NEXOGENESIS
STREAMLINING WATER RELATED POLICIES

# Deliverable 3.2

# Final report on the complexity science and integration methodologies

**Lead: UTH**
**Date: May 2023**

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# Project Technical Report

| Project Number | Project Acronym | Project Title |
|---|---|---|
| 101003881 | NEXOGENESIS | Facilitating the next generation of effective and intelligent water-related policies, utilising artificial intelligence and reinforcement learning to assess the water-energy-food-ecosystem (WEFE) nexus |

| Instrument: | Thematic Priority |
|---|---|
| H2020 RIA | LC-CLA-14-2020 |

| Start Date of the project | Duration |
|---|---|
| 01 September 2021 | 48 months |

| Organisation name of lead contractor for this deliverable | Document version |
|---|---|
| UTH | 1 |

| Dissemination level | Deliverable Type |
|---|---|
| **Public** | **eport** |

| Authors (organisations) |
|---|
| Chrysi Laspidou (UTH), Alexandra Spyropoulou (UTH), Alexandra Ioannou (UTH), Dimitrios Kofinas (UTH), Nikolaos Mellios (UTH), Konstantinos Ziliaskopoulos (UTH) |
| **Reviewers (organisations)** |
| Stefania Munaretto (KWR) |





NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

**Abstract**

Deliverable 3.2 is the main and primary outcome of Task 3.1 and outlines the WP3 methodology. It focuses on the conceptual level of the Complexity Science integration models for each Case Study within the NEXOGENESIS project. System Dynamics Modelling (SDM) will be carried out using the STELLA Architect environment, which was chosen after the in-depth review of 5 Complexity Science methodologies, as the most suitable method for NEXOGENESIS's application of complexity science.

At each Case Study workshop, the stakeholders assisted in developing the conceptual models, which were subsequently presented in D3.1. In this report, Causal Loop Diagrams (CLDs) have been described in detail and were designed for all the Case Studies in accordance with the conceptual maps provided in MS11 (Complexity science tools progress report for all case studies). These CLDs will feed the SDMs for all the Case Studies. The WEFE nexus system's behavior and response will be assessed utilizing the ongoing sensitivity/uncertainty analysis process and will be reported in D3.6.

Keywords: causal loop diagrams, trade-offs, nexus, transboundary, case studies



NEXOGENESIS STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# List of abbreviations

CS – Case Study
WP – Work Package
D – Deliverable
M – Milestone
CLD – Causal Loop Diagram
SD – System Dynamics
SDM – system Dynamics Modelling
CA – Cellular Automata
MFA – Material Flow Analysis
FCM – Fuzzy Cognitive Maps
ABM – Agent Based Modelling
CI – Computational Intelligence
SFD – Stock-Flow Diagrams
WEEE – Waste from Electrical and Electronic Equipment
WEFE – Water-Energy-Food-Ecosystems
WEF – Water-Energy-Food



NEXOGENESIS STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# Table of Contents





NEXOGENESIS STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# List of Figures



# List of Tables





This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# 1. Introduction and purpose of the Deliverable

The primary objective of the Work Package 3 (WP3) is to review and select appropriate complexity science methodologies suitable for all the NEXOGENESIS case studies (linked to Task 3.1). Initially the following complexity/integration methodologies were considered: System Dynamics Modelling, Cellular Automata, Fuzzy Cognitive Mapping, Material Flow Analysis, and Agent Based Modelling.

This deliverable (D3.2) is an important outcome from Task 3.1, reviewing in detail all the aforementioned complexity science methodologies assessed with regards to the Nexus that have the potential to be used in NEXOGENESIS and reports on the finally selected methodology to be used. The outcome of this Deliverable will be used in Task 3.2, 3.3 and 3.4.

System Dynamics Modeling was chosen as suitable methodology for NEXOGENESIS's integration of Complexity Science for the following reasons:

i) Its graphical context makes it understandable to users and stakeholders, facilitating the validation process;
ii) It may incorporate several types of data and components into a single model and is highly adaptable;
iii) It can be immediately translated to Python, which makes it appropriate for the kind of modeling needed within the NEXOGENESIS project.
iv) It can utilize external data and model output as necessary, downscaled to appropriate levels benefit from the theme models' aggregated, downscaled outputs (Tasks 3.2, 3.3 and 3.4, and linked to WP2).

As a result of the aforementioned factors, NEXOGENESIS selects System Dynamics Modeling (SDM) as the ideal integration technique for Complexity Science for all Case Studies and all the simulations will be implemented in the STELLA Architect environment. The creation of the Conceptual Complexity Science models, which will serve as instruments for the SDMs' development, was the initial phase. To be compatible and useful as tools for the quantitative SDM models, the Conceptual Complexity Science models have been developed and drawn by each Case Study team with the help and assistance of all the key individuals involved in the Case Studies including stakeholder, with continuous consultation and participation to several meetings, both virtually and in person.

In this report, Causal Loop Diagrams (CLDs) are described in depth for all the Case Studies. CLDs were designed in accordance with the conceptual maps provided in MS11 (Complexity science tools progress report for all case studies). The CLDs (structure and components) are to be used as tools for the next stage of SDM development. The SDMs for all the Case Studies will be developed and presented in detail in D3.4 (Complexity science models implemented for all the Case Studies-Prototypes and explanatory report/manual for each CS, M23).



NEXOGENESIS STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# 2. Complexity science integration methods

## 2.1 System Dynamics Modelling

System Dynamics (SD) is defined as a method for studying the information feedback features of dynamic systems to show how structure, policies, decisions, and delays mutually affect development and stability (Drew, 1995). It is a strategy set up by Prof. Jay Forrester of MIT for addressing problems about the dynamic behavioral characteristics of complex systems (Forrester, 1961). It is associated with constructing quantitative and qualitative models of complex problem-solving situations and then trying out with and understanding the behavior of these models gradually (Coyle, 2000). The SD approach allows for the representation of decision-making policies and information flows while dealing with an extensive number of variables inside several interacting feedback loops (Forrester, 1992, 2009). SD modeling may prove efficient since it relies on the dependable aspects of system understanding while correcting for the untrustworthy aspects. SD models stand back for soft variables including impetus and beliefs, allowing engineering projects to be more effectively understood and managed overall. Understanding the dynamics of a system is the initial goal of system dynamicists when using modeling and simulation.

