexus questions asked in the previous paragraph. These hurdles include: difficulties in identifying relevant water-energy links; managing the trade-offs between increasing model details and solution efficiency; capturing life-cycle cross-sector feedback; synchronization of spatial and temporal scales; differences in the physical characteristics of water and energy; sparse data; and large uncertainties.

This paper presents the SPATNEX-WE (**SPA**tial and **T**emporal **NEX**us - **W**ater **E**nergy) model which attempts to address several of these issues. The model is a hard-linked partial equilibrium linear optimization model which tracks resource flows throughout the life-cycle of both the water and energy systems in equal detail. Keeping in mind the diverse needs of different users, the model is designed to be flexible, allowing customization of a weighted multi-objective function composed of costs, emissions, water consumption and withdrawals by the energy system and energy consumption by the water system. Given appropriate data availability, the model can be spatially dis-aggregated to the desired geographical boundaries. Different temporal scales can be used to characterize different processes such as monthly precipitation or varying demand levels specified for weekend or weekdays. Data is aggregated to the finest common spatial and temporal scales across the water and energy sectors. The two sectors are linked based on cross-sector life-cycle resource consumption, water temperature impacts on power plant cooling, a common objective function and via the management of multi-use reservoirs.

Section 2 reviews some of the existing models and summarizes recommendations from various studies. Section 3 discusses the methodology of SPATNEX-WE model and how it incorporates the recommendations made from the review. Section 4 develops a baseline case study for the country of Spain. In Section 5, the capabilities of the model are demonstrated by investigating a hypothetical future scenario. The performance of the model and benefits of integration are explored by comparing several model runs with and without water-energy inter-linkages. Detailed spatial and temporal variations in various parameters as well as the robustness of the solutions are analyzed as part of the outputs. Section 6 discusses some of the limitations of the model and possibilities for future developments. Finally, some conclusions are offered in Section 7.

2. Literature Review

Over the past decade several models have been developed to analyze the water and energy systems simultaneously and have been reviewed in Khan et al. 2017 [11]. The review finds that the most common approach to integration has been to include water constraints in already existing energy models [12] [13, 14] [15] [16] [17]. In these models, water systems are however under-represented and physical water resources often ignored. Few models [10, 18, 19, 20, 21] which do include more detailed water systems reveal other issues related to the dis-aggregation and synchronization of the two systems across different scales. A few studies focus on more general, broader links in the energy, water and other economic sectors using methodologies like the open source Global Change Assessment Model (GCAM), input-output analysis and life-cycle analysis [22, 23, 24, 25, 26, 27]. Other models integrate individual energy and water models in an iterative way using soft-links [20, 28] [29] which is often the most practical starting point for linking models based on different approaches [30]. However, soft-linked models do not guarantee convergence to optimal solutions and the difference between the individual model results produces noise which can be complicated to control. In general, current efforts seem to try to incorporate nexus links into their models guided more by convenience of the tools and expertise available in the particular research group, rather than through a methodological approach to identifying the most pertinent inter-dependencies. Key conclusions from the review paper show that there is still a need to further harmonize the differences in water and energy system equation structures; input parameters; and model variables over common spatial and temporal boundaries. Other areas needing development include better tracking of water quality changes, temperature impacts on power plant cooling and choosing the degree of detail to use in representing complex processes.

A balanced hard-linked water-energy nexus model, treating both resources more uniformly would require compromising between the distinct conventional modeling approaches established in the two sectors. The traditional approach to modeling complex and non-linear water system processes has been to use hydrological simulation models such as WEAP [31] to investigate different "what-if" scenarios such as changes in reservoir operation rules, allocation priorities, crop mixes and climate change impacts on both final demands and water availability. Simulation models are not restricted to any particular form of functional relationships, unlike optimization models in which all processes need to be modeled as compatible, often simplified, equations conforming to the chosen algorithms [32]. In water resources, optimization has primarily been used in making allocation priority decisions, often by maximizing the common economic benefits derived from different water withdrawals in Integrated Water Resource Optimization models (IWROM) [33]. Other models like OPTIMA [34] use a hybrid methodology to find pseudo-optimal solutions by combining the power of complex non-linear simulation programming with discrete multi-criteria methodologies on sets of feasible solutions. In the energy sector, both simulation models (LEAP [35], POLES [36]) and optimization models (MARKAL [37], TIMES [38] are already widely used in practice. Simulation models in energy systems tend towards more aggregated macroeconomic top-down approaches while optimization models tend towards dis-aggregated technology based bottom-up approaches. In bottom-up models, processes are defined from a technical engineering viewpoint while top-down models characterize technologies based on the shares of a given input in intermediary consumption, production functions, labor, capital and other parameters [39]. Operation and investment planning decisions taking into account the complexities of the water-energy nexus calls for a detailed techno-economic representation compatible across both sectors and lends it self well to a bottom-up, partial equilibrium linear programming approach close in spirit to the TIMES-MARKAL family of models.

In summary, the various links between the water and energy sectors can lead to unforeseen impacts of technology, infrastructure and regulatory decisions made in one sector on the other. In order to understand these potential impacts more holistic models are needed to capture the broader system encompassing both the water and energy sectors. Furthermore, nexus models need to be able to track variations in these impacts spatially, temporally and across the life-cycle chains of each sector. Key nexus links including water consumption by different energy processes, energy consumption by water processes, multi-purpose reservoirs as well as water quality and water temperature impacts on power plant efficiency need to be taken into account. Important compromises will need to be made between the detail and complexity of modeling different processes and making the model compatible across sectors, time scales and geographical boundaries. Furthermore, the large uncertainties associated with scarce data, future predictions of resource availability and demands coupled with a range of socio-economic pathways and climate change scenarios call for the need of some form of sensitivity analysis to check for robustness of proposed solutions.

3. Methodology

The SPATNEX-WE model is designed to address some of the key issues reviewed in Section 2. A balanced model representing both the water and energy sector life-cycle processes is developed with a flexible framework for choosing spatial and temporal scales as well as a multi-component objective function with adjustable weights. The program is a partial equilibrium linear-optimization model with a consistent framework across both sectors. As discussed above, representing the water system in linear equations requires simplification of several hydrological processes, such as the relationship between hydro-power generation and reservoir heads. The spatial and temporal variations of water consumption in the energy sector, energy consumption in the water sector, operation costs, investment costs and emissions are tracked throughout the life-cycle of both resources. Both water quality changes through different processes as well as water temperature impacts on power plant cooling efficiency are also taken into account.

The model is programmed in GAMS (General Algebraic Modeling System [40] and can be thought of as consisting of a single model with two hard-linked sub-modules: the energy module and the water module. Subsection 3.1 describes the overall scope of the proposed model. The various links between the two sub-modules are explored in subsection 3.2. Each sub-module is then described in further detail in subsections 3.3 and 3.4. Detailed equations for the full model are made available in the Supplementary Material.

3.1. Scope

The spatial boundaries considered in the model are flexible and can be dis-aggregated into sub-units according to the needs of the users. Water balance is tracked within each chosen spatial sub-division and water can also be transferred between the sub-units. A sub-region may have a runoff drainage outlet into another region and these flows are also tracked. Energy extraction and production capacity is identified for each sub-unit, making the two sub-modules spatially compatible. Energy production and investment decisions impact water demands from the energy sector in each unit, while water availability and temperature changes also impact the efficiency and feasibility of operating and investing in different energy technologies in each unit. The existing energy sub-module assumes a single node final energy delivery system without transmission congestion between the spatial-sub units. Both primary and final energy imports and exports are considered from and to this node.

The temporal scope of the overall model is a single year with further subdivisions in each sub-module. Temporal timescales in water systems can vary from minutes for rainfall and interception evaporation to years for groundwater flow, with a large variation between this range for other processes such as channel flow or sublimation. The water sub-module in the current model is divided into months but can be further distributed over finer time scales if needed. Water storage in the form of reservoirs, rain water harvesting tanks and groundwater aquifers allow management across temporal subdivisions. Given the current limitations of energy storage, and in particular electricity storage, the energy sub-module uses a finer temporal dis-aggregation with monthly time periods, weekdays and weekends as well as five load-level characterizations from peak to off-peak hours. Both water and energy demands and production are then balanced over the common timescale of the month. If finer common temporal divisions are desired then chronological demands for each time period in each spatial unit will be required.

Thus, the model is divided into common spatial and temporal subdivisions over which all input parameters, equations and outputs to be synchronized across the water and energy sectors are then either dis-aggregated if they exist on a larger scale (e.g. countrywide to river basins or annual data to months) or are aggregated if they exist on a finer scale (e.g. individual plants to river basins or daily data to months).

Processes in the model for both the energy and water systems are modeled for the whole life-cycle of each resource. The energy sub-module considers different forms of primary energy carriers which can be transported and converted to final energy products according to the needs of a variety of different energy service technologies which serve to satisfy exogenously defined demands for various services. Similarly the water sub-module considers exogenous demands for different qualities of water which can be extracted from a range of sources and then processed through different conversion, purification and delivery technologies.

3.2. *Nexus Links Framework*

Based on the conclusions from Section 2 and the findings from the water-energy nexus review paper by Khan et al. 2017 [11], five key links were identified as the most important to model between the water and energy sectors. Each of these links is explicitly modeled as constraints in the model and can be turned on or off as desired. A conceptual framework for the links is shown in Figure 1 and they are also listed below:

- i Multi-purpose reservoirs providing water for electricity, other sectors and storage.
- ii Energy consumed by water processes such as desalination or pumping.
- iii Water withdrawn and consumed by energy processes such as bio-energy irrigation or power plant cooling.
- iv Water temperature impacts on power plant efficiency.
- v A multiple objective function considering costs, emissions, energy in water and water in energy.

Brief descriptions of these links are provided below with detailed equations presented in the Supplementary Material.

In Figure 1 the link relating water temperature and power plant efficiency is defined as shown in Equation 1a in which the reduction in efficiency is translated into a reduced effective capacity for each generating process, region and time period. The linear correlation of efficiency decrease per unit increment in degrees Celsius has been found to range from 0.01% up to 0.12% [41]. In the existing model, changes in water temperature are an exogenous input, which need to be entered based on the assumptions and predictions made for the particular climate-change and socio-economic scenario being analyzed. Based on the cooling technology employed by each power plant (Once-through, tower or dry cooling), changes in water temperature result in a corresponding change in plant efficiency. Future developments of the model will add additional endogenous local impacts on water temperature as it passes through different processes supplementing the water temperature change impacts from external events.

