



Operationalizing the Nexus Approach: Insights From the SIM4NEXUS Project

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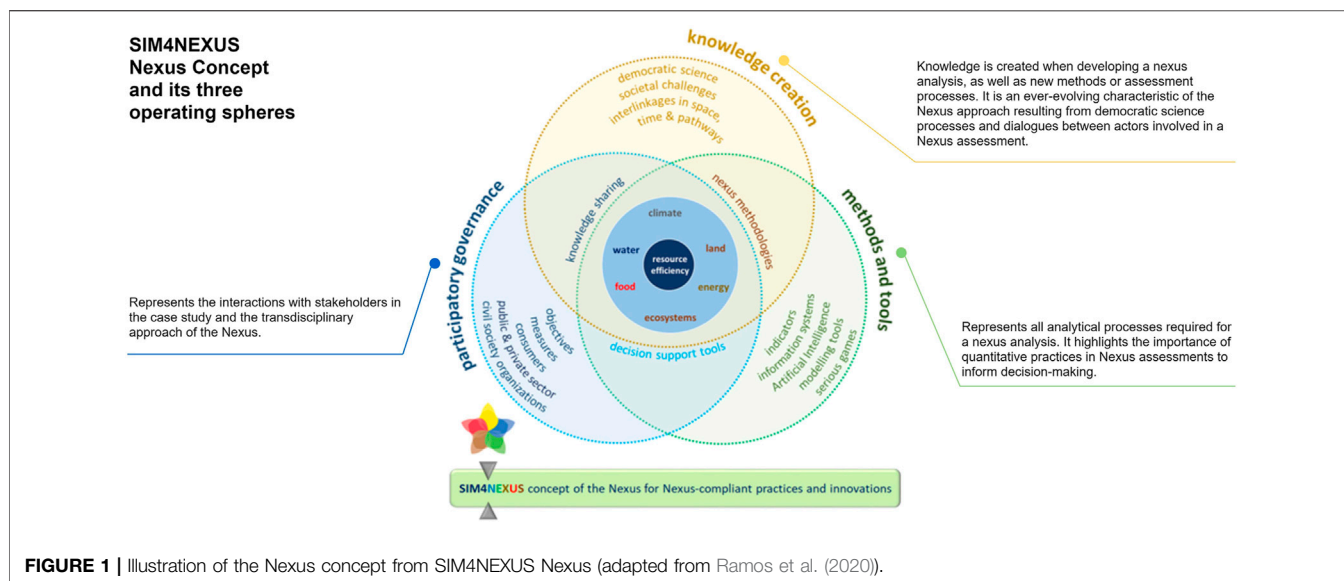
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Over the past decades, the understanding and assessment of cross-systems interactions have gained momentum in research and policy-support. As such, scientific literature on Nexus assessment methods and applications continues to grow, followed by numerous state-of-the-art reviews. Among the flexibility and variety of Nexus approaches, comprehensive, transferable and accessible methodologies with operational potential are missing. To address this gap, we introduce the SIM4NEXUS approach, which emerged from twelve test cases. Fledged from practice, the approach is a unique output in the Nexus research field. It is informed by the development of twelve case studies, which differ in spatial scope, socioeconomic and biophysical contexts, and Nexus challenges. The studies were conducted under similar conditions (e.g., timeframe and multidisciplinary teams of experts and dialogues with practitioners from policy and business). We find that transdisciplinarity and the integration of qualitative and quantitative methods are vital elements in Nexus assessments for policy support. Additionally, we also propose steps to advance Nexus assessments: 1) integration of the policy cycle in research (including monitoring and evaluation, and offer support during the implementation process), 2) multidisciplinary collaboration with different levels of engagement and financial support, 3) inclusion of ecosystems and other relevant dimensions (e.g., health) in the Nexus. Ultimately, the SIM4NEXUS approach provides practice-based guidance on conducting a Nexus assessment, and we recommend it for future Nexus assessments by the research community, institutions, and private actors.

Keywords: nexus, nexus approach, nexus assessment framework, resource management, sustainability, resource efficiency

1 INTRODUCTION

Natural resources, including materials or substances occurring naturally in the environment, are not always used sustainably. The intensification of human activities and increasing demands, driven by population growth and economic development, add pressure to these reserves, raising questions regarding the environmental impacts and the feasibility of maintaining current resource management practices. This motivates the need to understand better how resources can be more efficiently managed without compromising the environment and the life of future generations. Since resources are used across systems, an integrated multi-systems perspective is needed in planning processes.



The term “Nexus” relates to the identification of interactions between different entities (Liu et al., 2018) and the understanding of cross-sectoral dynamics (i.e., multi-systems thinking), whereas the “Nexus Approach” represents the effort of assessing it. In its application to the analysis of resource systems, it gained momentum with the Bonn Nexus Conference (Hoff, 2011), although the importance of assessing cross-sectoral challenges was highlighted in the Global Risks Report 2011 (World Economic Forum, 2011), and the importance of the quantitative analysis by Bazilian et al. (2011) and IAEA (2009). The Nexus approach seeks knowledge and understanding of systems interactions, what factors influence them, how to recognize and assess trade-offs and synergies, and, in this way, reconcile the interests of the different sectors which are part of the domains (i.e. systems) that constitute the Nexus context. A Nexus analysis is a multi-objective approach, which means that it does not seek for optimization in one of the interlinked systems solely, rather than a balanced combination of good solutions in all involved systems upon a Pareto-like front (Wicaksono et al., 2019).

In this paper, we summarize and derive insights from work conducted in SIM4NEXUS, a project funded by the European Commission under the Horizon 2020 programme that investigated the Water-Energy-Food-Land and Climate (WEFLC) Nexus and which was operationalized in twelve Case Studies. The research and innovation project searched for new scientific evidence on sustainable and integrated management of resources in Europe and elsewhere and adopted the Nexus concept in testing pathways for a resource-efficient and low-carbon Europe (Brouwer et al., 2020a).

The Nexus approach is embedded in the investigation of interlinkages between the Nexus systems of water, energy, food, land and climate, and aimed to create synergies and reduce trade-offs, as motivated by the sustainable and integrated management of natural resources. The latter is not possible with the current lack of policy integration and coherence;

thus governance is a pivotal component in the Nexus approach (Howells et al., 2013; de Strasser et al., 2016; White et al., 2017; UNECE, 2018). A new vision for the Nexus concept emerged from this work (Figure 1). The WEFLC dimensions are at the center of the concept, representing the Nexus approach where all spheres overlap, with its focus on resource efficiency. The overall intersection results in innovations (social, policy, technical, business), and Nexus compliant practices. Ecosystems are added, as this dimension is considered crucial from the case study work. Hence, we recommend Nexus practitioners to also consider “Ecosystems” be part of the Nexus concept. Climate change is implicit in the climate dimension. Other than the operating spheres of Knowledge Creation, Methods and Tools and Participatory Governance (Figure 1), we highlight the importance of their intersections. These indicate the spheres are mutually dependent and do not operate in isolation.

The cross-overs between Knowledge Creation and Participatory Governance refer to knowledge sharing through stakeholder participation activities, as well as bilateral consultations. They are aimed to empower stakeholders empowerment, and to streamline Nexus knowledge to actual socio-economic contexts. The crossovers between Knowledge Creation and Methods and Tools enable the evolution of methods and tools to advance the Nexus concept. The Methods and Tools and Participatory Governance crossover reveals stakeholder requirements on tools, and shares Nexus insights and findings to the stakeholders through simulation, quantification and finally the popularization of the Nexus assessment. This intersection can also support the design of funding mechanisms and business models.

Nexus assessment frameworks, or Nexus approaches, consist of a set of overarching steps (including methods and tools to be adopted) that guide a Nexus assessment. Several Nexus approaches are described in the literature. They primarily focus on the process of conducting an assessment, are rather flexible in their design and are not constrained by a modelling

framework or tool. Aimed at the assessment of water-energy-food (WEF) interactions, the WEF approach (Flammini et al., 2014), proposed by the Food and Agriculture Organization (FAO), is structured in three distinct components: 1) context analysis, from which results a qualitative analysis which feeds on the next phase; 2) quantitative assessment, based on matrix analysis of Nexus sustainability and resource use efficiency indicators to compare implications of interventions, and 3) response options, which translate into strategic visions and governance aspects (policy, regulations, institutions). Stakeholders are foreseen to be involved in all phases. The components can be performed independently, although “response options” would benefit from a “quantitative assessment”. A key feature of the approach is the definition of Nexus indicators which can inform about the performance of Nexus interventions, under a specific context. The Climate, Land, Energy, and Water systems (CLEWs) approach (Howells et al., 2013; Ramos E. P. et al., 2021) consists of five main phases: 1) CLEW systems’ profiling, 2) pre-Nexus assessment, 3) analytical approach, 4) analysis of results, and 5) findings and recommendations. Quantitative analyses are performed in phase 3 and can be qualitative and/or quantitative. The single-model quantitative approach, using open source software, is the most commonly deployed method and applied to national-level studies. The CLEWs methodology often involves stakeholder participation, including capacity development and Nexus dialogues, although it is not considered a requirement. The Transboundary Basin Nexus Assessment (TBNA) methodology (UNECE, 2015; de Strasser et al., 2016; UNECE, 2018), considers the Nexus of water, food, energy and ecosystems in transboundary watercourses. It is split into two interacting tracks: the technical (often quantitative), and the governance analysis. The CLEWs approach is adopted for the technical component and most basins’ analyses are based on sectoral model soft-linking (UNECE, 2018). The methodological tracks converge into six main steps: 1) socioeconomic context; 2) key sectors and key actors; 3) analysis of key sectors; 4) intersectoral issues; 5) Nexus dialogue; and 6) solutions and benefits. Stakeholder participation is necessary, and essential, for the elaboration of the transboundary Nexus assessments, since the ultimate aim of the assessments is to foster collaboration and promote dialogue between countries sharing the watercourses for the integrated management of resources at the basin/aquifer system level. Another approach is the integrated Water-Energy-Food (WEF) Nexus framework, introduced by Mohtar and Daher (2016), which focuses on using Nexus analytical approaches to facilitate multi-stakeholder dialogue. It is structured on three components: 1) WEF Nexus analytical platform; 2) Supply chain dialogue, involving different types of supply chain actors; and 3) political economy dialogue. Several Nexus tools are available that can be used for stakeholder participation in the assessments. One example is the WEF Nexus 2.0 tool (Daher and Mohtar, 2015), a comprehensive yet accessible scenario-based tool with the capacity to support decision-making processes. A transdisciplinary approach is recommended for defining quantitative boundaries of the systems, importance indices, and communication purposes. On a different approach, (Giampietro et al., 2009; Giampietro,