Traditional techniques are valuable for resolving detailed operational difficulties inside the process, while SD is especially useful for getting insights into the patterns displayed by dynamical systems along with the structures underlying them. Closed-loop modeling has been shown to be the most effective in developing comprehension of the dynamic behavior of complex systems. This understanding is aided greatly by the concept of modeling the systems or challenges under study in continuous mode and at relatively high aggregate levels (Forrester, 1997). Traditional approaches emphasize a careful examination of the system. The SD technique is holistic in nature with an emphasis on the input/output principle that occurs throughout the system. SD's fundamental drawback is that it does not give a framework or approach for designing organizational structures as patterns of relations among organizational actors, encompassing the division of activities and functions (Schwaninger and Rios, 2008). Another constraint of SD is the organization's ability to absorb variation or complexity. SD provides a method for dealing with variation that enables modeling at multiple sizes of a problem or system (Odum and Odum, 2000).

SD focuses on identifying the primary stock variables that will be affected by the relevant flows at a specific resolution level or maybe numerous resolution levels. Parameters and extra variables will likely have an impact on these. SD approach, while allowing for conceptualizing and modeling at different scales, does not give a formal procedure for an organization to deal with external complexity, namely building a structure capable of absorbing that complexity (Schwaninger and Rios, 2008).

Validation of the fundamental presumptions, which are often based on individual personal experience, figures out the trustworthiness of traditional models. The presumptions offer a means for dealing with subjective difficulties that are difficult to quantify, but they are often implicit and overly relied on. The problem of this more traditional technique is that the assumptions are not always relevant, resulting in a model that is disconnected from reality. A SD model is confirmed by comparing it to earlier models. Even a precise copy of past behavior,



NEXOGENESIS STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

as in any modeling exercise, will not ensure precise prediction of a new model's behavior. Models are distinguished by their uniqueness, and extreme caution is needed when projecting prior experience, regardless of modeling methods (Rodrigues and Bowers, 1996).

SD is a complex system modeling and simulation technique that has numerous applications in science and engineering (Sušnik et al. 2012, 2013, 2021; Laspidou et al, 2019; Bakhshianlamouki et al. 2020; Laspidou et al., 2020; Purwanto et al. 2021; Ioannou and Laspidou, 2022; Wang et al. 2023). While experts in the field handle most model development, recent improvements have focused on bringing system dynamics closer to rapidly emerging fields such as data sciences. A few distinct approaches were recently investigated to enable modeling stages such as model structure development, model calibration, and policy optimization. However, an integrated method that supports the procedure for modeling throughout the board is still lacking. Using computational intelligence (CI) approaches, the proposed support system enables data-driven inference of causal loop diagrams (CLDs), stock-flow diagrams (SFDs), model equations, and model parameter estimation. The System Dynamics Modeling (SDM) approach's main goal is to help develop complex models where human intervention is insufficient. Such complex models were developed in the context of quantifying systemic resilience (Ioannou and Laspidou, 2022), to quantify the state of biodiversity (Laspidou and Ziliaskopoulos, 2022), and with the aim of being used as a practice guide and as a basis for planning (Ramos et al., 2022). The ability of humans to store and analyze an increasing amount of data, and then apply CI approaches to transform this data into valuable information, is causing a revolution in the SD field. SD is an effective modeling technique for complicated dynamical systems (Azar, 2012).

The scientific field of SD renders a framework for modeling complex and dynamic systems. Understanding the connections between SD model structure and model behavior in complex model formulations is a significant difficulty in the field of SD modeling (Richardson, 1996). A long sequence of model tests of increasing sophistication and insight leads to profound comprehension. SD is a policy modeling methodology founded on decision-making, feedback mechanism analysis, and simulation (Drew, 1995). Decision-making targets on how decision-makers will take actions. Feedback is concerned with how information created provides perspectives on decision-making and influences future decision-making in comparable instances.

Contrary to a real system, simulation offers decision-makers with a tool to operate in a virtual environment where they may examine and analyze the implications of their decisions in the future. Thus, SD has the potential to simulate real-world systems, apparently with some assumptions, in order to improve understanding of complex systems, dynamic complexity, and policy resistance sources in order to construct highly successful policies (Forrester, 1992).

Typically, complexity is described in terms of the number of system components or the number of combinations that must be considered while making a choice. This is referred to as combinatorial complexity. Even simple systems with minimal combinatorial complexity can exhibit dynamic complexity (Bayer, 2004). Dynamic complexity is the outcome of the interplay of system parts over time. Even systems with modest combinatorial complexity can have significant dynamic complexity. Complex behavior is observed in dynamic, strongly linked, feedback-governed systems that are non-linear, adaptive, paradoxical, and policy resistant.



NEXOGENESIS STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 101003881

## 2.2 Cellular Automata

A Cellular Automata (CA) is a discrete model that was initially theoretical but is now used in fields ranging from physics to biology, geography to ecosystems, software engineering to regional science. As Miller (2009) states, CA are discrete spatio-temporal dynamic systems based on local rules. CA is the most basic modeling framework for demonstrating complexity. CA can display extraordinarily sophisticated behavior and development with simple conditions and rules. They are intrinsically appealing as geographical models since they map precisely onto the raster grid of a geographical information system, involve just regional interconnections among cells, and are simple. Nonetheless, they have the ability to model and reproduce incredibly complicated behavior as well as displaying emergence (Batty 2000).

Stanislaw Ulam invented CA while working at the Los Alamos National Laboratory in the 1940s. John von Neumann focused on addressing the issue of self-reproducing systems. Von Neumann recommended the kinematic model, which envisioned a robot that could be rebuilt from replacement components.

CA models, which are frequently employed in complex system analysis throughout fields of study, that simulate worldwide repercussions based on regional relationships between different individuals of a population. The CA technique is able to disentangle difficult research challenges. A series of studies were presented in the 1980s that extensively investigated an undiscovered class of one-dimensional CA that was named elementary CA (Wolfram 1986). The revelation that what is now known as "complex systems behavior" may be simulated from the most basic of CA sparked a flurry of research in both the physical and social sciences into the breadth of what CA might model. Wolfram extended his research and published A New Kind of Science in 2002 (Wolfram 2002). Wolfram contends in the book that findings regarding cellular automata are not isolated facts but have implications for all disciplines of science. Wolfram established that practically any calculation can be simulated using a one-dimensional CA, and he investigated applications across fields.

Batty (2000) examined the geo-computational variations of CA that can be used to simulate urban and comparable systems. He pointed out that rigid CA models are at one end of a functional continuum, while simple Cell Space models, which are just raster grids containing limited amounts of states that shift over time, are at the other. He distinguished cell space models, that are not strictly CA models, and the idea of loosening the CA assumptions. The addition of action-at-a distance, which is disallowed by rigorous CA's usage of the von Neumann or Moore neighborhoods solely, is essential to all relaxations. A literature review covers CA development in urban area modeling and other geographical territories, and several valuable sources are given (Batty 2000).