The link between hydroelectric production and reservoir outflows is defined in Equation 1b. For each spatial sub-unit the percentage of electricity producing reservoirs is established. Hydro electricity produced is correlated to the outflows in each period, by a correlation variable defined for each region. The volume of water in the reservoirs is then managed by the model based on the overall program constraints and the weighted multi-objective function. Water is released from hydro-power reservoirs to simultaneously produce energy and meet other sector demands.

Energy consumption is tracked through each water process based on the volume of water and any additional parameters, for example the pumping head for groundwater or the net head for long distance transfers. Equation 1c presents an example in which the energy needed for groundwater pumping is calculated as the amount of water pumped times the head times gravity times the pump efficiency times a conversion factor for the desired units. Other water processes consuming energy include desalination, purification, waste-water treatment and local distribution.

Both water withdrawal and water consumption are tracked in energy processes as shown in the example Equation 1d. Water withdrawal and consumption parameters per GWh of energy produced need to be established to calculate these flows.

A linear optimization program is used to minimize the objective function which is composed of costs, emissions, energy consumption by the water system and water consumption and withdrawals by the energy system. Costs are composed of operation costs, annualized investment costs, emission costs, export revenues, import costs and non-served resource costs. Equation 1e is a generalization of the multiple objective function. In the water system, paying for energy is not included in the operation costs since the price for energy is not fixed. The costs for energy use in the water system are reflected through energy consumption feedback to the energy system and the sub-subsequent operation costs of processing that energy. Likewise, prices for water or the "water value" in the energy system are endogenous to the model. Investment costs for new infrastructure, power plants and other technologies are based on the estimated lifespan, principal amount per unit of capacity and the interest rate to calculate an amortized annuity. Emission costs are based on carbon emissions from each process per unit of GWh produced and an exogenous carbon price which can be adjusted according to the local regulations. Non-served water and energy resource costs are set by final demand sector and also serve as allocating sector priorities. Increasing residential non-served water costs relative to agricultural non-served water will divert water to residential users before agriculture users in scarcity situations.

$$P_{eff}(r,b,p) = P_0(r,b) \times \Delta T(b,p) \times (1 - R_t(r)) \tag{1a}$$

$$E_h(b,p) = X(b) \times Q_h(b,p) \times R_h(r) \tag{1b}$$

$$E_{gw}(b,p) = Q_{gw}(b,p) \times h(b) \times g \times \rho \times \eta_{gw} \times R_{gw} \tag{1c}$$

$$F_{cons}(r,b,p) = E(r,b,p) \times R_{cons}(r) \tag{1d}$$

$$O_{tot} = \sum_i (O_{sub}(i) \times W_{sub}(i)) \tag{1e}$$

Where..

r : Energy production process, b : Spatial sub-unit, p : Temporal sub-unit,
i : Object function sub-components (costs, emissions, water consumption,
water withdrawals, energy consumption),
P_{eff} : Effective Capacity, P_0 : Original Capacity, ΔT : Change in temperature,
R_t : Correlation of temperature with effective capacity, E_h : Hydroelectricity,
X : Percentage of electricity producing reservoirs, Q_h : Reservoir outflow volume,
R_h : Correlation of outflow with hydroelectricity production, E_{gw} : Groundwater pumping energy,
Q_{gw} : Groundwater outflow volume, h : Groundwater mean head, g : Gravity,
ρ : Density of water, R_{gw} : Units conversion coefficient, F_{cons} : Water consumed,
E : Energy produced, R_{cons} : Water consumption parameter, O_{tot} : Total objective function value,
O_{sub} : Objective function sub-component value, W_{sub} : Objective function sub-component weight

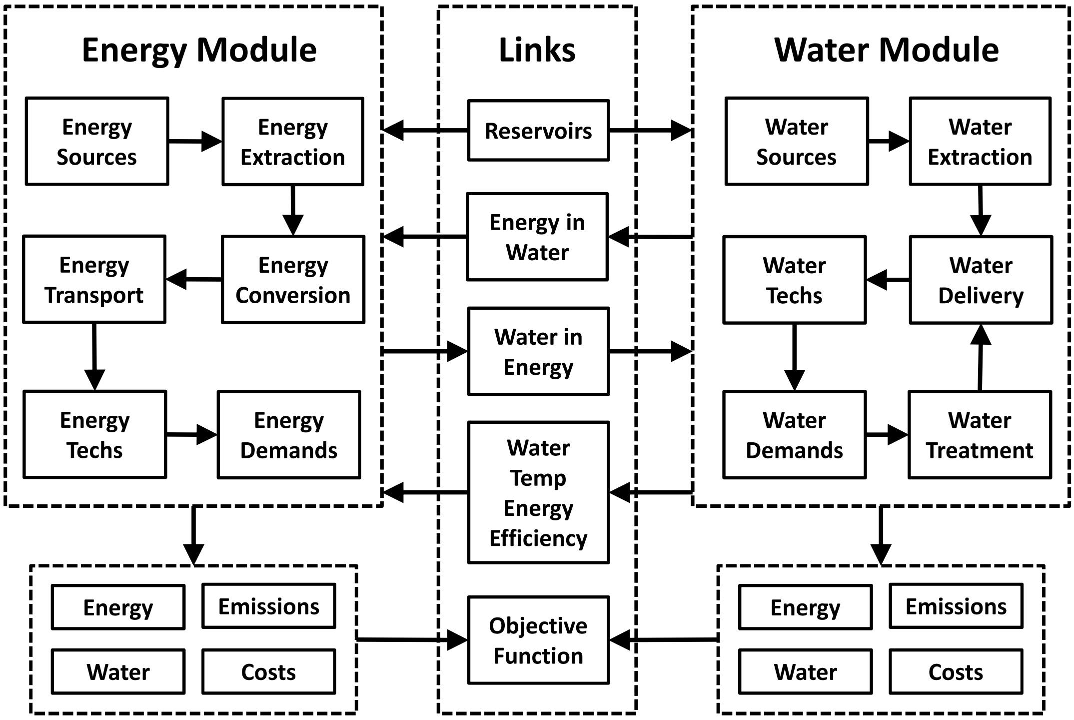

Figure 1: Conceptual model links between the energy and water sub-modules.

3.3. Energy Model Framework

The original energy sub-module, was developed at the Institute for Research Technology, Comillas Pontifical University. A brief description of this original model is provided here and a detailed description can be found in the studies by López-Peña et al. [42, 43].

Figure 2 adapted from López-Peña 2014 [42] shows a conceptual diagram of the energy system model. Flows of different energy forms represented by the multi-colored sankey diagram are tracked through four broader energy system process sub-categories represented by the four large vertical rectangles labelled Primary Energy, Conversion of Energy, Transportation of Energy and Demand Sectors. The flow paths of different colors represent the flow of different forms of energy carriers such as nuclear power, oil, gas, coal or electricity. The flow paths enter and leave different smaller boxes, representing particular technologies such as oil refineries, integrated combined cycle coal gasification, open cycle gas turbines or solar photovoltaics. Each technology is located within the larger categories of Primary, Conversion, Transportation or Demand Sector. The existing energy sub-module includes 22 primary energy carriers (e.g. nuclear, coal, gas, solar etc.), 77 conversion energy technologies (e.g. combined cycle coal, gas turbines, co-generation plants, wind etc.), 16 transportation energy technologies (e.g. centralized electricity, gasoline, diesel, distributed heat etc.) and 10 final demand sectors (e.g. industrial mining, residential, services, air transportation etc.). New technologies and sub-sectors can easily be added to the module and will require the corresponding cost and performance parameters. The dotted line around the sankey diagram and sub-category boxes indicates the model spatial boundary, from which energy can be exported or into which energy can be imported.

The demand sector processes are further subdivided into "Energy services" and "Energy Service Supply Technologies" to allow for demand side management. Final demands are allocated for different "Energy Service" processes such as the number of kilometers for inter-urban land transport or heating for residential buildings. The model considers 38 different "Energy Service" categories for the different demand sectors. To satisfy each of these demands the model provides options for 263 different "Energy Service Supply Technologies" such as district heating, fluorescent light-bulbs, natural gas boilers or biomass boilers. Each ESST has a different efficiency and cost. The energy sub-module is divided into twelve months, each of which is further divided into working and non-working days. Each day has sub-categories corresponding to five load levels.

As done in several other water-energy nexus models in the literature [12] [13, 14] [15] [16] [17], water constraints were introduced into this energy model in order to study the impacts of water shortages on the energy system in the study by Khan et al. 2016 [44]. However, these models lack a physical water system representation and provide water availability as an exogenous input. This hampers consideration of the water system processes and the corresponding feedback between the water and energy systems. This paper advances this previous work by developing a compatible water system sub-module allowing endogenous water resource management and feedback via the established inter-links discussed in subsection 3.2.