2013), propose a multi-scale integrated analysis of societal and ecosystem metabolism (MuSIASEM) framework that explores the interrelations between societal and natural systems and how they influence one another when interpreted as a metabolism. The analytical approach is structured around three main components: a fund-flow analysis of production-consumption socio-economic processes, a multi-level production-consumption analysis (“Sudoku effect”), and impredicative loop analysis. The approach addresses the challenge of old-fashioned quantitative approaches, which require updating, by keeping the versatility for the analysis to adapt to the changing systems, and by including quantitative elements adaptable to different dimensions and scales and semantic categories. Authors’ refer to the framework as a “multi-purpose grammar” due to its boundless applicability characteristic (Giampietro et al., 2009), supported by the numerous applications found in the scientific literature.

The Nexus approaches described share similar elements. They all consider the scrutiny of systems, the identification of interactions, and the need to identify critical interlinkages. Quantification is another common characteristic necessary for comparing alternative futures of resources’ management, policy options or changes in natural systems. Stakeholders’ involvement is also deemed key, and approaches contemplate different engagement options (e.g., interviews, consultation workshops, surveys, capacity development). The approaches also differ. One noticeable difference is the Nexus dimensions considered. Some focus on services, such as energy, water, and food, while others look into systems more from the resource’s angle, which is the case in CLEWs. Another difference is the analytical approach. The FAO-WEF approach proposes an assessment based on indicators that align with the specifics of the Nexus context under study. One method suggested in the WEF Nexus framework is informed by sustainability indicators, while the CLEWs framework considers flexible quantification methods. The governance analysis and its interconnection with the technical Nexus analysis are distinctive characteristics of the TBNA methodology. The WEF Nexus framework also discusses stakeholder dynamics in more detail than other approaches. MuSIASEM follows a very different approach to the others. It applies to any combination of systems (it is not linked to a specific set of Nexus dimensions) and can be applied at any scale using the same methods.

1.1 Gaps in Nexus Assessments Frameworks

Several Nexus assessments reviews have been conducted that compare approaches under different criteria. The reviews examine not only the methods used in an assessment but also the process in itself. We select some of these reviews and try to overcome some gaps in the existing frameworks that can improve Nexus assessments. We focus on three categories referring to the general approach and to intrinsic and extrinsic elements.

Regarding general gaps, Albrecht et al. (2018) find that quantitative approaches are often preferred in Nexus assessments. Few combine qualitative methods, while Endo et al. (2017) state that the Nexus approach is yet to be

formally recognized and its complexity requires clarification. The thin interface between policy and science, and the challenging incorporation in decision-making processes, is also frequently mentioned (McGrane et al., 2018; Wiegleb and Bruns, 2018; Dargin et al., 2019). The coverage of Nexus systems also varies, and many studies tend to focus on a reduced number of systems (Endo et al., 2017). Nexus assessments also commonly prefer techno-economic and biophysical analyses, and the consideration of social science methods and aspects is limited (Kling et al., 2017; Albrecht et al., 2018).

Other gaps in Nexus approaches refer to intrinsic elements in the approach. One such gap is the lack of standard procedures, methodologies, and models (Fernandes Torres et al., 2019; Liu et al., 2017) with the capacity to adequately identify and assess the influence of Nexus interlinkages. Understanding the systems' Nexus is vital and necessary for the approach's success, and such understanding should be shared by the actors involved (McCarl et al., 2017a; Ramos E. et al., 2021). On modelling tools, Kling et al. (2017) highlight the need for model validation, while (Liu et al., 2017; McCarl et al., 2017a) suggest the need for a unifying integrated model or procedures for multi-model integration, particularly due to the challenge of reconciling differences (temporal and spatial resolution) across sectoral models. The identification of interlinkages, access to information, and terminology are another core gap in Nexus approaches. Although some approaches inform on interlinkages more broadly (Flammini et al., 2014; Ramos E. P. et al., 2021), others are specific to applications. Liu et al. (2017) note that Nexus interactions would benefit from clarification, and (Endo et al., 2017; McCarl et al., 2017b) pinpoint that clarification on the complexity of the Nexus is needed. On terminology, another challenge relates to common semantics between actors involved in the assessment to realize effective collaboration (Kumazawa et al., 2017). On the issue of data and information gaps, Lawford (2019) suggests the development of an integrated data and information service in support of Nexus assessments. The need to realize interoperability between models and model integration is pointed out by (Liu et al., 2017). Improved interdisciplinarity and transdisciplinarity practices in Nexus assessments is necessary to address sustainability challenges (Mauser et al., 2013; Ghodsvali et al., 2019). In the perspective of Kling et al. (2017), gaps in Nexus knowledge can be overcome through multidisciplinary¹, and (Endo et al., 2017) justify the development of disciplinary integration for reducing Nexus-wide trade-offs and synergies. Additionally, coordination between different actors can be critical in data production (Liu et al., 2017). Ontology engineering is proposed by Kumazawa et al. (2017) as an approach with the potential to support interdisciplinarity efforts. However, although considered an obvious requirement, the practicality of transdisciplinary approaches is yet to be understood. Limitations to multi-stakeholder participation may prove difficult, particularly in

different geographical contexts (e.g. language) (Ghodsvali et al., 2019).

Governance, financing and funding, and approach's timeframe and vision were identified as extrinsic gaps to advance Nexus approaches. These may be more challenging to address than the intrinsic ones since they depend on external factors and conditions beyond reach to practitioners. A significant obstacle to the operationalization of the Nexus approach is its application in decision-making contexts and governance (Al-Saidi and Elagib, 2017; Dargin et al., 2019). Bridging the gap between science, and policy- and decision-making, requires approaches to incorporate options that can mitigate and respond to this issue. The inclusion of transdisciplinarity practices, e.g. multi-stakeholder involvement, is paramount. Such inclusion should clarify how natural and social systems interact and how systems are managed and governed, including understanding the nature of stakeholders' "thresholds" to decisions (Ghodsvali et al., 2019). Only then synergies can be effected via integrated governance (Liu et al., 2017). Increased collaboration between stakeholders and researchers is also pointed out by (Dargin et al., 2019), in addition to strengthening the first phases of the assessment process in terms of diagnostic, guidelines and knowledge transfer opportunities to facilitate the shared understanding of the Nexus approach. Another aspect that needs consideration is the shared risks in innovative governance mechanisms and reconciling sectoral, political, and power interests (Gallagher et al., 2016). Linked to integrated governance are the approach's timeframe and long-term implementation vision of the implementation. Its long-sighted implementation requirement (Cremades et al., 2019) not only battles with existing sectoral policy integration challenges (Venghaus et al., 2019) but navigates through asynchronous policies and strategies commonly coupled with cyclic policy mandates. On the discussion of the concept of transdisciplinarity, (Ghodsvali et al., 2019), explain that effective transdisciplinarity requires the change to remain. Decisions may have conflicting implications and effects on society and places, depending on the decision context (Romero-Lankao et al., 2017; Engström et al., 2021). Thus, for the Nexus approach to promote a governance transition, it should explicitly contemplate this aspect in its structure. Commonly, assessments close with "conclusions and recommendations", which is the step from when stakeholders may need assistance and follow up on the solutions identified. If the follow-up study of interventions, or test cases, is not possible to implement, the Nexus study could be side-lined. The previous gap can be related to the project orientation and limited funding to advance the Nexus approach. Not only do assessments require financial support for researchers and practitioners, but they may also require financing of the recommendations (Hoolohan, et al., 2018; Cremades et al., 2019). In one way, an economic and cost-benefit analysis could provide an estimate of economic implications, but may not be enough. Nexus financing, and the roles of public and private sectors, is discussed by (Markantonis et al., 2019).

¹Tress et al. (2005) define multidisciplinary as the interaction between different disciplines for a common goal but with different discipline objectives.

TABLE 1 | The SIM4NEXUS case studies and indicative diversity factors (GL: Global, CO: continental, TR: transboundary, NA: national, RE: regional) (Peel et al., 2007; Brouwer and Fournier, 2017; Fick and Hijmans, 2017; Eurostat and European Commission, 2019).