Above mathematics, CA implementations were mainly concerned with having CA adapt to regional variance than with definitional accuracy. Automatic techniques for learning to empirically create guidelines from seen trends, self-modification or modification of rules generated by aggregate system activity, and the addition of "ghost" states that are classified among strict classes have all been proposed as techniques (Clarke, 2014).

Obtaining accurate and trustworthy information to assess the process of diffusion is probably one of the most difficult issues that diffusion scientists encounter. The development of new products is a complex process that often includes an extensive amount of people engaging with each other over a period of time. Unfortunately, researchers frequently only have access



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

to gathered adoption data for study, as is typically the case using market-level models of diffusion (Sultan, et al., 1990).

As computer systems become increasingly powerful and user-friendly, the ability to model huge and complex systems allows insights previously unimaginable. The complexity of the marketing environment, with so many consumers and merchants interacting, suggests that Cellular Automata will be an important tool for marketing analysis in the approaching decade.

CA can be valuable in contexts other than the diffusion process. Models in which users are influenced by diverse brand advertisements in addition to the beneficial and adverse responses of other consumers, for example, can assist to supplement the game theory research on competitiveness. Consumer and network membership responses to new distribution methods can aid in the analysis of new avenues like electronic commerce. "Relationship marketing" tactics, whereby the marketing mix is adjusted to someone's preferences and long-term earnings are monitored, can be improved.

## 2.3 Fuzzy Cognitive Maps

Fuzzy Cognitive Maps (FCMs) are representations of knowledge and reasoning inference networks that use circular digraphs. FCMs have attracted significant scientific attention during the last decade and are commonly utilized to evaluate causal complex systems derived from the merging of fuzzy logic and neural networks. FCMs can be used in a wide range of applications, including computer science, engineering, environmental sciences, behavioral sciences, medical, business, computer systems, and data technology. Their dynamic properties and learning capacities render them indispensable for activities such as modeling, analysis, policy making, forecasting, and so on (Papageorgiou, 2011).

An FCM is made up of a collection of quantitative 'causal conceptions' or parameters, Sj, as well as directed 'edges' or arcs linking pairs of parameters. Each edge is linked with a weight, Wji, which stands for the way the parameter Sj at the originating end of the arc affects the parameter Si at the opposite end (Kosko 1992). Variables might reflect logical statements, random events, or managerial. FCMs can incorporate feedback loops, enabling for the modeling of complex interactions between systems, based on how the edges are constructed. Comparing this method to rule-based systems that depend on fuzzy sets, this is its main benefit.

Several sample areas of use were chosen to show how FCMs were used and are illustrated in the following. Recently, much FCM implementation research has been done in business and management, 23 in engineering and control, 67 in computer science, and two in medicine (Papageorgiou, 2011). In behavioral sciences, Andreou et al. presented the usage of the genetically evolved certainty neuron fuzzy cognitive map (CNFCM) as an extension of CNFCMs, with the goal of overcoming the latter's fundamental drawback, specifically recalculating the weights associated to every notion whenever a new strategy is selected (Andreou et al., 2003). Additionally, Acampora et al. proposed a novel approach for designing ambient intelligence systems that uses a multiagent structure and an innovative variant of FCMs theory assisting from timed automata theory to generate a collection of dynamical intelligent agents which utilize computational intelligence to identify action patterns that can maximize environmental variables such as user comfort or energy savings (Acampora & Loia, 2009).

FCM-based decision-making methodologies in the field of medicine, particularly for healthcare support of decisions tasks, encompass a combined framework for therapy planning



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

management in radiotherapy (Papageorgiou et al., 2008), a model for impairments of language (Georgopoulos et al., 2003). FCMs were applied for recognizing pattern problems by Papakostas et al. (2008). For mining time-related data related to healthcare, Froelich and Wakulicz-Deja (2009) presented an FCM technique. Using the intracellular biochemical pathway, Rodin et al. (2009) built a fuzzy influence diagram to simulate cell activity in system biology.

FCMs find a wide range of applications in the engineering sector, particularly in controlling and predictions. FCMs were used to model and assist with a plant management system, to build a framework for failure modes and impact research, to optimize fuzzy logic controllers (FLCs), to represent a control system's supervisor. Stylios and Groumpos researched the FCM for modeling complex systems and controlling supervisory control systems (Stylios and Groumpos, 2004). For training FCMs to simulate industrial process control problems, Papageorgiou et al. (2006) used learning algorithms based on nonlinear Hebbian rules. On an area of heating network, Lu et al. (2010) used an FCM-based control technique and provided a method for developing the FCM model using supervised object-oriented least squares and previous data sets. Ioannou and Laspidou (2023) quantified and investigated the influence of Water-Energy-Food Nexus on the 17 Sustainable Goals using the FCMs analysis revealing either synergies or trade-offs that can contribute to enhance sustainability.

The FCM methodology is being well demonstrated in the literature as an extremely valuable tool for modeling and analyzing complicated dynamical systems. It is a simple cognition tool that can successfully reflect knowledge and reasoning. There is numerous application research on FCMs in various sectors, extensions of FCMs, or modifications. FCM applications are rapidly expanding. FCMs are useful as the decision-makers consider their representation of a specific issue to determine its suitability and may prompt the implementation of any modifications that are required.

## 2.4 Material Flow Analysis

A methodical assessment of the flows and stocks of materials inside a structure that is described in both time and space is known as a Material Flow Analysis (MFL). It links a material's sources, routes, and in between and final sinks. MFA acts on several timescales and scales. To enable multifaceted decisions on current systems or situations, resources, or items may be linked to their costs and environmental implications. The preservation of materials as stock in the built environment and cross-border resource trade are both considered by regional metabolism (Kennedy & Hoornweg, 2012; Baynes and Wiedmann, 2012). According to this conceptualization, Clift et al. (2015) stated that cities are complex systems that depend on their external surroundings for contributions of resources and for assimilation of pollutants and generate structured environments at the cost of growing disorder, i.e., environmental disruption beyond their limits. For instance, Barles (2014) conducted a territorial metabolism on the Midi-Pyrénées and Ile de France regions of France. These databases cover local resource extraction, transportation of goods (such as biomass, minerals, and fossil fuels), and outflows to the environment (such as emissions to the air, water, and soil). This regional-scale data is helpful to decision-makers in terms of waste management policies, dematerialization policies, etc., and it raises issues regarding the contributions of various industries, such as food, agriculture, and construction.