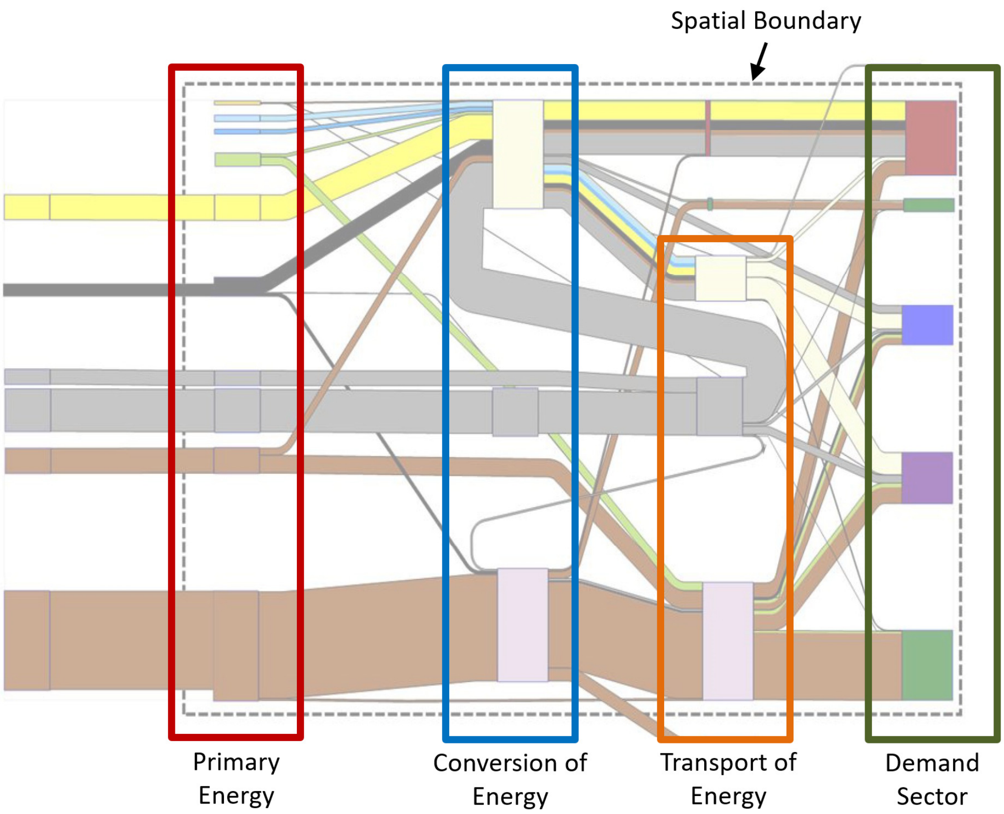

Figure 2: Energy sub-module conceptual framework (Adapted from López-Peña 2014 [42]). Sankey diagram multi-colored paths representing flows of different energy carriers (e.g. nuclear, oil, electricity etc.) passing through the smaller boxes representing different energy technologies (e.g. oil refineries, gas turbines, solar photovoltaics etc.). Larger boxes indicate different phases of the energy life-cycle (e.g. Primary energy, conversion of energy etc.). Dashed line represents the spatial boundary.

3.4. Water Model Framework

The water sub-module can be conceptualized as presented in Figure 3 showing the flow of water through different processes. Each node represents a mass-balance equation with the different colored lines representing parameters and variables. All flows into a node must equal all flows out of the node. Water can be of different qualities such as saline, potable, untreated, waste or recycled water.

This system is applied to each spatial sub-division over the chosen temporal sub-divisions. In Figure 3 the different boxes represent water entering or leaving the chosen spatial boundary. Yellow boxes represent exogenous parameters which define water entering the system and comprise of precipitation and ocean water. Green boxes represent water leaving the spatial boundary as runoff, environmental flows or waste water. Final demand consumption and non-served water are represented by the dashed-line box. At each node water can also leave the system either as evapotranspiration indicated by red lines or as leakages (green lines representing process leaks and pink lines representing distribution leaks). Certain nodes also have storage capabilities indicated by a blue line. Storage capabilities include snow and soil moisture at the "Precipitation Balance" node, ground water aquifer storage at the "Ground Water" node, reservoir storage at the "Reservoir" node and rainwater harvesting storage at the "Rainwater Harvesting" direct and central nodes. As seen in the figure a distinction is made between "Direct" users, who use water directly from the system and "Central" users, who are provided water by a central administration. Purification, waste water treatment and reclaimed water redistribution is included as a service provided by the central administration.

For each spatial and temporal unit the mass-balance is checked according to Equation 2. Changes in storage for every temporal sub-unit occur as a result of the difference between water entering the system (from precipitation and desalination as well as transfers and runoff from other regions) and water leaving the system (as evapotranspiration as well as transfers and runoff leaving each region). Evapotranspiration is composed of interception evaporation, snow sublimation, plant transpiration, surface evaporation, soil evaporation and water consumed or evaporated as part of different conversion, distribution, treatment and end-use processes.

$$\delta S(b,p)/\delta p = P(b,p) + D(b,p) + I_{in}(b,p) + Q_{in}(b,p) - V(b,p) - I_{out}(b,p) - Q_{out}(b,p) \tag{2}$$

Where..

b : Spatial sub-unit, p : Temporal sub-unit, S : Storage, P : Precipitation

D : Desalination, I_{in} : Inter-basin transfers in, Q_{in} : Runoff in

V : Evapotranspiration, I_{out} : Inter-basin transfers out, Q_{out} : Runoff out

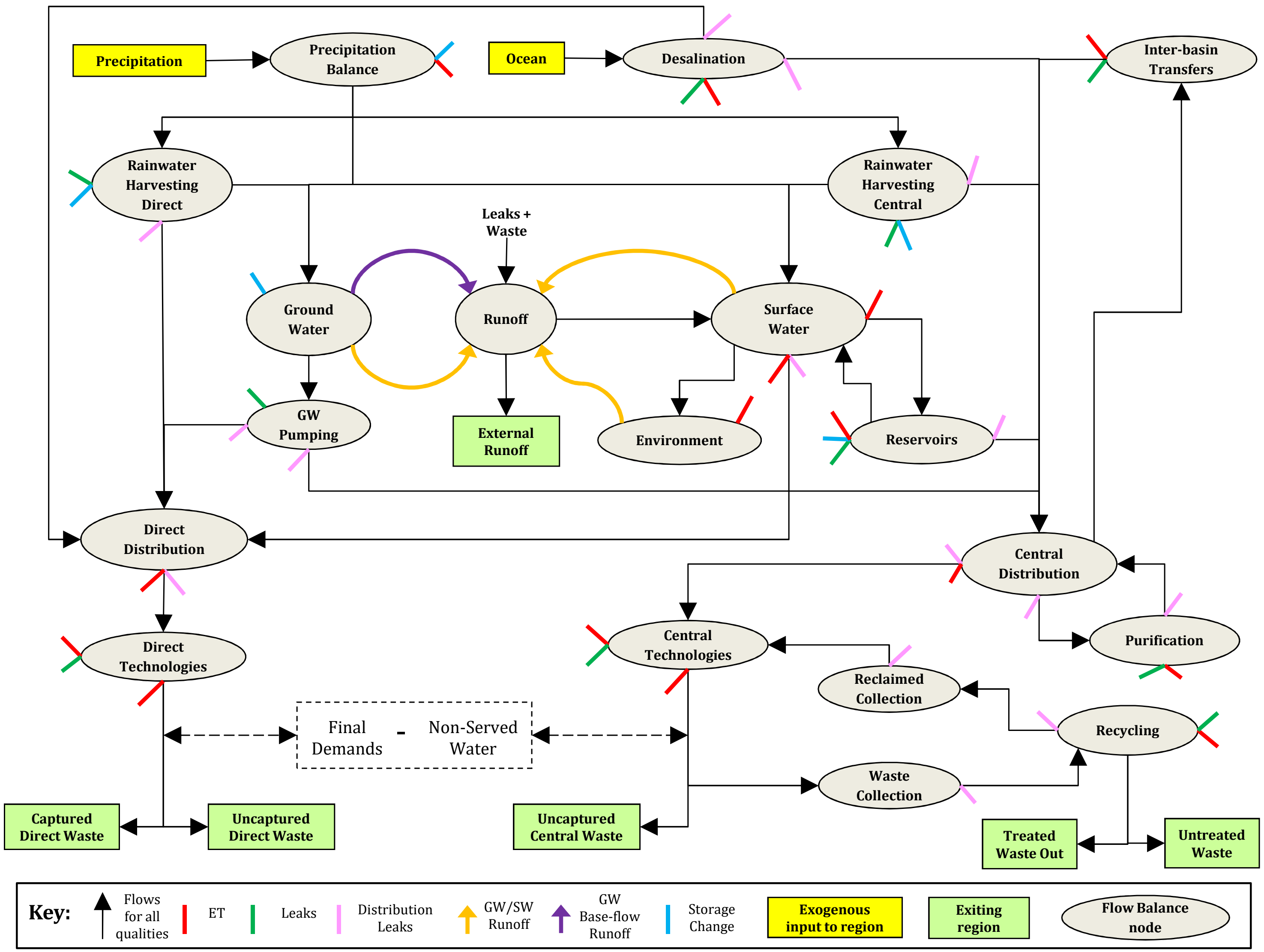

Figure 3: Water sub-module conceptual framework showing the flow of water volume tracked through different water processes.

As an example, Figure 4 shows a close-up of the desalination node. The mass balance for this node is defined as shown in Equation 3a. Each of the lines in Figure 4 is represented by a term in Equation 3a. Comparing Figure 4 and Equation 3a it can be seen that $Q_{o2d}(b, d, q, p)$ represents the flow of water from the ocean to the desalination system. In all the equations q represents the quality of water which can change after passing through a node. In this example water of "saline" quality is treated through desalination processes to produce water of "potable" quality. The mass balance is maintained for the total volume of water regardless of the quality. Several desalination processes can be defined and are contained in the set named d. Each d process will have its own costs, losses, energy consumption and ability to process water to different qualities. Similarly the other flow lines from Figure 4 include water passing through desalination processes to central distribution captured by the variable Q_{d2C} and to direct users in the variable Q_{d2D}. Leakages for each d process are captured by the Q_{d2L} term and leakages in the distribution systems by Q_{C2L} and Q_{D2L}. Finally for each d process some water will be consumed or evaporated and is captured by the Q_{d2V} term.

Apart from the flow balance term, each process is also characterized by additional equations such as Equation 3b and Equation 3c which define other constraints. Equation 3b limits the flow of water through desalination processes to less than the sum of existing desalination processing capacity P_0 and newly invested capacity P_{Inv}. Equation 3c calculates the energy consumed by each desalination process based on the amount of water flowing to the distribution systems and the predefined energy parameters, $N(d)$.

Each node is defined by similar equations which maintain mass balance and also calculate energy, leaks, evapotranspiration and costs. Equations for each of the other nodes from Figure 3 are provided in the Supplementary Material.