CS	Scale	Geography	Climate (Köppen-geiger Classification)	Main Economic Activity	Critical nexus Challenge
1. Sweden	NA	Northern Europe, North Sea, Baltic Sea	South: humid continental North: cold, without dry season and with cold summer	forest products, hydropower, forest fuels	climate change impact on water resources, forest ecosystems and interlinkages
2. Latvia	NA	Northern Europe, Baltic Sea	cold, without dry season and with cold summer	agriculture, wood products, food processing, chemicals	low-carbon development and resource-efficiency policies
3. Netherlands	NA	Western Europe, North Sea	temperate without dry season and warm summer	agriculture, food industry, industry, services, tourism	the role of biomass in the transition to a low carbon economy and impact on water, food, land, climate
4. Eastern Germany-Czech Republic-Slovakia	TR	Central Europe	West: temperate without dry season and warm summer East: humid continental without dry season and with warm summer	agriculture, industry	precipitation retention as a driving force of climate-resilient landscapes, land use antagonism between bioenergy and food production
5. Counties of Devon & Cornwall, United Kingdom	RE	Southwest of the United Kingdom, Northern Europe, Atlantic Ocean, North Sea	temperate without dry season and warm summer	tourism, agriculture	cost, environment and security in water supply
6. France- Germany	TR	Upper Rhine region, Western, Central Europe	temperate without dry season and warm summer	industry, agriculture	the consequences for aquatic ecosystems and rivers, bioenergy, energy crops, land uses, water quality and quantity
7. Andalusia in Spain	RE	south of the Iberian peninsula, Southwestern Europe	Mediterranean, Temperate with dry, hot summer	agriculture, fishing, animal husbandry, forestry, energy	water-efficient irrigation, agricultural energy
8. Sardinia in Italy	RE	west of the Italian Peninsula	Mediterranean, Temperate with dry, hot summer	tourism, mining industry	limited resources under sustained socio-economic development
9. Greece	NA	South-Eastern Europe, Mediterranean Sea	Mediterranean, Temperate with dry, hot summer	agriculture, maritime industry, tourism	cross-sectoral implications of single-sector strategies
10. Azerbaijan	NA	Eastern Europe, Western Asia, Southern Caucasus region, Caspian Sea	diverse, cold semi-arid humid continental, humid subtropical, temperate oceanic	oil and gas products, agriculture, food production	lack of diversification in energy sources, food security, dependency on TR water resources, potential role of RES
11. European	CO	Northern and mostly Eastern Hemisphere	mainly temperate, diverse	diverse, services, industry, agriculture, tourism	the impact of transition to a low carbon economy on the Nexus
12. Global	GL	n/a	n/a	n/a	identify and assess Nexus issues at the global scale with focus on the SDGs

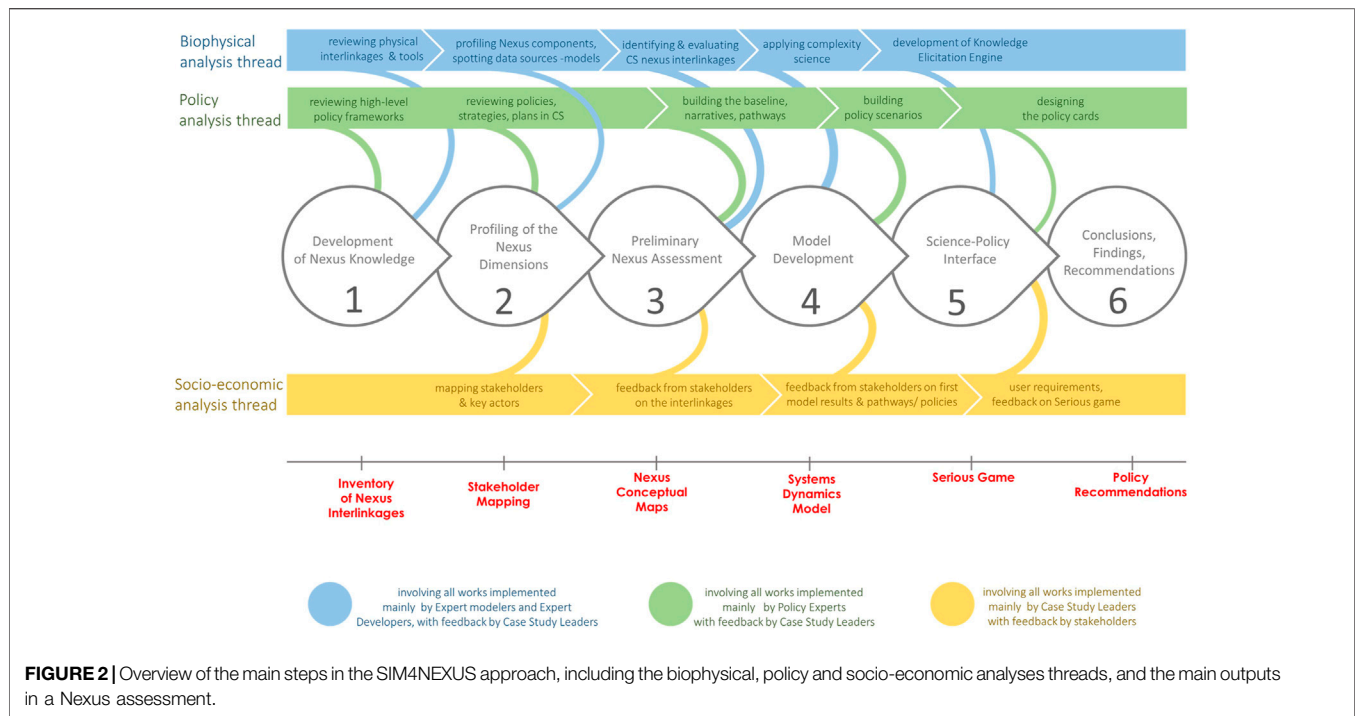
1.2 Unique Characteristics and Contribution

The Nexus approach designed from the SIM4NEXUS project is a unique contribution to Nexus research. An early version of the approach was informed by the FAO-WEF and CLEWs approaches, and was throughout the 4 years of project. One case study (Greece) operated as a front-runner and showcase for the other case studies.

The SIM4NEXUS approach was designed, validated and updated from the twelve case studies implemented, considering diverse geographical, biophysical, socio-economic and political contexts, and covering different spatial scales (e.g. regional, national, transboundary, continental and global scales). Very importantly, except for the case of Azerbaijan, case studies are led by locals, giving a unique advantage in the approach, considering that a foreign team would need to surpass a series of contextual difficulties (i.e., language, cultural distance, context knowledge). An overview of case studies is presented in **Table 1**. More information on the cases is available in **Supplementary Appendixes A and B**.

In order to test robustness of the approach our focus is on different spatial scales (regional, national, transboundary, continental and global). The biophysical nature differs across scales, as well as the input and output flows from the system boundaries in place. This can be depicted in the imports and exports of food and energy in all the different scales. The scale diversification in case studies plays an equally important role, if not more, in the socio-economic and the political analyses, since it shapes differentiated stakeholder maps and policy level—EU, national, regional—frameworks, respectively. Nexus A number of additional artificial and functional differences, such as the availability in data, the stakeholder participation, the capacity and expertise in tools of the different working subgroups, the resources, etc. complete the full diversity of the case studies in place.

In this paper, we present the consolidated view of the main tasks necessary to perform a comprehensive Nexus assessment through the SIM4NEXUS approach. The approach is informed by Nexus-related research and tested against twelve Nexus



assessments. Our ultimate aim is to release and transfer the SIM4NEXUS approach to the research, planning and policy communities², using the learnings and experience from the case studies. By doing so, we aim to contribute towards the operationalization of the Nexus approach, meaning its uptake and effective use in decision making.

2 MATERIALS AND METHODS

The SIM4NEXUS approach is grounded in the practice of twelve case studies that have worked under the same project showcasing geographical, social and economic diversity. They are implemented in different scales: regional, national, transboundary, European and global. This is a unique output in the Nexus approach field. To our knowledge, no other research initiatives or projects have combined so many cases, and so varied, over the same period, and involving the same and diverse teams of experts. The work in the cases was dynamically iterated within the project activities and developed in collaboration with stakeholders. Ultimately, the approach provides guidance on how to conduct a Nexus assessment and informs on the key methodological steps of the process. We recommend the approach for use in the development of future Nexus assessments by the research community, institutions, and private actors.

²By planning communities we refer to actors which engage in planning processes within the sectors which operate in the different Nexus dimensions. Such “planning communities” can be local stakeholders responsible for a municipality, private utilities, farmer associations, etc.

2.1 Description of the SIM4NEXUS Approach Steps

The SIM4NEXUS approach is presented in this section and includes three phases. It was reached following a 4 years project and completed in 2020. Initially, it was informed by existing frameworks, such as CLEWs (Howells et al., 2013; Ramos E et al., 2021) and the WEF Nexus assessment methodology by the FAO (Flammini et al., 2014), review of other approaches to the Nexus. It was then shaped according to several activities conducted in the project for the development of the Nexus assessments in each case study. A first comprehensive version was reached halfway the project. The framework was then reviewed and updated, taking stock of the continued work of the case studies until spring 2020.