Both territorial ecology and industrial ecology use territorial metabolism. However, MFA techniques depend on the mass-conservation rule and inadequately take into account flows of



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

intangible capital when they are applied alone (Buclet et al., 2019). More integrative frameworks, such as industrial ecology, have emerged over decades to get around this constraint. Large and complex territorial systems are taken into consideration in territorial metabolism, industrial, or territorial ecology while meso-level activities and their effects on the territory are studied.

MFA provides a solid foundation to serve as a reference framework with relation to the physical aspect of circular economy. MFA has made a name for itself as one of the primary industrial ecology tools (Kalmykova et al., 2018; Geng et al., 2012) in worldwide (Fischer-Kowalski et al., 2011), regional (Chen et al., 2013), sectoral (Allesch and Brunner, 2015), and commercial (Habib et al., 2014) studies. It is also a crucial component of most circular economy evaluations (Eckelman and Daigo, 2008). Furthermore, MFA Sankey diagrams have demonstrated to be highly effective for public interaction (European Academies Science Advisory Council, 2015), which is a critical aspect because circular economy methods engage a variety of stakeholders, such as individuals (Ghisellini et al., 2016). If a system's mass flows are arranged in a regular pattern, circular economy indications may be established explicitly in relation to those flows. Pauliuk (2018) recently presented an overall MFA scheme at the organizational and product life cycle level. Such systems and indicator formulations have been provided and created for economy-wide MFA for an extended period (Fischer-Kowalski, 2011; Matthews et al., 2000; Eurostat, 2001). They represent the system at a coarse level, making it challenging to fit complicated systems to this framework.

MFA is acknowledged as an appealing decision-making tool, notably in the areas of resource management and waste management, because of the strict methodology used by developed nations to tackle diverse waste streams. MFA covers four main steps: (i) identifying the main MFA concerns; (ii) analysis of the system to identify the pertinent matter process, indicator elements, and system limits; (iii) qualifying mass flows of matter and indicator compounds; and (iv) identifying weak points throughout the entire MFA system. A graphical representation and analysis of the MFA diagram is then used to analyze the whole procedure after this step. The method is inexpensive and can be utilized for estimating product inventories for the production, transportation, and disposal of waste from electrical and electronic equipment (WEEE) as well as the chemicals it emits (De Meester et al., 2019). MFA is a reliable method industrialized nations use with an input and output assessment framework to manage diverse waste sources. The value chain's issues and gaps may be found using this technology, and appropriate management solutions could be developed. It is advantageous for waste streams that are complex and diverse, like WEEE, that include both useful and detrimental components. Also, MFA is described as a framework used to evaluate the flow of matter supported by material stability and adheres to the material preservation law (Allesch and Brunner, 2015).

## 2.5 Agent Based Modelling

Agent-based models (ABMs) are a group of mathematical models used for modeling the behavior, interactions, and actions of autonomous single or group entities, with the aim of examining the effects of a single agent or a particular type of behavior on the system as a whole. According to Miller (2009), the agents are autonomous entities that try to achieve a specific set of objectives. A country, a property owner, a citizen, someone renting, an agricultural producer, a consumer, a car, or even a person out for a stroll can act as an agent. Contrary to Cellular Automata, the goal of ABM is frequently not to produce aggregate structures or maps but rather to investigate variations in system behavior caused by agent



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

features (like the number of various kinds of agents) or rules. One example of a multi-agent model is a habitat model, which may include plants, animals that eat the plants, and predators that devour the animals. Multi-agent systems have multiple agents. ABMs combine evolutionary computer programming, complex systems theory, concept of games, and stochastic modeling techniques. ABMs are known as "individual-based models" in ecology and biology.

In an effort to model the behavior of the entire system and forecast the patterns of complex events, ABMs imitate the actions and interactions of numerous agents. Although they function freely, agents respond to their surroundings, the system's overall qualities, and other agents. An ABM includes (i) agents that are mentioned at particular model scales (granularity) and formats, (ii) decision-making algorithms that are frequently provided by censuses and surveys in the actual world, (iii) learning or adaptive rules, (iv) a method for engaging the agents, such as sampling, moving, and interacting, and (v) an environment that can both influence and be impacted by the agents. ABMs have their roots in von Neumann, Ulam, and Conway's work. Thomas Schelling's urban residential segregation model (Schelling, 1971) was a groundbreaking agent-based model for urban systems. The work represented the fundamental idea of agent-based models as autonomous agents interacting within a defined context and with an observed aggregate consequence, albeit not being computational.

Niazi and Hussain (2011) conducted a review of the most recent ABM literature. Parker et al. 2003's survey, which was the outcome of a workshop (Parker et al., 2002), was a significant study in geography. A number of studies released by the Santa Fe Institute were also influential (Gimblett, 2002). The application of agent-based modeling has been quite multidisciplinary. ABM was previously used to simulate consumer behavior, epidemics, biological warfare, traffic congestion, building and stadium evacuation, and organizational behavior. In these situations, a system encrypts both the interactions between individual agents and their behavior. In some geographical applications, field research, interviews, or census data have been used to support the models to infer behavioral features and decisions using qualitative techniques.

ABMs have recently been used to model a variety of regional science problems, including crowd behavior throughout rioting and events in the outdoors (Torrens, 2012), corporate innovation (Spencer, 2012), commuter behavior (McDonnell and Zellner, 2011), ecology and habitats, illness, and land use changes. The need for merging agent-based and complicated network-based models has been made clear by the latest studies on agent-based models. There has been a demand for more effective validation, as well as a need for models with reused parts, tools for evidence of conception and design, descriptive agent-based modeling for creating descriptions of agent-based models using templates, and complicated network-based models.

The Schelling model is an illustration of a typical ABM application (Schelling, 1971). Many ABMs and theoretical debates on ABMs have been built on the foundation of this straightforward model of segregation, which was first offered as a game simulation. The model shows how a person's attitudes about their neighbors might result in racial segregation in urban areas. The concept, in which agents represent homeowners who relocate to the city, has been used extensively to analyze the residential segregation of ethnic groups. The model is succinctly stated as described by Benenson et al. (2009), wherein the six behavior rules are listed, presuming that the model is an ensemble of agents of two types, B and W, scattered over a grid.