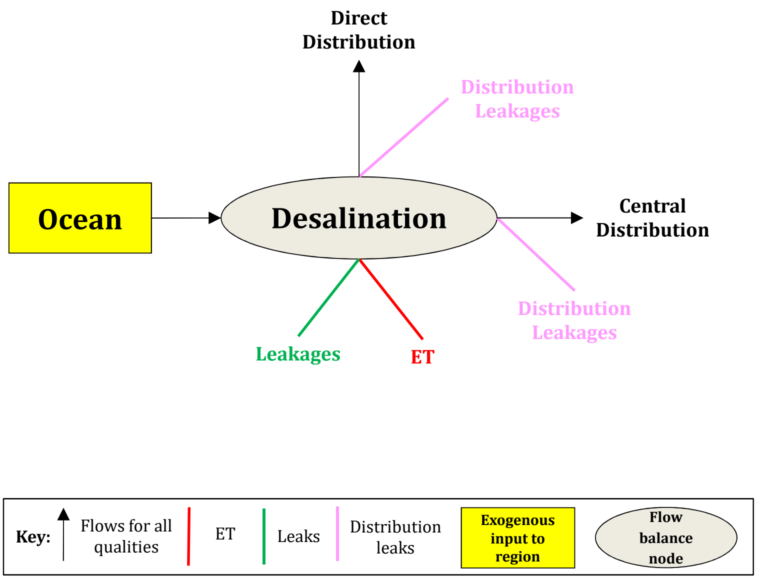

Figure 4: Close-up of desalination flow balance node from Figure 3.

$$\sum_q Q_{o2d}(b,d,q,p) = \sum_q (Q_{d2C}(b,d,q,p) + Q_{d2D}(b,d,q,p) + Q_{d2L}(b,d,q,p) + Q_{C2L}(b,d,q,p) + Q_{D2L}(b,d,q,p) + Q_{d2V}(b,d,q,p)) \tag{3a}$$

$$\sum_q Q_{o2d}(b,d,q,p) < P_0(d,b) + P_{Inv}(d,b) \tag{3b}$$

$$E_{dsal}(b,d,q,p) = (Q_{d2C}(b,d,q,p) + Q_{d2D}(b,d,q,p)) \times N(d) \tag{3c}$$

Where..
b : Spatial sub-unit, d : Desalination type, q : Water quality, p : Temporal sub-unit
Q_{o2d} : Water flow ocean to desalination, Q_{d2C} : Water flow desalination to central distribution
Q_{d2D} : Water flow desalination to direct distribution, Q_{d2L} : Water flow desalination to Leakages
Q_{C2L} : Water flow central distribution to Leakages, Q_{D2L} : Water flow direct distribution to Leakages
Q_{d2V} : Water flow desalination to evapotranspiration, P_0 : Initial desalination capacity
P_{Inv} : New desalination capacity investments, E_{dsal} : Energy in desalination processes
N : Energy consumed by desalination per unit volume of water processed

4. Reference scenario definition and validation

An example application of the model is developed for the case of mainland Spain. Spain is chosen as a case study because it has well managed river-basin authorities with detailed historical data for both energy and water. Furthermore, Spain is an interesting case for the water-energy nexus since it already suffers from regional water scarcity concentrated in the South-East which it can address with several different water technology options such as desalination, re-use or long distance transfers, each with different possible impacts on the energy sector. Spain also has access to a well balanced energy mix with renewable technologies, nuclear, traditional fossil fuels and bio-fuel, all possible candidates for further development, each with their own possible impacts on the water sector. Finally, Spain has a well developed network of about 1200 dams offering storage capacity of about 55,000 hm^3 allowing for several opportunities for managing the water-energy nexus. The model can easily be applied to other countries or regions after replacing the relevant input parameters with those of the area of interest.

The baseline scenario is created to try and simulate the behavior of the water and energy systems in recent years. Estimates for the existing installed capacity and process parameters for the Spanish energy system are taken from López-Peña 2014 [42]. Estimates for the existing water system capacity are taken from various sources including the Spanish Ministry of the Environment (Ministerio de medio ambiente, Gobierno de España) [45] [46], the Spanish National Commission of Energy (Comisi'on Nacional de Energía) [47], the Centre for Public Works Studies and Experimentation (Centro de Estudios y Experimentación de Obras Públicas (CEDEX)) [48], the Spanish National Transmission System Operator - Red Electrica (Red Eléctrica de España) [49] and the Spanish Ministry of Food and Agriculture (Ministerio de Agricultura, Alimentación y Medio Ambiente, Gobierno de España) [50].

The common spatial sub-unit across the water and energy sectors is chosen as the river basin and the common temporal sub-unit is chosen as the month. Spain is divided into fifteen river basins as listed in Table 1 and shown in Figure 5. The key exogenous input parameters (Rainfall, energy demand and water demand) are based on average historical values. The historical mean precipitation from 1941 to 2010 from the

Spanish Ministry of the Environment [51] is used. Energy demands in the model are specified by indicating the demand for energy services such as the number of passengers travelling a specific distance as discussed in Section 3.3 on the energy sub-module methodology. The demands for different energy services are adjusted so that the final energy to different sectors is similar to that of recent years. The exogenous water demands by sector are calibrated against the values provided in the online database of the Spanish Ministry of the Environment [52].

Table 1: River basins in Spain.

Basin	**Map Label**	**Area (km^2)**	**Coast (km)**	**Rivers (km)**
Galicia Costa	GalCosta	13,217	2,120	2,875
Miño-Sil	MinoSil	17,592	0	4,473
Cantabrico Occidental	CantbrOc	17,436	807	3,839
Cantabrico Oriental	CantbrOr	5,807	266	1,282
Duero	Duero	78,860	0	13,539
Tajo	Tajo	55,764	0	10,130
Guadiana	Guadiana	55,389	34	8,046
Tinto,Odiel y Piedras	TintOdPdra	4,751	214	871
Guadalquivir	Guadalquivir	57,228	73	9,701
Guadalete y Barbate	GuadBarbte	5,928	280	1,195
Cuencas Mediterraneas Andaluza	CMedAndlz	17,948	652	2,145
Segura	Segura	18,897	395	1,469
Jucar	Jucar	42,958	588	5,386
Ebro	Ebro	85,567	148	12,495
Cuencas Interna de Cataluña	CICat	16,494	795	2,786

With the input parameters set no additional infrastructure or capacity is allowed to be installed. The model is then run and key outputs are validated against historical values. The model optimizes the choices of energy and water technologies to meet the demands based on resource and capacity availability. Given the uncertainty, assumptions and level of aggregation across the sectors it is only attempted to roughly mimic historical values for the baseline case. In Figure 6a the energy production from different sources is compared with historical values from 2000 to 2014 (EIA and World Bank) [53]. The water model is checked by comparing the evapotranspiration generated per basin per month against historical values from 1941 to 2010 [46] as shown in Figure 6b. Evapotranspiration in the model is composed of precipitation evapotranspiration (which aggregates interception evaporation, snow sublimation and plant transpiration), surface and soil evaporation as well as water consumed or evaporated as part of different conversion, distribution, treatment and end-use processes. Finally one of the key advances made in this model is that of tracking energy in the water system and water in the energy system. These nexus results are compared with the values published in Hardy et al. 2012 [54] for the Spanish water and energy systems, as shown in Figure 6c for the water consumed and withdrawn by energy processes and Figure 6d for energy consumed by different water processes. Water withdrawal and consumption parameters used in the model are based on the values presented in Khan et al. 2016 [44]. The model assumes that nuclear power plants use tower cooling with lower water withdrawal but higher water consumption compared to once-through cooling systems. Water withdrawal parameters for gas and coal in the model are about three times higher than those used in Hardy et al. 2012, the same for hydroelectric production and about one-tenth for nuclear power technologies. Water consumption parameters are similar in both studies for different energy technologies except for nuclear power plants which have a consumption parameter about 1.6 times higher in the model than that in Hardy et al. 2012. In both studies hydro-electric reservoirs are the largest consumers and withdrawers of water in the energy sector. Energy consumption by the water sector in the model is about four times greater than that of the Hardy et al. 2012. This difference can be attributed to the differences in water volumes being processed considered in the two studies. While both Hardy et al. 2012 and the current model use similar final water volume demands, the current model takes into account considerably more water being processed at earlier stages of the water cycle in order to deliver this final volume. The additional water needed at these earlier stages is due to losses and evapotranspiration during processing and transportation.

Figure 5: River basins in Spain.