The SIM4NEXUS approach is structured into six main steps: the *Development of Nexus Knowledge*, the *Profiling of the Nexus dimensions*, the *Preliminary Nexus assessment*, the *Model development*, the *Science-Policy interface*, and finally the *Conclusions, findings and recommendations*. The following description of steps and sub-steps constitutes a synthesis of the workflows in all the case studies and uses as a baseline the national case study of Greece that operated as a frontrunner. **Figure 2** depicts the six main steps, the main tasks involved in the three workflow threads: the Biophysical, Policy, and the Socio-economic analyses, as well as an abstract timeline of the main assessment outputs. A detailed description of this process follows as structured into the aforementioned six main steps and shown in **Figure 3**. Important to clarify that the framework is not an automatic process, nor is there automation in its implementation (other than inherent automatic tasks specific to the modelling tools, the SDM and the activities for the development of the

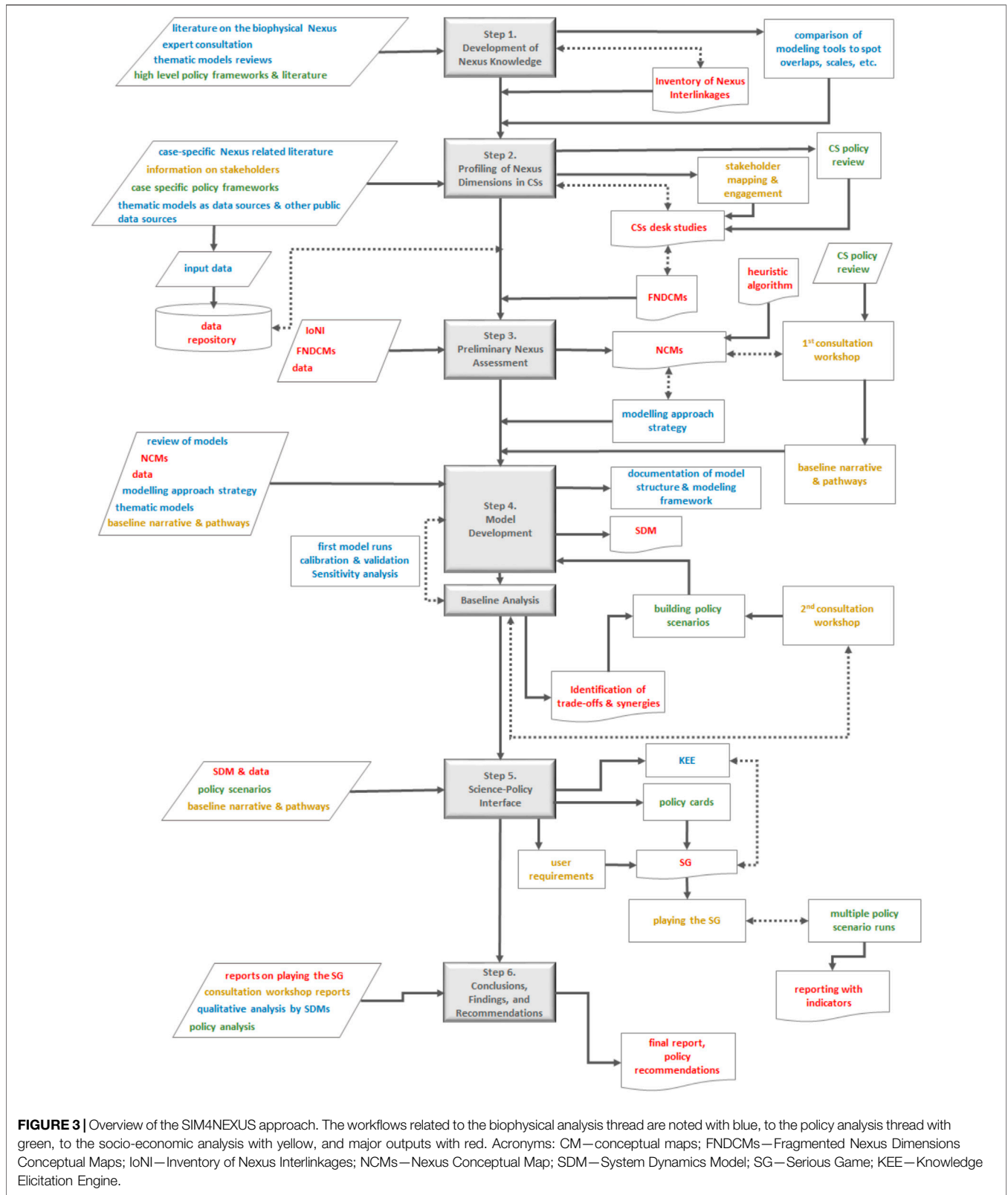


FIGURE 3 | Overview of the SIM4NEXUS approach. The workflows related to the biophysical analysis thread are noted with blue, to the policy analysis thread with green, to the socio-economic analysis with yellow, and major outputs with red. Acronyms: CM—conceptual maps; FNDCMs—Fragmented Nexus Dimensions Conceptual Maps; IoNI—Inventory of Nexus Interlinkages; NCMs—Nexus Conceptual Map; SDM—System Dynamics Model; SG—Serious Game; KEE—Knowledge Elicitation Engine.

Serious Games (SGs)). Serious Games are interactive video games that expand beyond recreational purposes and aim at skills and knowledge development by their users through problem-solving (Manero et al., 2015; Pilote and Chiniara, 2019; Sušnik and Masia, 2020).

The first step of the SIM4NEXUS Approach is the Development of Knowledge in the Science of the Nexus. This step is implemented in three sub-steps:

- 1) *Building the Nexus knowledge*: refers to the process of developing Nexus approach knowledge by the experts involved in the assessment. This is critical for understanding the complexity of the analysis and for clear communication with stakeholders throughout the Nexus assessment, and when communicating the assessment outcomes to different audiences.
- 2) *Modelling tools to assess the Nexus*: A virtual “toolbox” is set up with all relevant state-of-the-art tools and other approaches that are available for quantifying the Nexus. A comparison is performed of modelling tools regarding their capacity to cover the different Nexus dimensions, coverage of spatial and temporal scales, semantics and ontologies and overlaps in the tools are identified.
- 3) *Preparation of the background knowledge on the Nexus*: An Inventory of Nexus Interlinkages (IoNI), all possible systems interactions, is created (Laspidou et al., 2017), as well as a method for visualizing interlinkages in an assessment through building a Nexus tree (Laspidou et al., 2018), which can be complemented by a heuristic algorithm to quantify the relative strength of interlinkages (Laspidou et al., 2019).

Key outputs of the first SIM4NEXUS approach step are the IoNI, the review of modelling tools and integrated assessments, and a review of high-level policy frameworks and papers.

The second step is the Profiling of the Nexus Dimensions in the case study and corresponds to the assessment of Nexus systems (Water, Energy, Food, Land, and Climate), their trends, the status of sectors, and the identification of sectoral challenges. Six main tasks are included in this step:

- 1) *Characterization of the Nexus dimensions*: characterization of all involved Nexus dimensions systems (domains and sectors) for the case studies, using publicly available sources and expert knowledge.
- 2) *Policy and governance analysis, consisting of* a thorough review and understanding of policies, strategies and plans implemented or to be implemented in the near future per Nexus dimension, or across domains, at all scale levels (regional, national, continental, and global) in each case study.
- 3) *Collection of data and sorting*: Raw non-processed data and simulated data (assessment of available modelled data for the case study, from Step 1.ii) if necessary are collected. The data may refer to resource uses, stresses, availability, spatial and temporal distributions, etc.;
- 4) *Mapping of stakeholders and key actors and first stakeholders' consultations*: The key players are identified in this step, and the stakeholder engagement process initiates. At the same

time, some first impression of the stakeholders on what shapes the Nexus map regarding resources, sectors and processes hotspots is recorded. The latter is done mostly via unilateral consultations.

- 5) *Identification of sectoral challenges*: Inputs from points i) to iv) result in the identification of sectoral challenges, which can be operational and/or at the institutional level. An example of an operational challenge would be the transition to a low-carbon economy, while an example of an institutional challenge would be the absence of inter-ministerial communication for co-designing a strategic plan for the environment, the energy, and the agricultural sectors. Challenge-implicated interactions in the systems Conceptual Maps (CM) should be identified, when possible. The DPSIR framework can be used in this step to assist in the structuring and interpretation of the information collected, from each Nexus dimension perspective.
- 6) *Assessment of thematic models outputs as data sources*. This is implemented to assess the potential need to obtain extra data or identify missing data to cover possible gaps in data sets. Key outputs of the second step are the sectoral assessments and Nexus systems conceptual maps, the policy analysis, the stakeholder mapping, the identification of main and/or potential data sources, and identification of the case studies hotspots regarding processes and resources.

The third step of the SIM4NEXUS approach is the Preliminary Nexus Assessment. This step develops from the outputs of Step 2, such as the desk-study and the systems conceptual maps, which are analyzed in an integrated manner following the sub-steps described below. In summary, this step includes:

- 1) *Scanning the systems for the identification of Nexus interlinkages*: The IoNI produced in Step 1 and the Nexus systems CMs produced in Step 2 are necessary for this step, since they are scanned to spot any interlinkage that can be considered relevant in each case study. Identifying interlinkages and assessing the complexity and extent of the interrelations among domains for the CSs leads to the drafting of Nexus CMs (NCMs) that are used later in the first consultation workshop.
- 2) *Preliminary estimation of the strength of the interlinkages*. The data collected are used for a first estimation of the most relevant interlinkages from the perspective of each system. The share of resources uses, and their flow from sector to sector, are quantified. This quantification may serve to filter the relevant interlinkages or reveal some important hidden interlinkages that were not perceived as critical. This preliminary Nexus quantification will also reveal the comparative spatial and temporal distributions of uses, processes and availability of resources and will help define the proper time step and granularity of the following modelling exercise according to the uniformity of the distributions. For a more systematic and standardized process of the preliminary estimation of the strength of the interlinkages, a Heuristic Algorithm for ranking the Water–Energy–Food–Land Use–Climate Nexus

Interlinkages is developed by Laspidou et al. (2019). This sub-step leads to the update of the NCMs draft.