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

ABM have the ability to develop systemic models that span disciplines, according to Bithell et al. (2008, p. 625), so that comparable mathematical methods may be utilized to manage the spatial search procedure, handle irregular boundaries, and exhibit the shifting characteristics of systems where the "preservation of heterogeneity within space and time is essential." They point out that finding rulesets that most accurately reflect the values and aspirations of people acting as agents while still allowing for system exploration is a key problem for ABM. ABMs are particularly suitable, according to Clifford (2008, p. 675) when decisions or actions are dispersed among certain areas and when structure is thought to develop through interpersonal interaction. Regarding this novel and exploratory modeling paradigm, he urges a rediscovering and reconsideration of the richness and depth of knowledge in the model-building business more generally. Some have made an effort to connect ABM with other theoretical systems; for instance, Neutens et al. (2007) connected ABM with temporal and spatial geography. In order to simulate urban growth, Andersson et al. (2006) connected networks, agents, and cells. Additionally, according to O'Sullivan and Hakley (2000), the use of ABM supports a modeling bias to a self-centered view of the social world and overlooks many of the influences that impact actual financial and human systems from the top, such as management and governance. According to Read (2010, p. 329), agent-based models occasionally offer just a veneer of, rather than meaningful involvement with, social behavior.

# 3. Causal Loop Diagrams

System dynamics modelling was chosen as the most effective way for integrating complexity science into NEXOGENESIS. It is highly adaptable and can incorporate various forms of data and components in a single model, meeting the requirements for the sort of modelling required for the project. Additionally, the graphical environment makes it simple for the users to understand interdependences among components, which makes the validation process with experts and stakeholders easier. For the conceptualization of each Case Study's model, Causal loop diagrams (CLD) will be developed.

Causal loop diagrams (CLD) are a qualitative approach applied in the process towards developing quantitative system dynamic models. CLDs are very useful in helping non-expert stakeholders develop better understanding of the interconnections in complex systems, shedding light on critical feedback loops and connections that may otherwise not have been apparent, and thus starting to get a better appreciate of how the whole system behaves, and how it may response to imposed changes. They contribute to breaking traditional silo-thinking. CLDs are able to be applied as a stand-alone system and not necessarily need to be supported by computer simulation in developing subject and solving selected problems (Wolstenholme, 1999). Causal effects among variables in CLDs are connected by arrows with polarity either positive (+) or negative (-) to indicate their dependency (Sterman, 2000). Connectors function to deliver information from one variable (A) in the system to other (B). The arrows with a "+" sign show that change (increasing/decreasing) in A causes change (increasing/decreasing) in B in the same direction. Meanwhile, the arrows with"-" signs indicate an opposite direction from A to B (i.e. if A goes up, B goes down). System dynamics behaviour can also take the form of feedback loops, with self-reinforcing behaviour (positive feedback loop) and self-balancing behaviour (negative feedback loop) being the result. Normally, a positive feedback loop represents the (exponential) continuity of growth or slowdown, while a negative one consists of causal links that try to fill the gap between desired and current condition (Mirchi et al., 2012), often leading to oscillatory or "goal-seeking" behaviour. Another important notation in CLDs is



NEXOGENESIS STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

delay caused by differences in time scales of system responses or restrictions in given parts of a system (e.g. production capacity may lead to delays between orders and manufacture of a product). Table 1 summarizes visual representation of CLD's notation.

*Table 1.Elements in causal loop diagrams. Modified from (Mirchi et al. 2012)*

| Notation | Description | Example |
|---|---|---|
| A → B (+)<br>Connector | change in A, causes change in B in the same direction. If A increases/decreases, B also increases/decreases | Temperature → (+) Evaporation<br>Cultivated land → (+) Water demand |
| A → B (-)<br>Connector | change in A, causes change in B in the opposite direction. If A increases/decreases, B also increases/decreases | Infiltration → (-) Run-off<br>Groundwater table → (-) Pumping cost |
| R or (+) | Reinforcing or positive feedback loop, if it contains an even number of negative causal links | Birth Rate → (+) Population → (+) Birth Rate (R) |
| B or (-) | Balancing or negative feed back loop, if it contains an odd number of negative causal links | Population → (+) Death Rate → (-) Population (B) |
| ⫽ (+) or ⫽ (-) | Delay, the situation when the systems respond slowly in certain condition | Number of Plant Growing → ⫽ (+) Harvest Rate |

CLDs have been effectively used recently in the development of quantitative Water-Energy-Food (WEF) nexus models and also for non-expert communication of system complexity to improve understanding of system behaviour without the need to build a simulation model. Purwanto et al. (2019) develop a comprehensive CLD of the WEF nexus in Karawang Regency, Indonesia. This CLD was developed with local stakeholders from all relevant Ministries in the region in a group model building (Vennix, 1996) setting. Therefore, stakeholders were invested in the development process, and were in a better position to understand an interpret the final produced CLD. In the end, one CLD was produced for each of the water, energy, and food sectors, and these were finally combined to develop a CLD for the entire system (Figures 1 and 2).