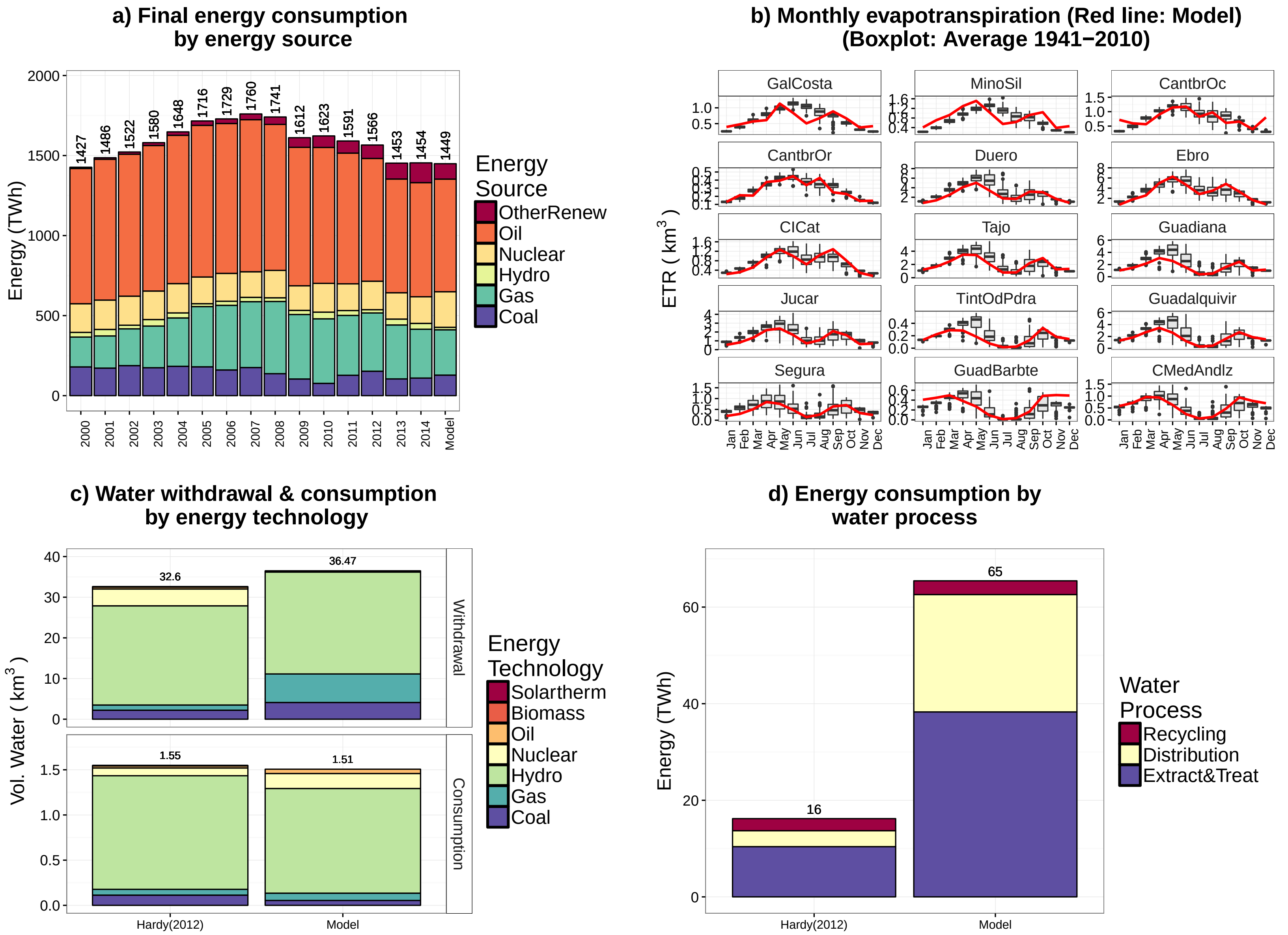

Figure 6: Baseline model outputs compared with historical data. a) Final energy consumption compared with historical data from EIA and World Bank [53]. b) Monthly evapotranspiration compared with historical data from the Spanish Ministry of Environment [46]. c) Water withdrawals and consumption by the energy system compared with data from Hardy et al. 2012 [54]. Differences in values due to different water withdrawal and consumption parameters. d) Energy consumption in water processes compared with Hardy et al. 2012 [54]). Differences in values due to larger volume of water processed in model at earlier stages of water life-cycle to account for losses and evapotranspiration.

5. Future Scenario

This section explores the advantages and opportunities of planning for future resource security using integrated modeling while at the same time demonstrating some of the capabilities and applications of the model.

Subsection 5.1 introduces the different model runs which will be used to demonstrate the differences between the integrated and non-integrated cases. Subsection 5.2 then demonstrates how a future scenario can be established for further analysis. In Subsection 5.3 the benefits of an integrated model are explored by analyzing the results from the hypothetical scenario from Subsection 5.2 with increases in water demands, energy demands and temperatures as well as a decrease in precipitation. The model is run in an integrated mode and compared with the model run in a non-integrated mode (representing the traditional way of isolated sub-sector water and energy management). For the given hypothetical scenario both modes are used to make investment plans in the water and energy sectors. With the new installed capacity, each plan is then subjected to the future scenario and the subsequent performance is then evaluated. In Subsection 5.4 the robustness of the two modes are checked in a sensitivity analysis matrix of performance indicators against variations in a number of uncertain variables.

5.1. Model runs definition

In order to analyze the impacts of ignoring water-energy nexus inter-links, several different runs of the model are planned as shown in Figure 7. The aim is to compare the capacity expansion plans of the model set to run in an integrated mode, in which the water-energy systems are interconnected, as shown on the right in Figure 7, with those of the model set to run in a non-integrated mode, as shown on the left. In the integrated mode the model calculates energy demands from the water sector and water demands from the energy sector endogenously and then optimizes technology investment and operation decisions (spatially and temporally) in both sectors accordingly. In this integrated mode the model also accounts for the impacts of water temperature changes on energy water cooling requirements. The non-integrated mode represents individual, sector-isolated approaches to expansion planning.

For each mode, the model is first used to calculate the corresponding optimal investment plan in the "Planning" phase runs as shown in the upper part of Figure 7. Next, the planned capacity is added to the original existing capacity and each of the plans is put to the test by running the model again for the same scenario as was planned for but this time without the option of new investments. This second phase is labeled the "Performance" phase and reflects the reality of a system in which the water and energy systems are interconnected.

5.2. Scenario definition

The model can be set up to compare different climate change and socio-economic scenarios. A scenario is defined using the input parameters shown in Table 2. As a simple example to demonstrate the outputs of the model, a hypothetical scenario is defined in which evapotranspiration potential is assumed to increase by 10%, temperature by 2.5 °C, while precipitation is assumed to decrease by 12%. These values are roughly based on predictions made for Spain for the years 2041 to 2070 by the Centro de Estudios y Experimentación de Obras Públicas (CEDEX) [48] for various climate change scenarios. Energy demands were assumed to increase by 35% and water demands by 10%. Given the wide range of possible socio-economic and climate change scenarios, no attempt is made here to simulate a particular scenario or year and the values chosen are arbitrary from within the range of values studied. The sensitivity to changes in these uncertain parameters are explored later in Section 5.4. Even though in this example the changes are allocated uniformly across the spatial and temporal boundaries, much more refined scenarios capturing local and seasonal changes could be analyzed by employing different values across the spatial and temporal sub-units.

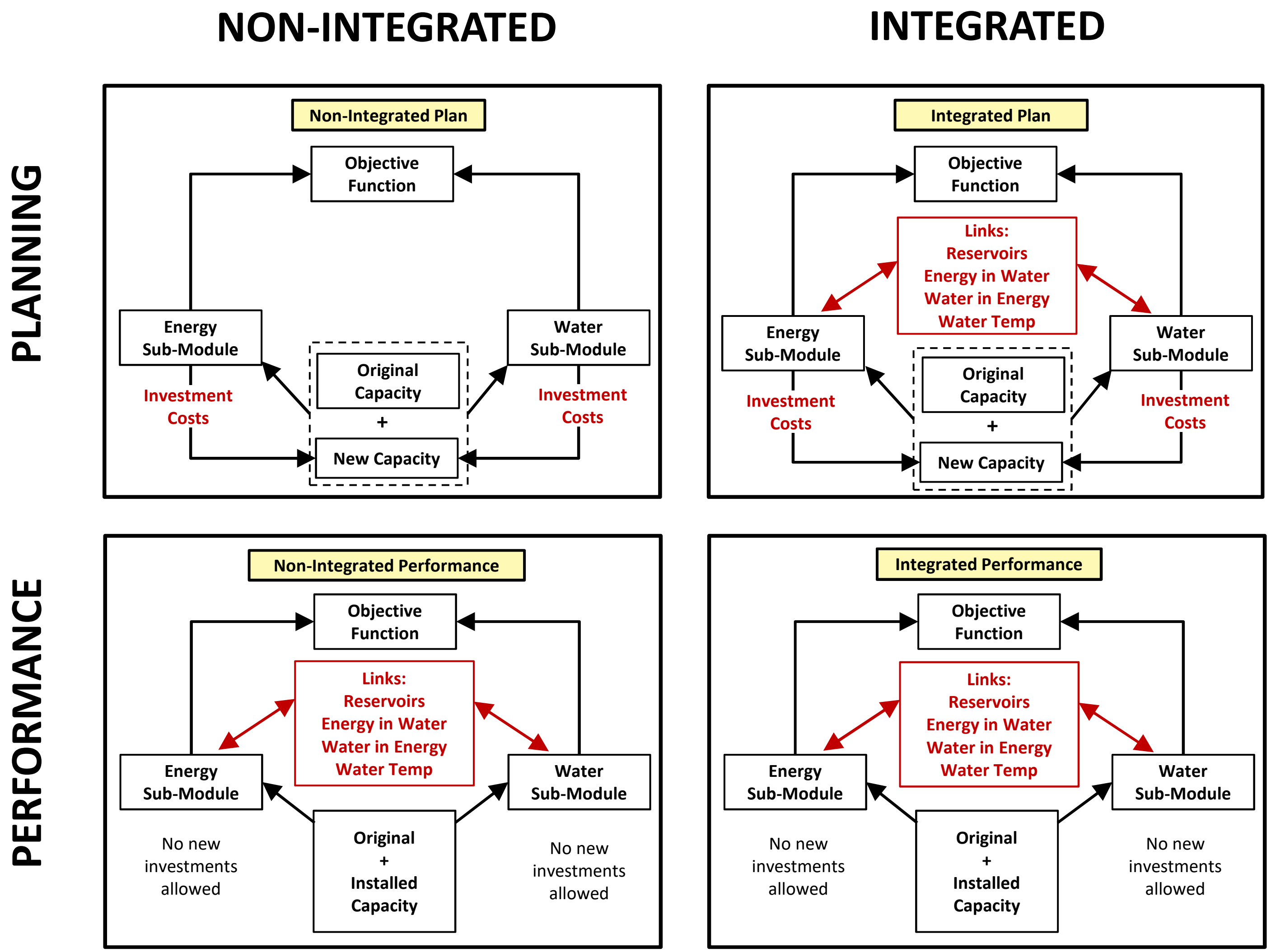

Figure 7: Model run definitions. Investments in new capacity is only allowed in the "Planning" runs. Planned investment capacity is then pre-installed in "Performance" runs. "Integrated" runs include the interlinks and feedback loops between the water and energy systems, while the "Non-integrated" does not.

Table 2: Scenario definition (Changes from baseline).

Parameter	**Example Scenario**
Evapotranspiration Potential	+10 %
Temperature	+2.5 °C
Energy Demands	+35 %
Water Demands	+10 %
Precipitation	-12 %

5.3. Nexus Results

Figure 8 gives a summary of the costs and investments made for each of the different model runs as shown in Figure 7. As seen in Figure 8a during the planning runs for the scenario described in Table 2, the "Integrated Plan" provides a plan which is about 3.2% more expensive than that of the "Non-integrated Plan" run. This is because it considers the different water-energy interdependent constraints via the programmed links. Taking water constraints into consideration, the "Integrated" run, invests in the more expensive and energy in-efficient but water-efficient dry cooling nuclear energy technology as seen in Figure 8d. This choice of energy technology allows the system more flexibility and thus ultimately lowers total costs during the performance runs in which the "Integrated Perf" run has total costs about 1.4% less (4.6 billion EUR in this case study) than that of the "Non-integrated Perf" run. In Figure 8b, we note that during the performance phase the "Integrated" mode is able to serve the final energy using the planned investments, with imports and operation costs remaining similar to those as planned. However, for the "Non-Integrated" performance mode, the new capacity investment decisions prove insufficient after water-energy nexus inter-dependencies are included and additional costs are incurred in the form of increased imports. In Figure 8b and c, "Installed Cap" costs in the performance runs refer to the planned investment costs and are not calculated during the performance runs but added on from the planning phase calculations. Figures 8e shows that water technology investments are similar for both runs with mostly desalination plants installed along coastal basins.