- 3) *Development of final NCMs*: this is a more mature version of the NCMs representing in a single diagram how the different systems depend on each other.
- 4) *Consolidated identification of critical interlinkages*: Comparison of (outputs from Step 1, such as sectoral challenges, preliminary interlinkages, policy analysis) and sub-steps i)–iii) (assessment of the significance of interlinkages, and CMs) for a consolidated identification of critical interactions, and by doing so, of Nexus-induced challenges;
- 5) *First consultation workshop* for stakeholder input and opinion on the status of the systems, sectors and challenges. This sub-step implements the validation and/or identification of critical interactions (consolidated in iv)) making use of the previous resources developed (NCMs, sectoral briefs, policy analysis summary, etc.). Details on the stakeholder and expert consultation processes can be found in Laspidou et al. (2019). In this step, the final NCMs are also validated by stakeholders;
- 6) *Formulation of the baseline narrative and identification of pathways that could be of interest to analyze*: This task involves the formulation of a “raw” narrative that characterizes the baseline case (or business-as-usual) related to how stakeholders perceive the development of the different sectors following current or expected trends. This is an important step to be used as a benchmark for pathways or scenarios of interest.
- 7) *Definition of the modelling approach strategy (e.g. selection of thematic models)*: This step builds on the previous steps (1 ii), 3 iv), and 3 vi)) and the consequent refinement of Nexus challenges and critical interactions. Thematic models and other quantification methods are identified based on their ability to cover the Nexus systems and, most importantly, to capture the cross-system dynamics related to the critical challenges identified in the case study. It will be important to assess data availability and access at this stage.

Key outputs of the third step are the NCMs, the identification of Nexus challenges, the definition of pathways, the first modelling requirements (what systems should be covered and with what level of detail), a heuristic algorithm for ranking Nexus interlinkages strengths, the preliminary selection of modelling tools, and the first version of the baseline narrative (storyline) of the case study.

The fourth step in the approach is Model Development. This step includes the use of the thematic models and System Dynamics Modelling (SDM). The latter is a complexity science approach that enables the quantification analysis of the qualitative information gathered in the previous steps (Laspidou et al., 2019; Sušnik and Masia, 2020). Such information is used in the SDM to mathematically characterise flows, stocks, tables and other simple features of the systems under investigation. The analysis helps capture complex and non-linear systems dynamics, allowing for performing scenario and

uncertainty analyses (Keyhanpour, et al., 2021). The main sub-steps in this phase are:

- 1) *Analysis of the information available for quantification*: In this step, analysts compare inputs from the previous tasks, particularly related to the Nexus interactions, pathways and NCMs.
- 2) *Implementation and development of the modelling approach strategy*. The selection of modelling tools, suggested in Steps 1 ii) and 3 vii), is evaluated and (re)defined (and decided upon). The choice of thematic models is also based on data availability and formulation gaps within the SDM. Inputs and outputs of models are compared, and harmonization of input data is performed to the extent possible.
- 3) *Literature review regarding the overall and in-parts model structure*: The whole modelling approach involves thematic models where needed, applies them for the baseline, and links them with all relevant variables through commonly accepted formulations. The final outcome is kept as simple as possible.
- 4) *Characterisation of the baseline in quantitative terms*: Drivers and narrative elements are analyzed for their representation in the models, and to guide the definition of assumptions coherent with the baseline and across modelling tools. Since the thematic models will unlikely cover all Nexus systems with an equivalent level of detail, it will be important that the detailed narrative produced as a starting point covers plausibly the evolution of the Nexus systems so that “baseline” dynamics across systems are well understood (step 3.f). This is an important step prior to the definition of scenarios.
- 5) *Data requirements are assessed and data availability evaluated*, in order to prepare baseline models for the CS. Modelling teams clarify the type of interactions and components of the narrative they could inform about. An important step in the modelling work is the analysis of the baseline results, represented separately in the diagram. Nexus trade-offs are identified as well as potential synergies across sectors and systems. Once the baseline is prepared, scenario development and implementation can follow.
- 6) *Data preparation and model development*: Data is collected and prepared to be used in the thematic models. The baseline of the models is prepared. Model runs are conducted and results analyzed. Depending on results, models may require to be improved to ensure the adequate representation of the functioning of the dynamics they represent.
- 7) *Building the policy scenarios*. Preliminary policy work is done here, with defining policy objectives and instruments. Policy scenarios are built according to the policy papers review and stakeholder participation.
- 8) *Preparation of the SDM structure (complexity science tools)*: Once the CMs are revised, based on activities in 3. a–f, the structure of the SDM is prepared. Data requirements of the SDM are mapped against models inputs and outputs and other relevant data available. The policy scenarios and the narratives shape the SDM structure and flow from inputs to outputs.

- 9) *Iterative model calibration and validation*: The runs will be used for calibration and validation. An iterative process between the SDM building (including thematic models) and the SDM runs lead to its structural improvement.
- 10) *Uncertainty analysis*: The dimensions of uncertainty, namely the location, the level and the nature, are identified by the involved modellers after defining all the modelling assumptions. The assumptions are labelled as contextual, structural, or parametric uncertainties (which are the locations of uncertainty). A series of sensitivity runs of the model is conducted to quantify the parametric uncertainties (Knobloch et al., 2019).
- 11) *The second stakeholder workshop* aims at informing stakeholders of the modelling outputs and discussing the first results. This may require updates or other iterations of the models. The workshop also initiates discussions on pathways and scenarios. The latter is done based on the selection of policies to be studied in combination with stakeholder input and feedback. SDM visualization tools are employed to show stakeholders what the potential of the tool is.

The key outcomes of the fourth step are the sectoral and/or multi-systems models, the repository of input and output data, the documentation of modelling assumptions concerning the characterization of the baseline, and the uncertainty analysis.

The fifth step corresponds to the Science-Policy interface. For results to be within reach of a variety of audiences (policy-makers and other actors of decision, in public and private institutions, academia, civil society, NGOs, etc.), they need to be packaged in a way that is simple and intuitive to interpret. In SIM4NEXUS, this is achieved with the Knowledge Elicitation Engine (KEE) in the format of an SG, which combines all efforts from the previous steps. The SG bridges the domains of science and policy-making, making the analysis accessible to a wider audience. In this way, users of the game are not required to have particular expertise or knowledge in any of the main components of the studies but will acquire knowledge on the Nexus by playing the SG. Tasks related to the development of the game include:

- 1) *Development of the Knowledge Elicitation Engine (KEE)*: This is the inference engine of an expert system (the SG in SIM4NEXUS).
- 2) *Conceptualization of the SG*: This task involves the development of Use Cases for the Serious Game, the design of the game structure, the moves that a player can implement, the rounds of the game, how a player wins, the tokens, etc. Special focus is given on the design of the policy cards, which constitute the players' option in the game that simulate in the visual environment actual resources management choices. This task also involves the creation of the Semantic repository.
- 3) *Definition of indicators*: In this task, established Key Performance Indicators (KPIs) are employed, and others are created from scratch to illustrate the Nexus systems' performance displayed in the game. These are designed to facilitate the understanding of the Nexus systems responses and the evaluation of the policies regarding the SDGs and Nexus coherency.

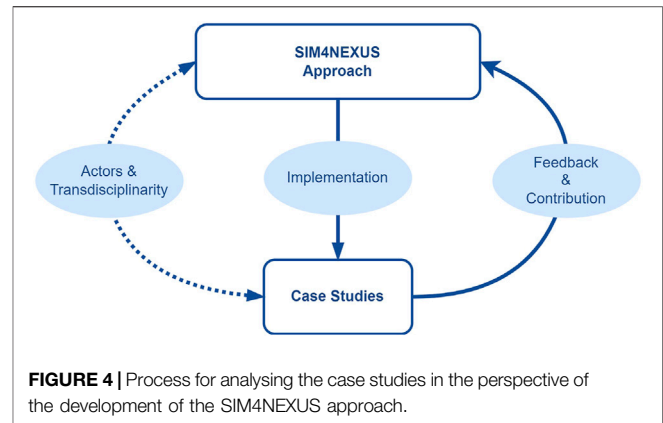


FIGURE 4 | Process for analysing the case studies in the perspective of the development of the SIM4NEXUS approach.

- 4) *Development of the visualization interface*: This task involves a lot of iterations among partners to provide for usability, commonly accepted aesthetics, etc.
- 5) *Instructions of how to play the game*: Instructions use popularized wording and are translated to all languages of case studies' stakeholders.
- 6) *The third consultation workshop* aims at presenting the game to the stakeholder group for feedback.

Key outputs of the step are the KEE, the SG, and the Nexus KPIs.

The final step naturally involves the formulation of Conclusions, Findings and Recommendations, based on the objectives of the pathways and scenarios investigated in each case study. Once the players play the game, they can manipulate the systems to explore different futures and collect messages that are specific to their choices. They will be able to infer on the coherency of policies based on the quantification analysis; the role of innovations; identification of trade-offs and synergies in the different scenarios; and assess potential solutions at the sectoral and cross-sectoral levels. This step can include the presentation of the SG in additional stakeholder consultation for the final version of the game. Other game dissemination activities include its application in universities and schools.

2.2 Methodology for the Analysis of the Case Studies

The SIM4NEXUS approach described in the previous section is the consolidated and generic version of the Nexus assessments process by the case studies. Dynamically developed, the approach provides an overall picture of how work is performed in different tasks constructing the way for the Nexus assessments. To distil learnings from the application and development of the SIM4NEXUS approach, we analyzed the cases from different viewpoints, as illustrated in **Figure 4**. Firstly, in terms of the actors involved and their role in the assessment process and transdisciplinary research characteristics. Secondly, in terms of the approach implementation. Lastly, how the work in the case studies is feedbacked to the approach is also examined. Findings from this analysis are presented in the Results section of the paper.

Nexus assessments aim towards knowledge integration from different disciplines in the investigation of Nexus challenges. With the involvement of more disciplines and actor types, assessments head towards transdisciplinarity practices. In the transdisciplinarity analysis of SIM4NEXUS case studies, we aimed at understanding the diversity of actors involved in each sub-step of the framework, their level of integration, and intensity of engagement.