NEXOGENESIS STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

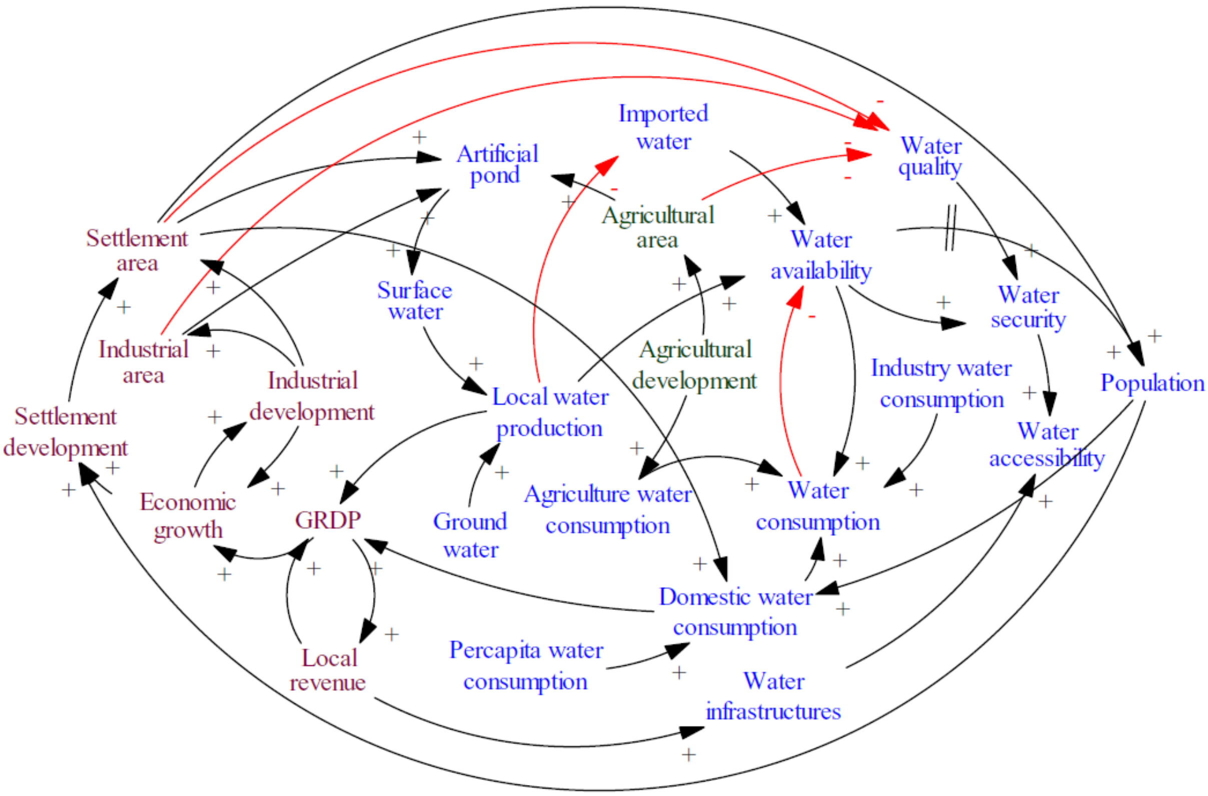



*Figure 1.The water-sector CLD from Purwanto et al. (2019).*

Ultimately, Purwanto et al. (2019) show the added value to local stakeholders of these CLDs without ever building a simulation model. The potentially wider-scale impacts of policy implementation can be 'tracked' through the system. As such these CLDs acted as an entry point for deep discussion about local policy development and the potentially wider effects of an individual policy on other unrelated nexus resource sectors.



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

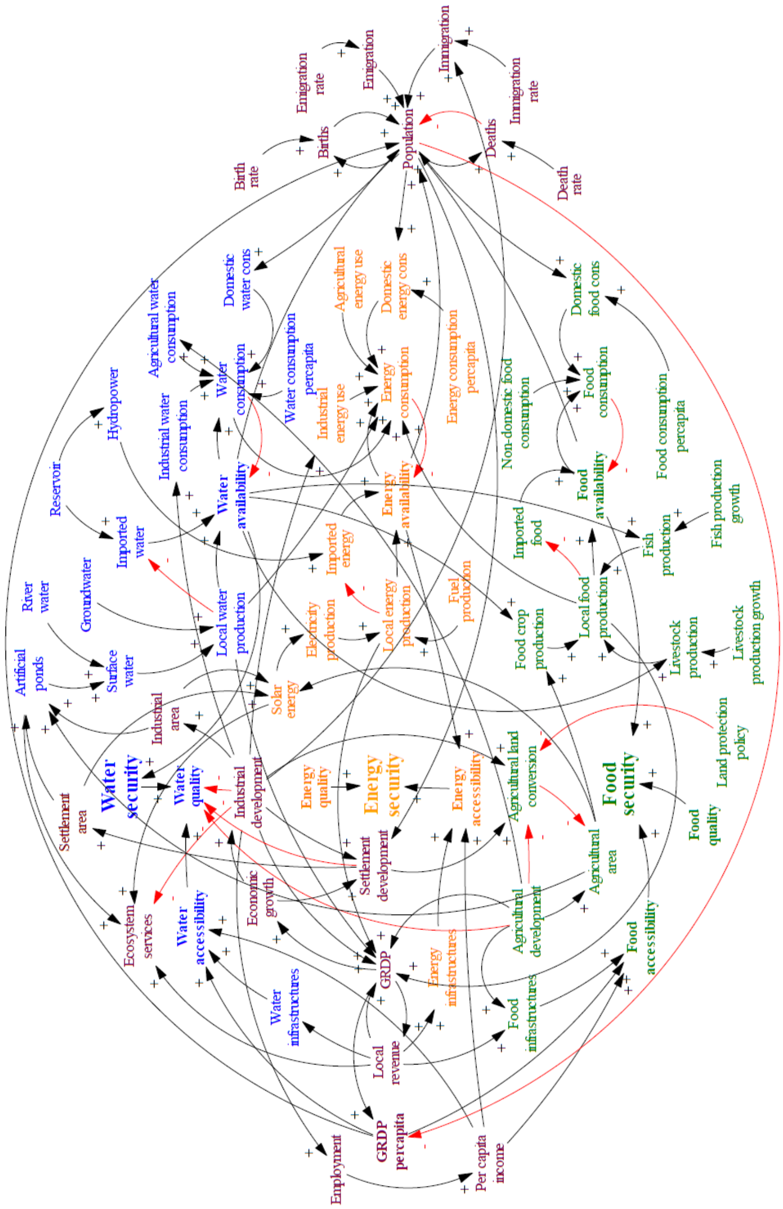


*Figure 2. The whole WEF nexus CLD from Purwanto et al. (2019).*

As a second example, more explicitly showing the connection between CLD and subsequent quantitative system dynamics model development, Sušnik et al. (2021) develop a quantitative system dynamics model exploring the WEF nexus in Latvia. As part of this process, a high-level, abstract CLD was also developed showing the main interconnections between WEF sectors (Figure 3).