Figure 9 shows the flows of energy and water through different processes to final demands for each run. As seen in Figure 9a, the "Non-integrated Plan" underestimates the total energy demands, because it does not account for the additional energy needs from water system feedback. This leads to a sub-optimal energy system plan in which, as seen in Figure 9b, during the performance phase, water constraints prevent the tower-cooled nuclear capacity in the "Non-integrated" from operating and forcing the system to switch to the more abundant gas powered technology options. Similarly, in the water system in Figure 9c, the "Non-integrated Plan" underestimates the final water demands because it does not take into account the additional water consumed by the energy sector. The difference is small, but as seen, in Figure 9d, this underestimation leads to changes in different water processes and higher overall water needs for the "Non-integrated Perf" run.

Figure 10 shows some key nexus results of process and temporal variations in the water consumed in energy processes and energy consumed in water processes. In Figure 10a and b we see how the "Non-integrated Plan" underestimates the energy needs of the water system and then during the performance phase it has a higher than expected consumption. This increase is a result of the additional water processing needs of the sub-optimal system. We see a similar result for the water consumed by the energy system in Figure 10c. The "Non-Integrated" performance run consumes more water as a result of the tower-cooled nuclear capacity in comparison to the dry air-cooled capacity available for the "Integrated" run. In all the runs water consumption by the energy sector is largely dependent on evaporation from hydro-electric reservoirs. Figure 10d shows the variation in total water consumed by the energy system throughout the year which also reflect changes in reservoir levels.

Figure 11 shows the spatial distribution of the same nexus results. Figure 11a shows the distribution of energy consumption in the water system to be similar for all the runs. The maximum energy consumption is concentrated in the Ebro basin which has the largest demand for agricultural water and therefore the highest energy required to process this demand. Figure 11b, shows the spatial distribution of water demands from energy technologies concentrated in the central basin of Tajo. This occurs because the Tajo basin has the largest amount of tower-cooled nuclear capacity as well as the largest reservoir capacity, both of which are the largest consumers of water. Furthermore, the higher quantity of tower-cooled nuclear capacity installed in the "Non-integrated" run leads to more water demands for this case.

5.4. Sensitivity Analysis

Given the large number of uncertain variables and assumptions of the model, a sensitivity matrix is created to evaluate the impacts of particular uncertain parameters on chosen variables. The sensitivity matrix shown in Figure 12 compares the results of the two runs for the performance phase. The vertical axis shows the percentage difference between the "Non-integrated" and "Integrated" runs for different performance parameters such as costs, energy consumption and water consumption while the horizontal axis comprises changes in different uncertain variables such as resource demands, emissions and precipitation. The sudden spikes and extremely high difference occur due to non-served energy or non-served water costs. The values for these parameters have been set to very high values to highlight when energy or water is not met.

In the first column of Figure 12 we see that the "Integrated" plan is significantly more stable than the "Non-integrated" plan for increases in energy demands. For the same increase in energy demands the "Non-integrated" plan results in higher non-served energy which increases its energy system costs dramatically as seen in the second row in comparison to the "Integrated" mode. The third row shows the difference in water costs also increases in a similar pattern but to a lesser degree. The "Integrated" mode remains stable up till about a 70% increase in energy demands after which point the differences in costs between the two runs starts to diminish. In the first column, fourth row, energy consumed by the water system decreases suddenly for the "Non-integrated" run as a result of the non-served water and energy at about 40% increase in energy demands resulting in less processing of the local resources. In the last row, water consumed by the energy sector is more erratic given the larger range of energy technology options as well as the opportunities to manage reservoir volumes. On average the "Integrated" run consumes less water in the energy system.

We see similar results in the second column of Figure 12 for decreases in emissions limits, where the "Integrated" plan remains stable up to a decrease of 50% in the emissions limits and then the differences start to diminish, reaching about a 25% difference in costs at 90% decrease in emissions limits. Again, these differences occur primarily due to non-served energy in the energy sub-system as seen from the cost differences in the second row, followed by additional cost differences from the water sub-system seen in the third row.

In the third column, second row, as water demands increase the difference between the energy system costs for the "Non-integrated" and "Integrated" runs also increases. This happens because additional water processing requires additional electricity and as seen in Section 5 the "Non-integrated" plan consists of additional tower-cooled Nuclear technologies which are more influenced by water constraints. The energy system in the "Integrated" mode plan with its investments in dry-cooled Nuclear technology is less dependent on the water system. The spikes in total cost differences (first row) results from the spike in water costs (third row) as a result of non-served water. The "Integrated" mode is able to avoid non-served water till about a 20% increase in water demands at which point the water costs for the runs converge. In the fourth row, as the water demands decrease the "Integrated" mode is able to decrease its water system energy consumption faster than those of the "Non-integrated" mode.

In the final column we see a spike in the difference in total costs at about a 30% decrease in precipitation. This occurs due to the "Non-Integrated" run not being able to meet final demands at this point leading to non-served water costs. For further demands in precipitation the "Integrated" run also fails to serve final demands and the results converge. The differences between the two modes for energy system sub-costs (second row) and the energy consumed by the water system (fourth row) remain below 5%. Water consumed by the energy system shown in the last row is more unpredictable but on average higher for the "Non-Integrated" case.

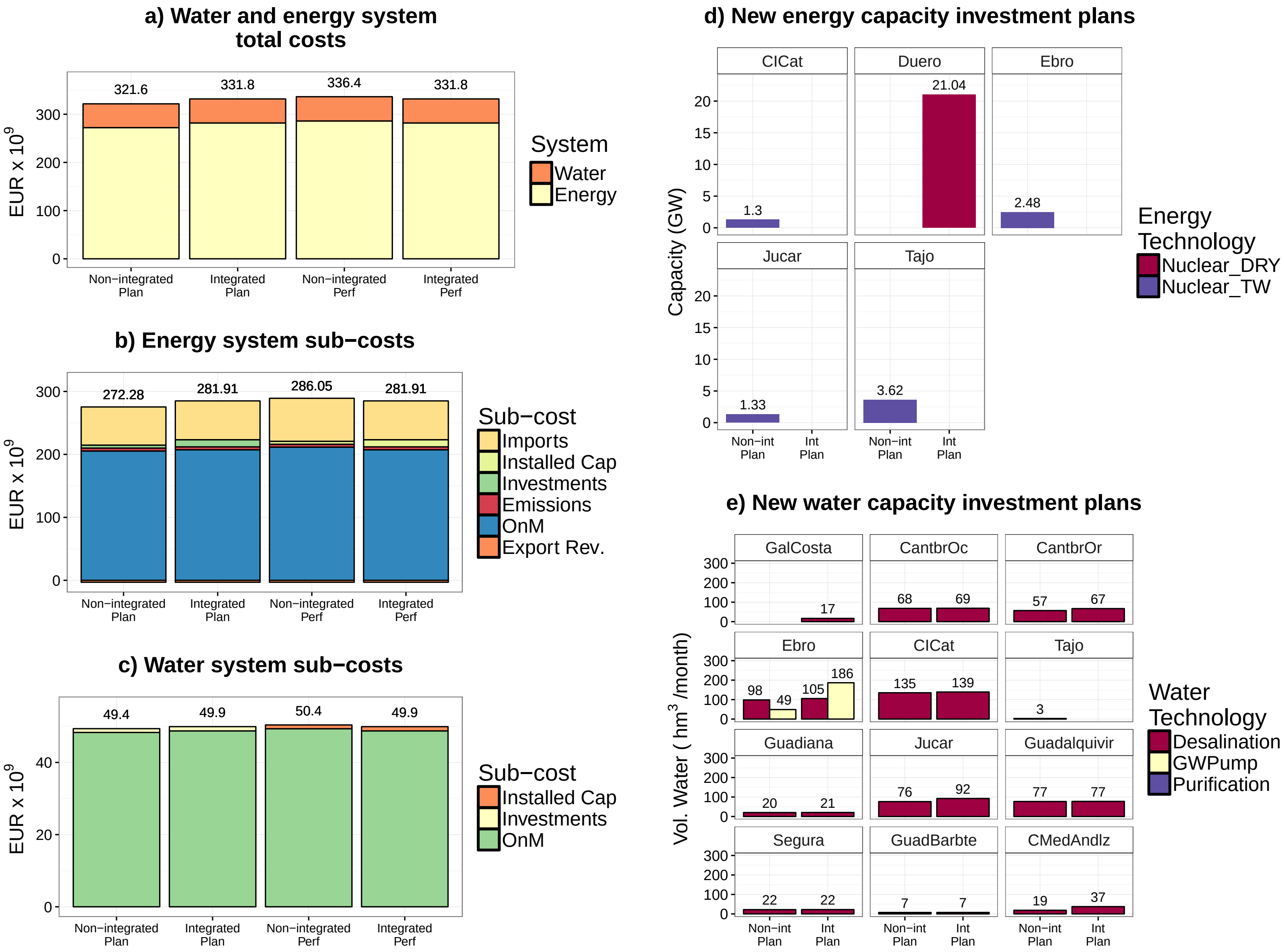

Figure 8: Costs and investments in the water and energy systems. a) Total combined costs for water and energy systems. b) Energy system sub-costs. c) Water system sub-costs. d) New energy capacity investments. The "Integrated" plan invests in more expensive but water-efficient dry air-cooled Nuclear technology. (Power plant cooling technologies: DRY - air cooled, TW - closed loop tower cooled, OT - once through cooled). e) New water capacity investments (1000 hm^3 = 1 km^3).