To validate the SIM4NEXUS approach steps and sub-steps, we examined how case studies had implemented them. An example of the case study analysis is presented in **Supplementary Appendix C**. The analysis enabled revising the steps suggested in an intermediate project deliverable (Ramos et al., 2019) and their update according to case studies' work until the spring of 2020. It is important to note that fewer inferences are made regarding Steps 5 and 6 as many deliverables were ongoing while developing the SIM4NEXUS approach. In addition, the Covid-19 pandemic induced constraints, affecting the organization of the last set of stakeholders' workshops.

Several project deliverables informed the comparative analysis, e.g., (Blanco, 2017; Brouwer and Fournier, 2017), bi-annual case study interviews carried out by Work Package 5 (Brouwer and Fournier, 2020a), and review and direct input from CSLs through the elaboration of case study tables for the approach's validation.

The comparison was conducted in two ways. Firstly, we assessed if cases had or not performed specific approach sub-steps, which informed if the step was or not relevant and if it had to be removed or updated. Secondly, we compared the descriptions provided by each case study on how sub-steps were conducted to assess. This comparison served to identify differences and particularities in the approach's implementation (e.g., an example is the fuzzy cognitive mapping for stakeholder participation developed in the case of Andalusia (Martinez et al., 2018)).

In the step and sub-step comparisons, we looked for systematic differences that informed their refinement or prompted changes to their location and, again, their relevance. An example of inference is that cases may have completed the task as planned in the project activities, but the specific task was not found to be relevant for their Nexus assessment. In the results section, we summarize the key findings of the comparison according to the categories in the Nexus concept (Brouwer et al., 2020; Ramos et al., 2020), described in the Introduction.

3 RESULTS

This section presents the results from the comparative analysis of the case studies in SIM4NEXUS. In summary, we assess actors' involvement, disciplinarity integration, and derive insights from the approach's implementation.

3.1 Actors' Involvement and Transdisciplinarity Analysis

Different actors were involved in diverse stages of the case studies and engaged with varying intensities. Based on the SIM4NEXUS experience, we identify six types of actor types: Expert Case Study

Leading teams (CSL), Expert Modellers (MOD), Policy Experts (POL), Expert Developers (DEV), Stakeholder (STK), and Other (OTH). The CSL is responsible for conducting and coordinating the case study, and in the majority of the SIM4NEXUS case studies, it is part of the case context. MODs develop mathematical models representing the Nexus systems and deal with modelling data inputs and outputs in the thematic models or the SDM. MODs also develop modelling frameworks that enable scenario analysis in the CS. POLs guide and assist the CSL in the policy analysis component of the assessment, which includes the policy coherence analysis, development of policy scenarios, and definition of policy cards for the SG. The SG is developed by DEVs, who liaise with actors engaged in SG development. Stakeholders (STK) are groups or institutions of interest that operate in the Nexus context of the case studies and are interested in the findings of the analyses. Lastly, the category "Other" (OTH) refers to actors external to the assessments' workflow but who contribute with knowledge and expertise throughout the assessment process. Examples of these actors include manuscript reviewers, the executive advisory board to the SIM4NEXUS project, and the scientific community in conferences or meetings.

After identifying actors and roles, an appreciation of their participation in each assessment stage was performed in **Table 2**. This evaluation was conducted by SIM4NEXUS project partners and was informed by the experience in the cases studies. Such knowledge is also documented in several project deliverables (Fournier, 2016; Munaretto, 2018; Brouwer and Fournier, 2020a; Echeverria et al., 2020; Sušnik and Masia, 2020). In the table, the engagement intensity is indicated using a color gradation from dark to light blue, linked to a numeric scale of 1–5, indicating high to low engagement, respectively. The results do not inform on the time effort of each task, but the timing of actors' participation and their expected level of engagement.

The results reveal the critical role of the CSLs. They are present in most assessment steps and with high participation intensity since they are responsible for the assessment development and the liaison with other experts and stakeholders. Modellers (MOD) are key in the model development step 4) and data preparation and tool selection for analyzing Nexus systems. They are also engaged in developing the SDM and providing modelling outputs for the Serious Game. Policy analysts are involved in the policy coherence assessment, identifying sectoral policy goals and instruments, in the model development stage for the definition of policy scenarios, and the Serious Game via the selection of system-level policy options the players can implement. As for the DEVs are primarily engaged in the Science-Policy interface step, which takes the format of a Nexus Serious Game or results' visualization tools. Due to their transversal role, stakeholders are present throughout the assessment process. Ultimately, they also test and play the SG, and thus are involved in retrieving Nexus (or integrated) insights. The involvement of "Other" actors can also be spotted in all framework steps since there could be opportunities for the engagement of external audiences to the CS throughout the Nexus assessment. One important role "Others" can play by testing the SG, contributing to its development and improvement.

TABLE 2 | Overview of actors involved in the different steps of the SIM4NEXUS approach and the intensity of their participation. Abbreviation meaning: CSL—CS Leading team; MOD—Expert Modeller(s); POL - Policy Expert; DEV—Expert Developer(s); STK—Stakeholder(s); and, OTH—Other actor(s). The color notation “x” expresses the degree of involvement of the actor type from high (dark blue color) to low (light blue).

SIM4NEXUS Approach Step	Actors					
	CSL	MOD	POL	DEV	STK	OTH
1. Development of Nexus knowledge						
a. Building the Nexus knowledge	1	1	1	1		
b. Screening of modelling tools and quantification approaches to assess the Nexus, and methods to compare policies	2	1	1			4
c. Preparation of the background knowledge on the Nexus	1					
2. Profiling of the Nexus domains						
a. Characterization of the Nexus domains	1					
b. Policy and governance analysis	1		1		2	
c. Identification of data requirements	1	1			2	
d. Mapping of stakeholders and key actors, and first stakeholders’ consultations	1				1	
e. Identification of sectoral challenges	1				1	
f. Assessment of thematic models outputs as data sources	2	1				4
3. Preliminary Nexus assessment						
a. Comparison of systems for the identification of Nexus interlinkages	1				2	4
b. Preliminary estimation of the interlinkages significance	1				2	
c. Development of the first version of the Nexus conceptual model	1					
d. Consolidated identification of critical interlinkages	2				1	
e. First consultation workshop	1				1	
f. Formulation of the baseline narrative	1		2		2	
g. Definition of the modelling approach strategy	2	1			2	4
4. Model development						
a. Analysis of the information available for quantification	2	1				
b. Implementation and development of the modelling approach strategy		1				
c. Literature review regarding the overall and in-parts model structure	2	1				5
d. Characterization of the baseline in quantitative terms	1	1				
e. Data requirements are assessed and data availability evaluated	2	1			2	
f. Data preparation and model development	1	1			3	
g. Building the policy scenarios	1		2	3	1	5
h. Preparation of the SDM structure	1			1		
i. Iterative model calibration and validation	1	1		1		
j. The 2nd stakeholder workshop	1		3		1	
5. Science-Policy interface						
a. Development of the Knowledge Elicitation Engine (KEE)		3		1		
b. The development of “Use Cases” for the game and creation of the Semantic Repository (SR) and policy cards	2		3	1		
c. Definition of indicators to illustrate the performance of the Nexus systems	1				1	4
d. Development of the visualization interface				1		3
e. Instructions on how to play the Serious Game	1			1		3
f. 3rd consultation workshop	1				1	
6. Conclusions, findings and recommendations						
	1		3		2	

Several types of stakeholders were engaged in the case studies through various participatory methods. These implied varying engagement intensities, from information sharing and consultation to consensus building. An overview of stakeholders involved in the case studies and participatory methods is shown in **Supplementary Appendix D**. Such information sheds light on the transdisciplinary character of the studies.

Transdisciplinarity research is characterized by high disciplinary integration (i.e., interdisciplinarity) combined with high engagement of non-academic actors, who work together for solving a common problem (Tress et al., 2005; Mauser et al., 2013). However, involving a diverse group of non-academic participants does not necessarily mean that a study is transdisciplinary if this engagement is mostly for consultation purposes, and coordination between different actors types is limited.

TABLE 3 | Analysis of the application of framework steps in case studies considering the activities reported in Deliverable 5.5 (Brouwer and Fournier, 2020b).

Framework Step	Findings
1 Development of Nexus knowledge	All cases completed the sub-steps in this step. The development of knowledge in the Nexus was important for all actors involved, and having a common understanding of the Nexus approach facilitated communication among the ones involved, including with stakeholders
2 Profiling of the Nexus dimensions	The majority of cases validated the steps. Differences here are verified in stakeholder mapping, which was more challenging for larger-scale cases (i.e., European and Global)
3 Preliminary Nexus assessment	<ul style="list-style-type: none"> • Different approaches were used to estimate interlinkages significance: quantitative (Lapidou et al., 2019) and qualitative, e.g., stakeholder consultation and conceptual maps' development • Workshops were not always conducted within the suggested work plan, suggesting these should be flagged in the framework as tentative • The cases refined the modelling strategy throughout the assessment process, specifically when certain data were not obtained from the selected thematic models. Thus, it is critical to understand modelling tools' capabilities to assess the Nexus context in the early stages of the assessment • Collaboration between actors is intensified in this stage. Better understanding by the case study team of thematic models and SG development is vital at this stage in support of stakeholder engagement activities
4 Model development	<ul style="list-style-type: none"> • The majority of the cases implemented the sub-steps described in the framework. Differences observed related to the availability of model results (some cases already had models that could be used, including SDMs, or modellers in the case study leading team). Data complementarity issues were identified in the characterization of Nexus domains by thematic models for populating the SDM developed based on the conceptual maps. Additional data collection was performed, and thematic models contribution was revised • Workshops were conducted but not always aligned with the work plan, partly due to the timing of the first workshop, different participation approaches followed, or information requirements from the cases to support ongoing tasks
5 Science-Policy interface	Most cases completed the tasks in this step, distilling insights from the case study and indicating policy options to tackle the Nexus challenges, fulfilling the purpose of the assessment. Learning was achieved in elaborating policy-relevant insights by case study teams Even though SGs were not developed for all cases, some could use other cases' examples in stakeholders' interactions. Some cases opted for other results visualization options (e.g., global case study). Experts' availability (modellers and developers) created a bottleneck that influenced the completion of tasks. In a single case study assessment involving a group of experts, such challenges would probably not occur
6 Conclusions, findings and recommendations	Conclusions and recommendations were included in several deliverables. Policy recommendations are structured regarding changes to policy outputs, policy contents, innovation, policy processes, and the policy-science interface. The corona pandemic emergency compromised the dissemination of results planned for the first half of 2020