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

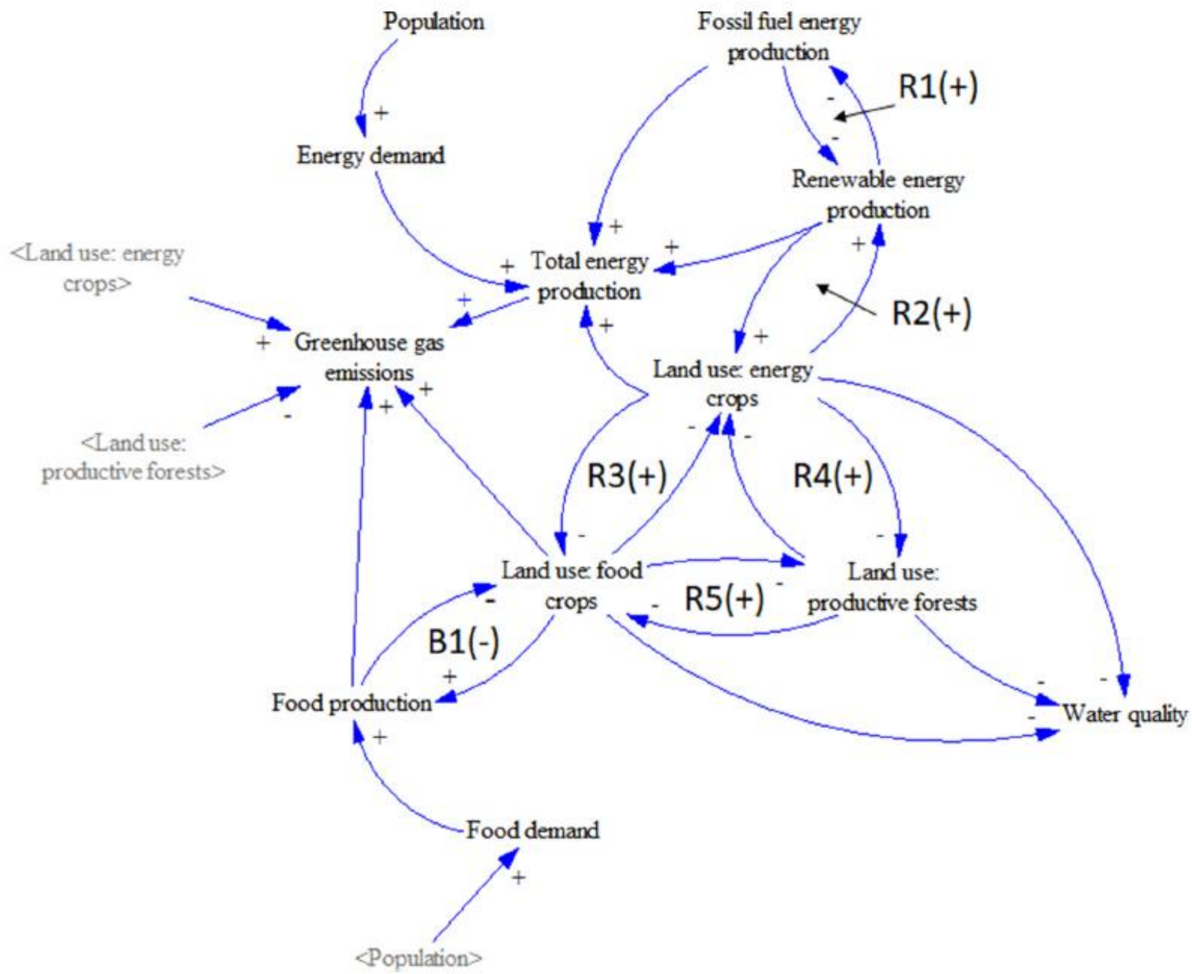



*Figure 3. The high-level CLD of Sušnik et al. (2021) showing the major connections and feedback loops in the water-energy-food nexus for Latvia.*

The Latvian CLD (Figure 3), was ultimately used to guide further development of a quantitative model to explore the impact of policy implementation on nexus sectors. As with Purwanto et al. (2019), it gave modellers and stakeholders a better understanding of critical system connections, and potential system behaviour.



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# 4. CLDs developed for the NEXOGENESIS case studies

This section presents the developed CLDs for each of the five NEXOGENESIS case studies. It is noted that an introduction to the cases is not given here, as these introductions are given in detail in Deliverable 3.1.

## 4.1 Case Study #1: Nestos/Mesta River Basin (Bulgaria – Greece)

The CLD of the Nestos River basin is illustrated in the following figure (Figure 4). The CLD is in essence a snapshot of all relationships that matter in the case study and portrays the processes through which the WEFE nexus aspect is represented.

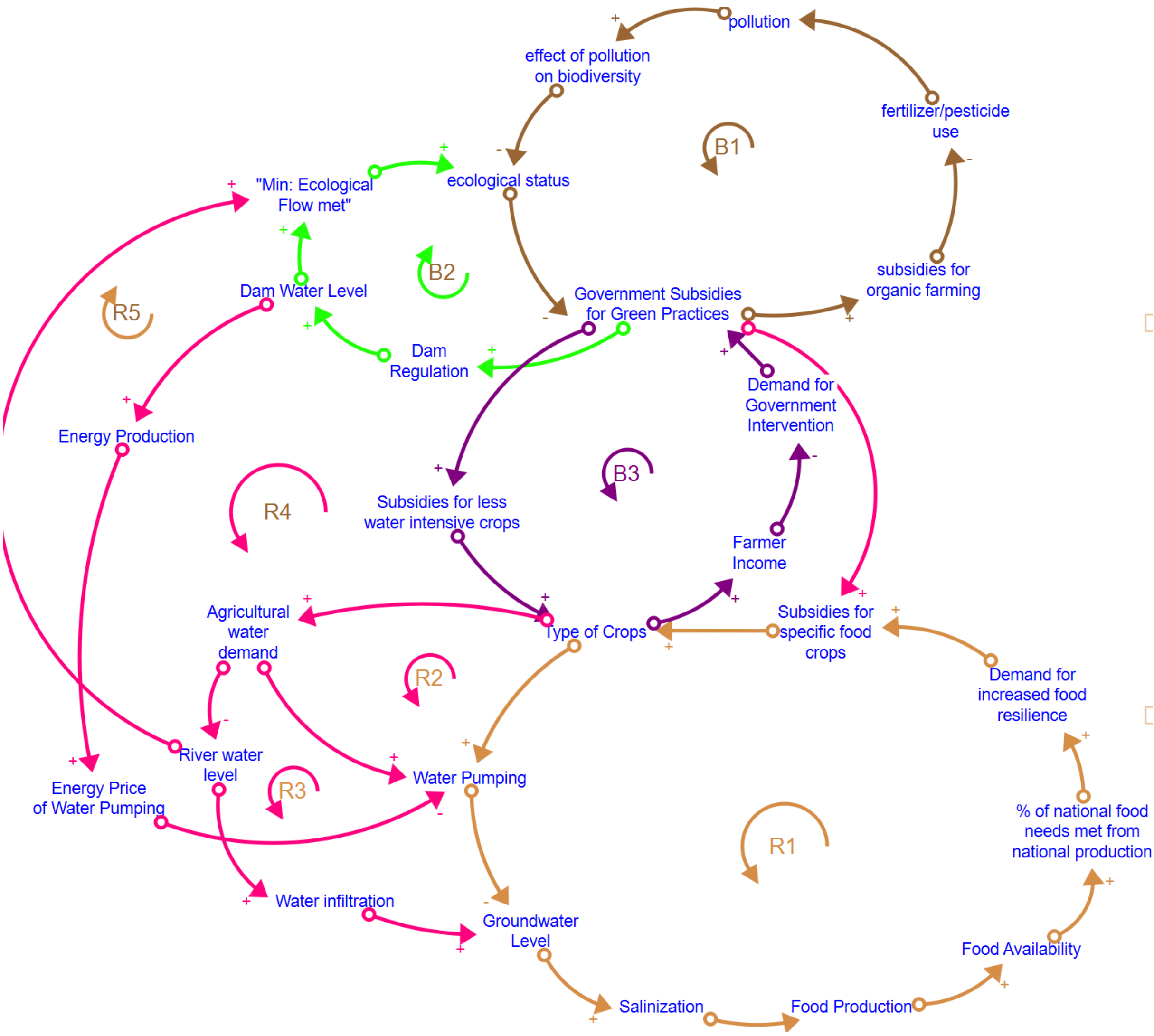



*Figure 4. Nestos/Mesta River Basin CLD.*



NEXOGENESIS STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

The main WEFE nexus concerns of this transboundary case study are attributed to the antagonistic character of the different types of water uses in the basin, including water for energy production through the operation of hydropower plants, water for irrigation, water for domestic/urban supply, water for food production, and lastly, water for the maintenance of the ecosystem. Since climate change is expected to magnify the tendency of water shortage in the years to come, mapping the causal relationships among evident and hidden variables/processes is of crucial importance towards understanding the system in a holistic manner.