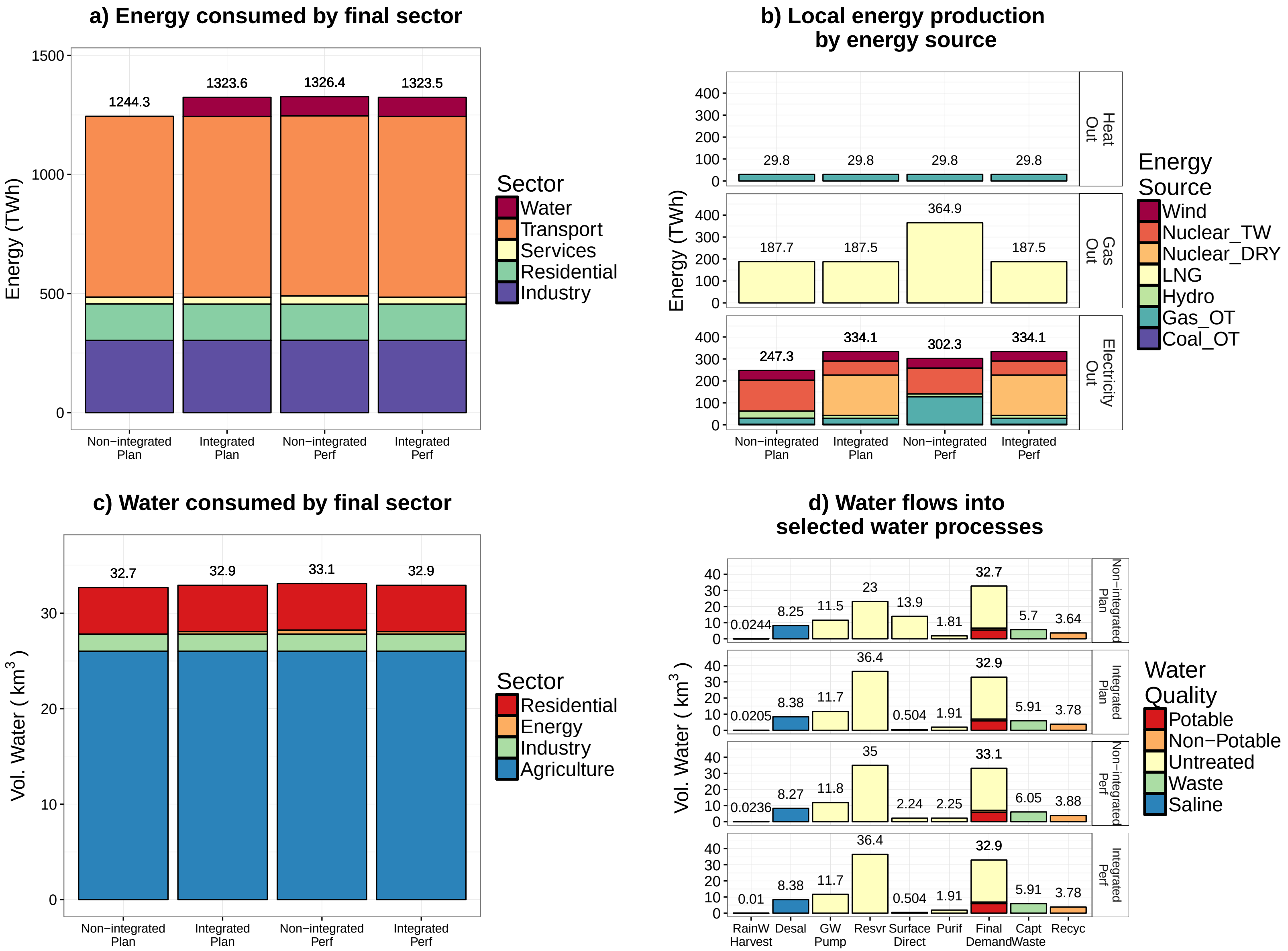

Figure 9: Water and energy production by source and final sectors. a) Energy consumed by final sector. b) Local energy production flows. In the "Non-integrated" performance, unplanned for electricity needs are met by additional gas plants (Power plant cooling technologies: DRY - air cooled, TW - closed loop tower cooled, OT - once through cooled). c) Water consumed by final sector. d) Water quality and quantity production flows into different processes. Does not show the losses and evapotranspiration in each process.

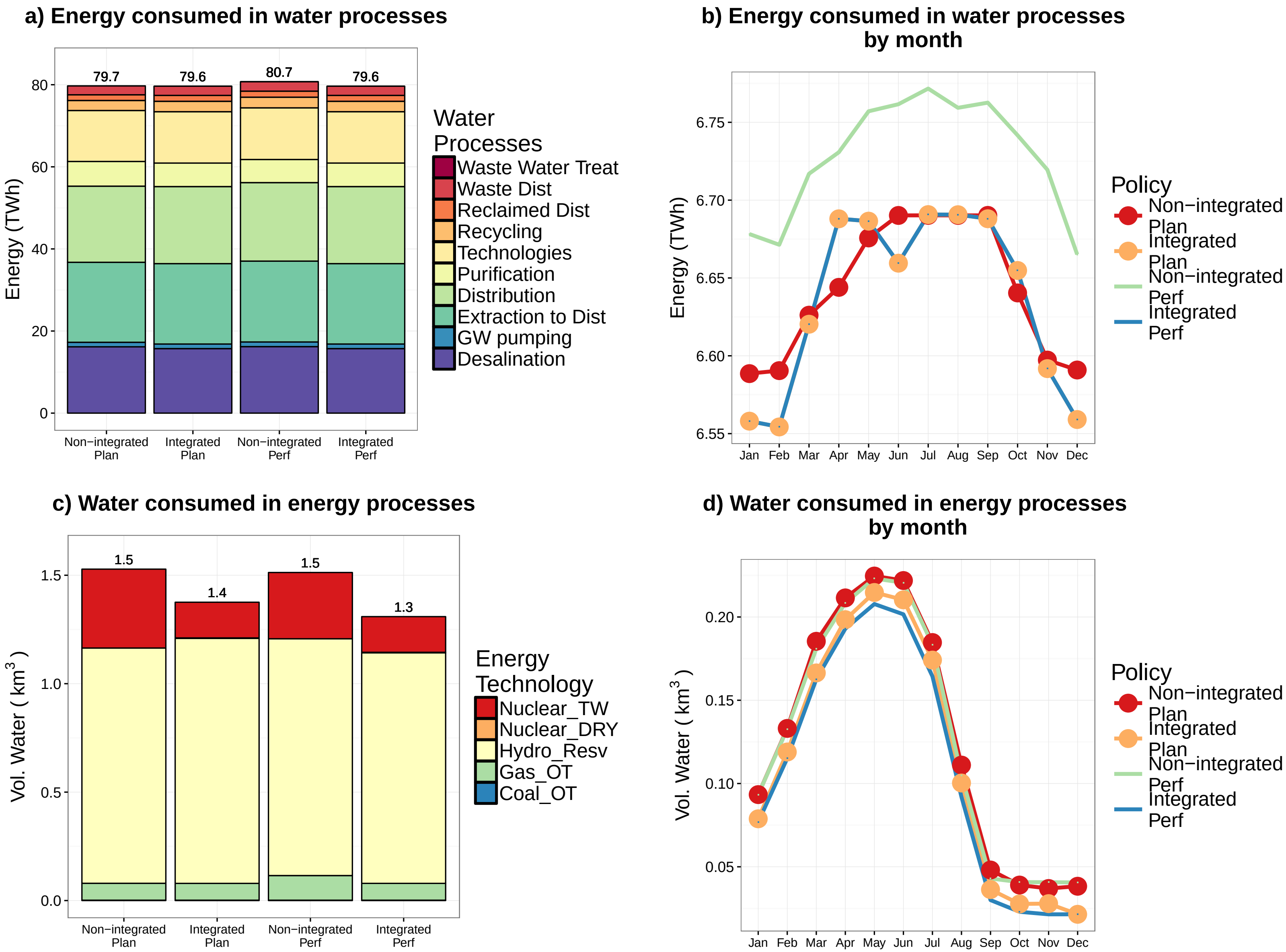

Figure 10: Water in energy and energy in water by process and temporal variations. a) Energy consumed by water processes. b) Monthly variations in energy consumption by water processes. c) Water consumed by energy processes (Power plant cooling technologies: DRY - air cooled, TW - closed loop tower cooled, OT - once through cooled). d) Monthly variations in water consumed by energy processes. Decline in water consumption primarily due to decreases in evaporation from reduced reservoir volumes.