In these circumstances, research can be considered “participatory” and “parallel”, as opposed to “transdisciplinary” and “integrative”, as explained by Tress et al. (2005) and Mauser et al. (2013). When research is focused on academic practitioners, the approach to disciplinary integration (e.g. cross-disciplinary, multidisciplinary or interdisciplinary) can vary, and depends on how a goal is planned to be achieved. For example, a cross-disciplinary study considers the perspective of another discipline when solving a problem within its disciplinary field. In multidisciplinary studies, different disciplines work together towards a common objective; in interdisciplinary studies, the integration of disciplines is required to answer a common question.

Reflecting on the transdisciplinary character of SIM4NEXUS case studies, we find that these can be of many types in terms of integrative approach—and not necessarily transdisciplinary. For example, larger spatial scale assessments, such as the transboundary, continental and global have a more challenging task in stakeholder engagement and closer participation due to the involvement of multiple countries, which then multiplies the stakeholders to be engaged from different management, political, and social contexts. These actors will unlikely share similar priorities, interests, values and decision-making power or influence, influencing the level of collaboration necessary for transdisciplinarity. In contrast, case studies of smaller

geographical scales, e.g., sub-national and national case studies, showed characteristics of transdisciplinarity. For example, in the Greek and Latvian case studies, transdisciplinarity was achieved by engaging a diverse group of non-academic actors; and in the South West United Kingdom (UK) case study, through a tight collaboration between academic and non-academic actors. In the latter, the case study leading team was a water systems company, and the integration of the Nexus approach was ambitious and aligned with the company's vision.

In conclusion, transdisciplinarity requires the engagement of a plural group of actors (academic and non-academic) who collaborate intensely in the investigation of Nexus questions. One way to achieve this is by planning stakeholder participatory activities that enable a higher collaboration between actors, such as the consensus-building, through the entire process of the Nexus assessment. Larger scale assessments would either benefit with more time for the assessment, or earlier engagement of actors in steps before its start. From the perspective of non-academics, the South West UK case study illustrated the advantage of collaborating with academic partners, supporting the importance of cultivating partnerships between business and private actors and Academia.

3.2 Application of the SIM4NEXUS Approach to the Case Studies

In terms of the implementation of the suggested approach steps and their relevance, we conclude that the work conducted in the cases is aligned with the approach suggested. A summary of this analysis is presented in **Table 3**. There was high accordance on the first four approach steps, and respective sub-steps. Differences exist mostly on the engagement of stakeholders and the timing of the organization of the workshops. In some cases, e.g., Global and European, the engagement proved to be more difficult than smaller scale or national case studies. In the case of Azerbaijan, since none of the partners was based in the country, subcontracting of national experts was conducted to facilitate access to national-context knowledge. All cases were able to arrive at conclusions and recommendations. **Table 3** should be analyzed in perspective with the involvement of different actors across the various steps, as presented in **Table 2**. The steps described in the assessment are very much in line with the activities developed and co-developed in several work packages. With the framework, we also aim to provide perspective on the purpose of these activities, which many times happened simultaneously but involving different types of experts.

3.3 Contribution of the Case Studies to the SIM4NEXUS Approach Development

Although cases were guided by the same approach, differences existed between the studies due to the diversity of contexts and challenges. In this comparison element, we searched for learning from the case studies practice. These contributed to the enrichment and transferability of the SIM4NEXUS approach. The findings were grouped according to the Nexus concept defining categories, described in **Figure 1**.

On Knowledge Creation, cases identified the opportunity of developing new methods to address the tasks in the different steps, depending on the resources available and the characteristics of the case. Some resulted in the application of methods to new problems (e.g., participation of stakeholders in the identification of key interlinkages in the case of Andalusia, (Martinez et al., 2018)), methods for the identification of interlinkages relevance (e.g. as in the case of Greece (Laspidou et al., 2019)), or the application of methods developed in the project (e.g., policy coherence analysis as in (Munaretto and Witmer, 2017; Papadopoulou et al., 2020)). Awareness of the Nexus interlinkages can be of value in policy design, and can increase the level of engagement of stakeholders in the analysis.

In relation to Participatory Governance, the category that embeds the interactions with stakeholders in the case studies, different ways of mapping and engaging stakeholders were followed. For example, in Andalusia, fuzzy cognitive mapping was used, while in the case study of Sweden, stakeholder mapping included a power/interest analysis (Brouwer and Fournier, 2020a). Also, challenges and opportunities of cross-sectoral collaboration were found. For example, in the Greek case study, the largest cotton production corporation expressed interest in creating the appropriate bonds to the water and energy sector, aiming at improving resource efficiency in its

production chain and getting certified accordingly. In the transboundary study of Germany, Slovakia and the Czech Republic, the team was engaged in a multi-country group of stakeholders for the preparation of pilot studies for landscape water retention. The cases recognized that the iterative process between local stakeholders and the research team (MOD, DEV, CSL) is key to identifying reasonable solutions to be investigated in the Nexus assessment. Thus, the clarification of roles and responsibilities, and also the timing of the communications, are important aspects which were then made more explicit in the SIM4NEXUS approach.

Methods and Tools represent the importance of quantitative practices (e.g., indicators, data, visualization tools, SGs, and modelling tools) in the SIM4NEXUS approach. These are essential to produce science-based evidence to inform sectoral planning. In SIM4NEXUS, new Methods and Tools were developed and therefore included in the approach. Examples include the application of Artificial Intelligence for the SG development, complexity science applied to the Nexus context, inter-comparison of thematic model results; and also the identification of critical data gaps in sectoral statistics. Also in this category are the creation of data repositories (i.e., cross-sectoral databases, both in terms of inputs and modelling results) and the combination of quantitative and qualitative information (e.g. incorporation of qualitative inputs from stakeholders to the quantitative analysis). The gamification of the Nexus is another important element in the approach, providing an opportunity to national stakeholders, e.g. from academia or ministries, for exploring the impacts of different sectoral policies on the Nexus. Additionally, the SGs developed can be used beyond the project timeframe in other projects or for educational purposes, and are now hosted by Watershare® (watershare, 2021).

4 DISCUSSION

In this section, insights from the analysis of SIM4NEXUS case studies are put in perspective with the Nexus approach gaps identified in the Introduction section. Additionally, we take stock of lessons learned from applying the approach across the twelve case studies and identify critical aspects for its operationalization.

4.1 The SIM4NEXUS Approach Compared to Other Frameworks

Similarities can be identified between Nexus approaches summarized in the Introduction, in particular to the FAO-WEF and CLEWs, and the TBNA regarding the policy analysis track and stakeholder participation. The SIM4NEXUS approach, similarly to the others, also defined indicators to characterize the Nexus performance, obtained from the models and used in the SG. In the latter, aggregated indicators inform on the Nexus “health”. The main differences between the SIM4NEXUS approach include the dedicated effort to build Nexus knowledge, which requires time, and the integration of thematic models, other modelling tools and data collection into a single modelling framework. The SDM, detailed to the

complexity level possible, is used to quantitatively describe the Nexus contexts in the case studies, following the Nexus conceptual maps.

The general Nexus approach gaps refer to the need to integrate quantitative and qualitative approaches, clarify the meaning of complexity, strengthen the science-policy interface and incorporation of the Nexus approach in policy, and the coverage of Nexus systems inclusion of social sciences. The SIM4NEXUS approach combines qualitative and quantitative methods, and it includes aspects from social sciences, policy analysis, and player behavior in gaming. Complexity is addressed through multiple iterations between the Nexus approach threads. Its transferability is evidenced by the application to multiple cases of different contexts and scales.

Intrinsic gaps relate to the lack of standard procedures, methodologies and models, the understanding of interlinkages and terminology, and the need for improving inter/transdisciplinarity. In relation to the standardization gap, the SIM4NEXUS approach contributes to addressing these gaps by introducing, applying and validating in multiple case studies the complexity science approach, developing SDMs that unified the Nexus models and complemented the representation of Nexus systems. Also, a methodology to rank the relevance of interlinkages is developed (Laspidou et al., 2019). Clarification on interlinkages and terminology is addressed through the elaboration of IoNI (Laspidou et al., 2017), the development of background information on WELFC Nexus, and the glossary of the Nexus (Ramos et al., 2019). The glossary aims at standardizing, to the extent possible, terminology which is frequently used in Nexus discussions and can facilitate communication with stakeholders and other audiences participating in an assessment. Regarding disciplinary integrative approaches, SIM4NEXUS considers a multidisciplinary team of experts with knowledge of different Nexus systems. Thematic models with a focus on different systems and with varying operating principles are used to simulate the Nexus in the case studies. Later, an SDM, which is based on the NCMs of each case study context, incorporates information from thematic models and is complemented by other information not modelled at the previous stage. Uncertainty analysis of the models is also performed (Knobloch et al., 2019). All the continued integrative approaches culminated with the development of an SG. Stakeholders are also engaged throughout the Nexus assessment, and local CSLs facilitate multi-stakeholder engagement.