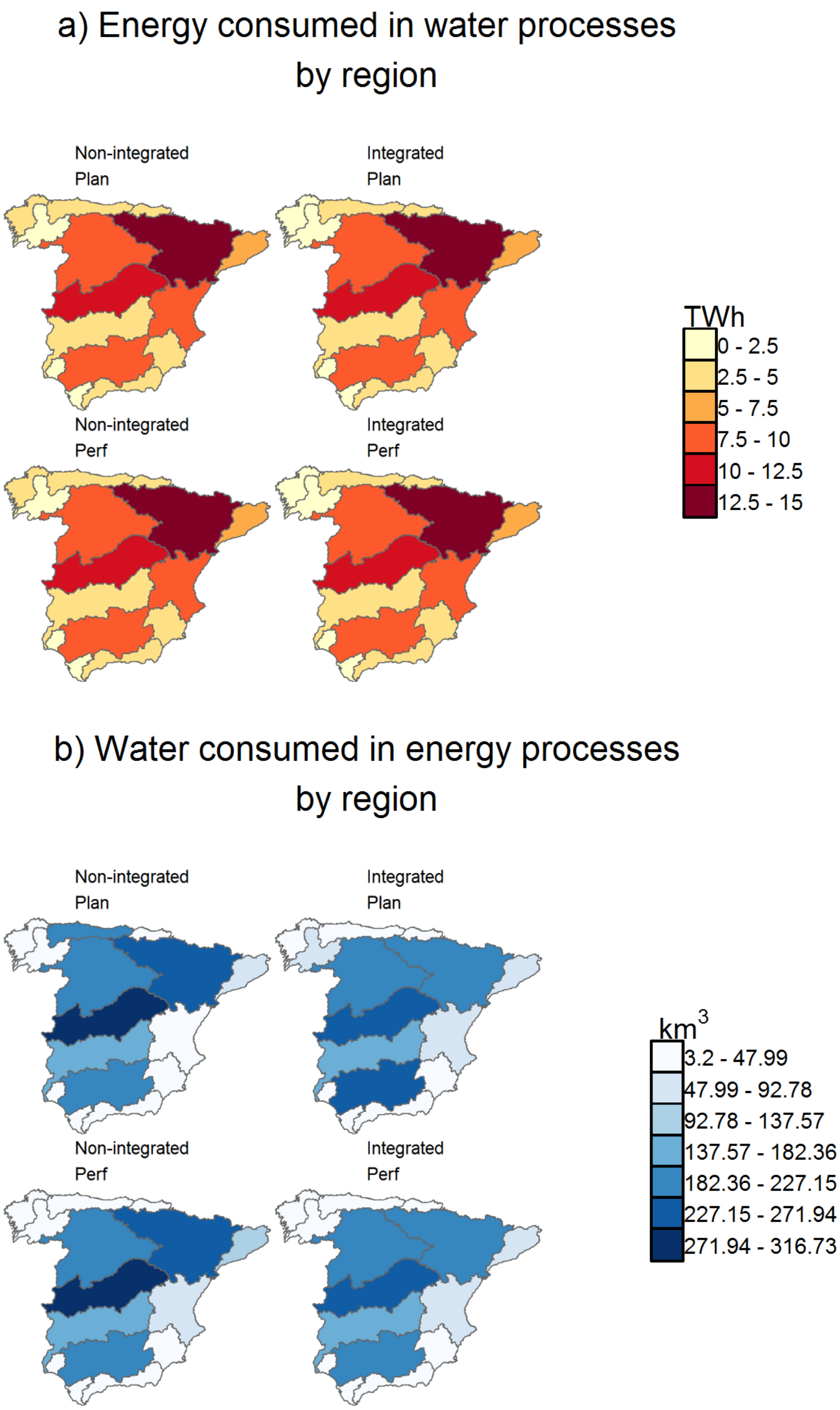

Figure 11: Spatial variation of water in energy and energy in water. a) Energy consumed in water processes. Largest energy consumption in the Ebro river basin due to the higher agricultural demands. b) Water consumed in energy processes. Largest consumption in the Tajo river basin due to the larger reservoir and tower-cooled nuclear capacity.

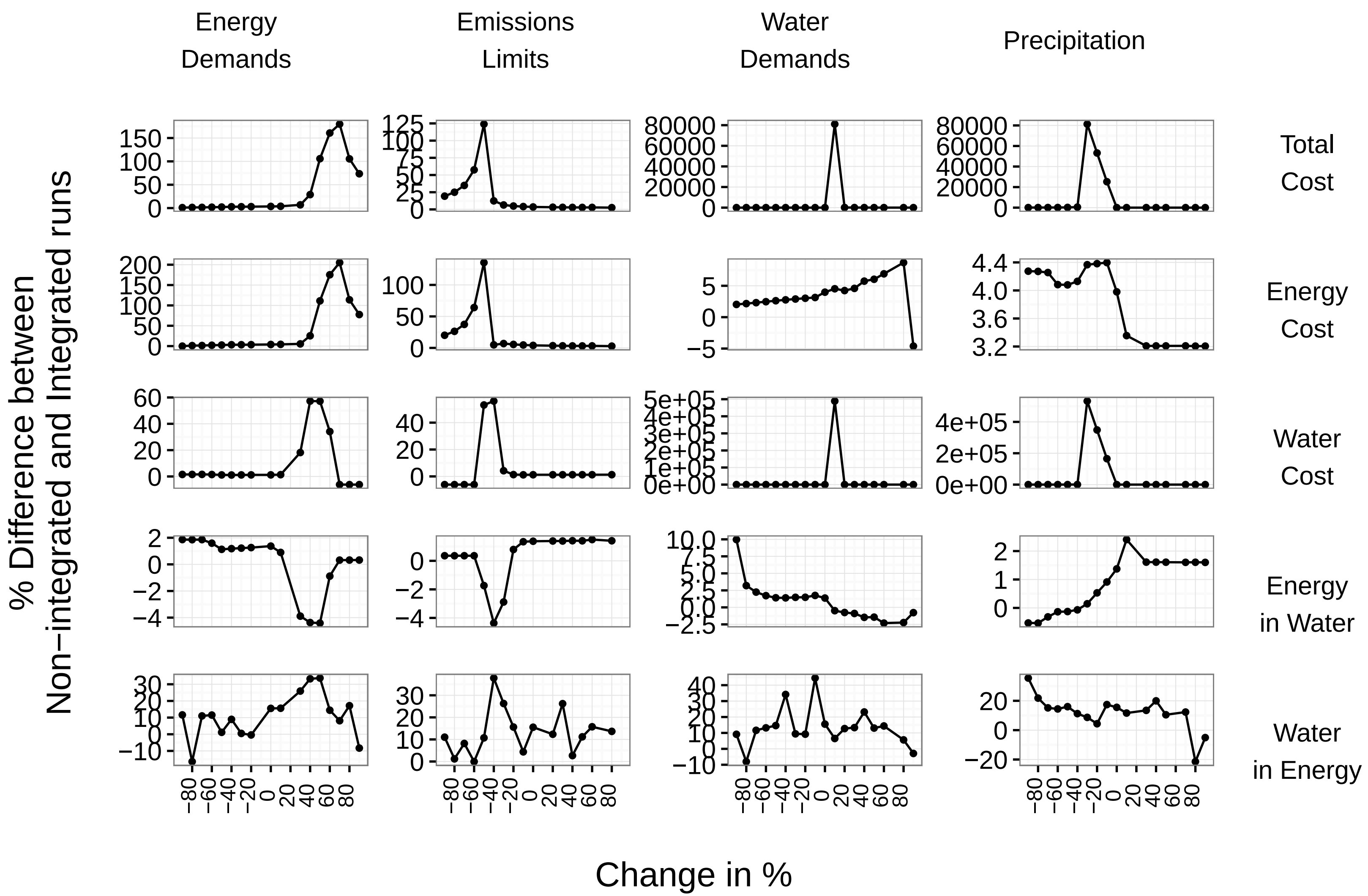

Figure 12: Sensitivity analysis matrix. Horizontal axis showing % changes in four uncertain parameters: Energy demands, emission limits, water demands and precipitation. Each column of charts in the matrix represents each of the uncertain parameters respectively. Vertical axis showing the % difference between the "Non-integrated" and "Integrate" modes for the value of one of four output variables: Total cost, energy cost, water cost, energy consumed in water and water consumed in energy. Each row of the matrix represents one of these output variables.

6. Limitations

As discussed before, the model is a linear optimization program which automatically leads to several limitations as a result of simplifying reality into linear equations which conform to the optimization algorithm. Several non-linear relationships such as reservoir hydro-energy potential or changes in groundwater heads are linearized. The impacts of these assumptions vary depending on the particular system being evaluated. For example, a constant head is assumed for reservoir hydro-energy output calculations and the resulting energy outputs, calculated from the linear correlation assumed, show increasing deviations from historical records as the amount of outflow increases. The deviations become significant only for outflows which are greater than one standard deviation from the historical mean from 1980 to 2012. The consequences of such assumptions are further intensified by the degree of aggregation of different processes over spatial and temporal sub-units.

Another limitation is that the partial equilibrium model in this paper focuses on the water and energy sub-sectors with other socio-economic parameters taken as fixed exogenous inputs. Future developments of the model can expand the model to include endogenous variable demands from other sectors such as the agricultural and food sector. It should be noted that any limitations apply to all the runs uniformly and given that the main purpose of the study was to evaluate the differences between the integrated and non-integrated runs these limitations play a smaller role in the final conclusions.

7. Conclusions

A review of past water-energy nexus studies showed that a more holistic approach, addressing both the energy and water systems more uniformly across their complete life-cycles was needed to tackle the increasing inter-dependent constraints across both sectors. In the past, creating such a model has been a challenge particularly because of the differences in the physical, spatial and temporal characteristics of the water and energy systems and their corresponding parameters.

This paper overcomes some of these issues by identifying key water-energy nexus links and then incorporating these into a single hard-linked linear programming model. The model addresses the highlighted research gaps and incorporates both the energy and water systems in an unbiased way, tracking flows in both systems throughout their entire life-cycles. Furthermore, the model outputs also capture the spatial and temporal variations in these life-cycle flows across different scenarios and model settings. Specific "nexus" outputs track use of water in energy processes and energy in water processes. Keeping in mind the needs of different stakeholders, the model is made flexible allowing users to modify spatial and temporal boundaries as well as to refine key process definitions and adjust the weighted multi-objective function as needed.

Applying the model for a case study in mainland Spain, for a specific future scenario (changes in ETP by +10%, temperature by +2.5 °C, energy demands by +35%, water demands by +10% and precipitation by -12%) shows that taking water-energy cross-sector dependencies into account result in additional constraints. Planning for these additional constraints require an additional 3.2% of the total water-energy system costs for the "Non-Integrated" run. However, when tested in the performance phase with increased demands and decreased water availability the "Integrated" plans prove to be more efficient from both an economic and resource perspective. For the current case study, final costs are 1.4% (4.6 billion EUR) cheaper, energy consumption by the water sector 1.4% (1.1 TWh) less and water consumption by the energy sector 13% (0.2 km^3) less for the "Integrated" mode versus the "Non-Integrated" mode. In an integrated mode the model considers possible water constraints and invests in water efficient dry-cooling technologies. The reduced water demands results in less processing of water and thus less energy. The model also allows for easy evaluation of spatial and temporal variations in the energy-water demands, production and cross sector inter-dependencies. The benefits of integrated analysis become even more important when considering uncertainty. A sensitivity matrix is used to show that an integrated plan is more robust for a larger range of uncertainty in demands and resource availability.

In conclusion, it is clear that integrated analysis can play an important role in helping to evaluate the impacts of water and energy policies across both sectors.

Acknowledgements

The study was funded by the Education, Audiovisual and Culture Executive Agency (EACEA) of the European Commission as part of the Erasmus Mundus Joint Doctorate in Sustainable Energy Technologies and Strategies (SETS). The authors would also like to acknowledge the support of the Fundacin Canal, Spain as well as the support provided by the International Institute for Applied Systems Analysis (IIASA) during the Young Scientist Summer Program (YSSP).

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