Extrinsic aspects related to governance, the understanding of a Nexus approach timeframe, and funding and financing of Nexus solutions influence the application and success of the approach. Regarding governance, in SIM4NEXUS, stakeholder participation is planned in several steps and considers the engagement of public actors from different levels of decision (local, regional and national). Participatory Governance is considered a pillar element to Nexus assessments. The SIM4NEXUS multi-stakeholder engagement process also facilitates communication between different stakeholder types and the possibility of gathering and understanding different decision level perspectives. In addition, the SIM4NEXUS

network of stakeholders allows participants and institutions to extend their networks, which can be of relevance for future work. In addition, policy analysis is performed to inform policy coherence, but also for the design of case-specific policy scenarios. The approach is also analyzed from how it can be integrated with the policy cycle for identifying entry-points and mapping interaction and collaboration opportunities throughout the process (**Supplementary Appendix E**). Several cases point out that the timeframe of the project influences stakeholder engagement. On the one hand, actors recognize that for the approach to have an impact on decision-making, tools need to be more mature in the first workshops. Quantitative analysis, for being meaningful and relevant to the level required for decision, need more time for development and stakeholder collaboration. However, recognizing the importance of cross-sectoral planning is already an important achievement, in particular, when many stakeholders are involved. Such findings support the importance of creating continuation projects that can foster cooperation and co-development between Nexus practitioners and stakeholders. Another aspect requiring attention is the voluntary nature of stakeholder participation and the difficulty of engaging decision-level stakeholders with limited availability. From another angle, tools and methods developed in SIM4NEXUS can continue being developed and applied. Such examples are the use of the SG in the Nexus oriented Erasmus+ SMARTENproject, the use of the SDMs in H2020 NEXOGENESIS, the adoption of the SIM4NEXUS Semantic repository by the NEXUSNETCOST Action and in general, the fact that teams that developed Nexus knowledge continue to disseminate and advance it. Thus, a long term vision needs to grow in different lines of work, so that collaborations are effectively transdisciplinary and the approach operational. In this perspective, the SG use in education or capacity development is recommended. Funding for Nexus projects, not only by research institutions, is in great part related to the challenge of operationalizing the Nexus approach. Given the effort magnitude of engaging so many experts, securing funding is challenging yet needed. From the implementation side, financing is required to test Nexus solutions and interventions and to support innovation. In the case study of Greece, where the banking sector was involved, credit solutions were discussed as a sector's contribution to making the Nexus approach operational.

4.2 Lessons Learned From the Application of the SIM4NEXUS Approach

A key step of the SIM4NEXUS approach is the understanding of the biophysical and socioeconomic Nexus context, its drivers, dynamics, and how it links to decision making. Developing this conceptual understanding is challenging and requires iterations. In SIM4NEXUS, this process was streamlined through the collaboration of different actors, but also through peer-review occasions (projects, conferences, meetings), unfolding other key steps, such as stakeholder engagement, modelling, scenario development, and participation in policy. The development of the conceptual model was a key output that translated scientific knowledge to the case studies. It also served to communicate with

stakeholders involved, enabling a set of consequent activities. The exercise of elaborating policy insights from a Nexus perspective was also critical. Knowledge was gradually constructed across all project activities and did not exclusively result from the quantitative analysis. Thus, combining quantitative and qualitative approaches in Nexus assessments is crucial to ensure a wider variety of solutions.

Regarding what is essential to apply a Nexus approach, flexibility in the implementation, in particular in the use of prescribed tools and methods, is listed high. Stakeholders may not be interested in adopting an established modelling tool if in-house robust tools exist and already inform decisions. However, Nexus knowledge is important and can be taken into consideration when using existing tools. Stakeholder participatory methods also need to be flexible and adaptable to the desired type of engagement. In terms of stakeholder participation, partners with existing networks were more efficient to engage stakeholders due to historical inter-institutional collaboration. Several cases noted that more workshops were needed to keep stakeholders engaged and for feedback and consultation on intermediary outputs of the analysis. Defining the analysis scope and expectations is also an essential component, since Nexus analyses are vast. A preliminary Nexus assessment helps define the analysis scope and prioritize what to investigate. Producing such a plan would support stakeholder engagement, more clearly understand what to focus on and when, plan for tool development, conduct an assessment of expert needs, and search for future funding. In addition, having a longer-term vision of the Nexus approach would contribute to knowledge transfer and the development of capacities at many different levels in the institutions involved and plan for the engagement of higher-level stakeholders.

Another critical point is to understand which tools are suitable, what type of coverage they provide, and to what detail (temporal, spatial and operative scales). Although thematic model suitability was performed in the initial stages of the case studies development (Fazekas et al., 2017), it was only after the finalization of conceptual models that a concrete understanding of interlinkages and quantitative inputs were specifically identified. Possibly the conceptual model should be designed before the tools were screened and chosen. Additional data collection, or use of other modelling tools, was performed to ensure SDM representation was covered. The challenge of model suitability highlights the importance of assessing tools and their documentation, methods for data integration, as well as data availability and accessibility, in the early stages of the Nexus assessment.

In SIM4NEXUS, five Nexus dimensions were selected (Climate, Land, Energy, Water and Food). As the project unfolded, several cases indicated that Ecosystems could be added as an extra dimension. This exemplifies the necessity for the Nexus approach to be plural and system-agnostic. When looking at resource efficiency and a transition to a low carbon economy, it makes sense that the resource systems (land, energy, and water), food system, and climate are interactively analyzed. However, practitioners may identify other relevant systems to analyze, depending on the Nexus context. Other systems, mainly from the economic sector, could be added, such as Tourism, which is found relevant in the cases of Greece and Sardinia, “Forestry” in the cases of Latvia and

Sweden, and Economic Growth or Employment, which are proven to be interlinked to the WEF Nexus in the Mediterranean (Markantonis et al., 2019). The dimension of Health is also growingly discussed as an entry to the Nexus complex. In this context, the Texas A&M Energy Institute has established the Water-Energy-Food-Health Nexus Renewable Resources Initiative (WEFRAH) in January 2020. Alternatively, the perspective could also be different and focus more on consumers’ behavior and choices; or have a business perspective to identify risks and vulnerabilities. Thus, other systems and viewpoints can be discussed and incorporated in conceptual models, based on their relative importance to the contextual challenges under scrutiny.

Frameworks, in general, lack the integration with the policy cycle and also a monitoring and evaluation component that could test recommendations and specific measures and support the decision making process. Addressing this gap implies a different intensity of actors’ engagement, the extension of the project timeframe, or the use of ready-made tools. Collaboration in planning activities should be better accounted for, for the Science-Policy interface to work. This could be achieved through capacity building on the tools and methods developed or establishing collaboration protocols between researchers and institutions of interest.

5 CONCLUSION

The management of resource systems, considering environmental, techno-economic and societal factors, is a multi-objective task. The Nexus approach can support sustainable development by providing an integrated systems perspective. The SIM4NEXUS approach constitutes a unique output in the Nexus research field. It results from the development of twelve case studies of different spatial scopes and socioeconomic and biophysical contexts developed within the same timeframe. It provides a solid basis for future assessments adopting a step-wise approach which considers the 1) development of Nexus knowledge, 2) profiling of the Nexus dimensions, 3) preliminary Nexus assessment, 4) model development, 5) science-policy interface and 6) conclusions, findings and recommendations.

Important gaps on Nexus assessments are addressed with the SIM4NEXUS approach, such as integrating biophysical and social aspects, combining qualitative and quantitative methods, clarifying Nexus complexity by considering different workflows in an assessment, and by demonstrating transferability in the application to multiple case studies. From the application of the cases, multiple challenges in the operationalization of the Nexus arose, such as the incorporation of the approach in the policy cycle, the understanding of the longer-term characteristics of the Nexus approach, and ensuring funding and finance mechanisms to support Nexus solutions.

The comparative analysis of the SIM4NEXUS case studies allowed for the identification of key aspects in Nexus assessments. These included the need to flexibly select Nexus systems to study and the implications of stakeholder engagement beyond the

assessment process through expanding networks and disseminating Nexus knowledge across institutions. The clarification of Nexus assessment outputs, systems coverage, and level of detail, are essential when performing an assessment and can assist with preparing subsequent Nexus complementary analyses.

The operationalization of the Nexus approach will take time and it will benefit from the realization of transdisciplinarity. The SIM4NEXUS approach can contribute to it in several ways. It can serve as a basis for planning, as it can serve as a guide for practice. Practitioners can select the steps that fit their prospective project, use the different steps to perform a needs assessment, or decide which step requires more or less effort. In line with the Nexus approach, the success of an assessment may depend on the identification of synergies, either through engaging partners with consolidated and relevant networks, by using existing quantitative approaches and methods, or through interdisciplinary practices by sharing objectives across projects.

DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/**Supplementary Material**, further inquiries can be directed to the corresponding authors.

AUTHOR CONTRIBUTIONS

ER, DK, FB and CL contributed to conception and design of the study. ER implemented the review of the existing nexus frameworks,

the identification of gaps, the comparison of the SIM4NEXUS framework to other frameworks, and the design of the methodological approach for the comparison of CSs. DK, ER and CL constructed the sequence and links of the methodological steps. ER, DK, CS wrote sections of the manuscript. DK and ER implemented the visualization. CL and FB implemented the supervision, project administration, funding acquisition. All authors contributed to manuscript revision, read, and approved the submitted version.

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SUPPLEMENTARY MATERIAL

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