One of the central challenges the basin faces is the safeguarding of water both from quantity and quality. Due to climate change which alters the hydrological and the climatic regime of the basin, preserving a minimum ecological flow in the river constitutes a challenge, since water demands to serve the aforementioned purposes are expected to increase. As for water quantity, the operating hydropower plant changes the flow regime of the river in order to produce energy and consequently it highly impacts the normal flow seasonality. In parallel, the adjacent agricultural activities consume significant water quantities, especially during summertime where the low precipitation and the high temperature regimes take place. As for water quality, the main challenges are found in agricultural nutrients and pesticides runoff, and the release of solid waste, plastics and sewage originating from the adjacent settlements.

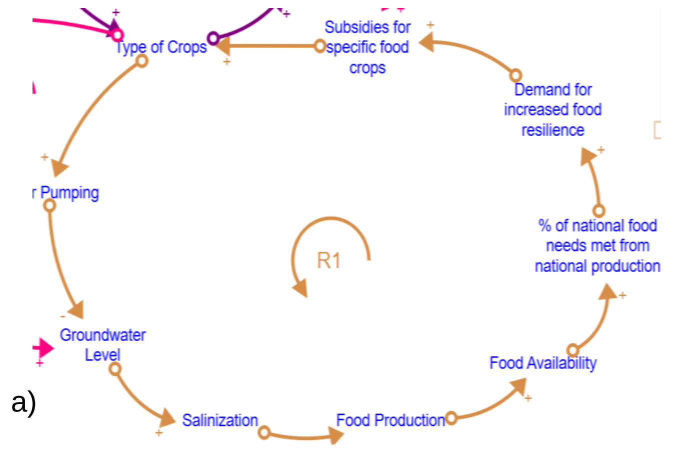
The CLD consists of five reinforcing and three balancing loops, which are presented in Table 2. The first three reinforcing loops deal with the agricultural sector which influences groundwater and river levels through water abstraction. The consequent depletion of groundwater tables leads to salinization effects which strongly affects crop yields and reduces food production and availability. Thus, increased food resilience is needed, and subsidies for specific food crops are expected for ensuring adequate food production and lower water demands for irrigation. The 4th reinforcing loop deals with the energy production from the hydropower plant which influences the energy price of water pumping and subsequently influences the crop types of the area. Thus, farmers' income will be influenced and the demand for governmental interventions will increase, leading to promoting green practices towards satisfying lower crop water demands and effectively regulating the dam. The 5th reinforcing loop deals with the Nestos River water level, which needs to meet a minimum ecological flow to ensure a good ecological status of the area. Thus, governmental subsidies for green practices and lesser water intensive crops are expected to take place, altering the types of crops and influencing the agricultural water demand. The 1st balancing loop deals with pollution and its effect on biodiversity and the ecological status of the area. This is expected to lead to subsidies for green practices and organic farming and subsequently to a reduction in fertilizers and pesticides use. The 2nd balancing loop copes with the ecological status which is strongly correlated to increased subsidies for green practices and consequently affects the dam water level regulation to meet the minimum ecological flow of the river. The 3rd and last balancing loop copes with the governmental subsidies for green practices and lesser water intensive crops which is expected to alter the type of crops cultivated in the area and farmers' income and; consequently the demand for governmental interventions will increase.

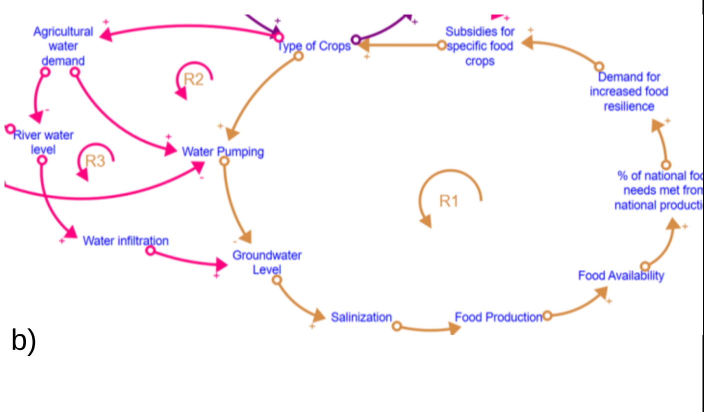
All loops are schematically depicted in the first column of Table 1, while the corresponding pathways are summarized in the second column.

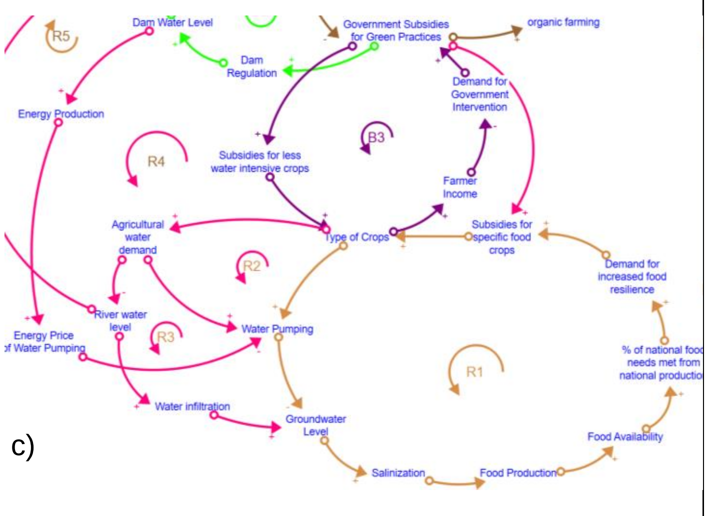


NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

*Table 2. The reinforcing and balancing loops of the Nestos/Mesta River basin CLD.*

<table>
<tr>
<td>

a)</td>
<td>R1: Water Pumping-> Grounwater level-> Salinization-> Food Prod-> Food Availability-> % of national food needs met from nat prod-> Demand for Increased Food Resilience-> Subsidies for specific food crops-> Type of crops</td>
</tr>
<tr>
<td>

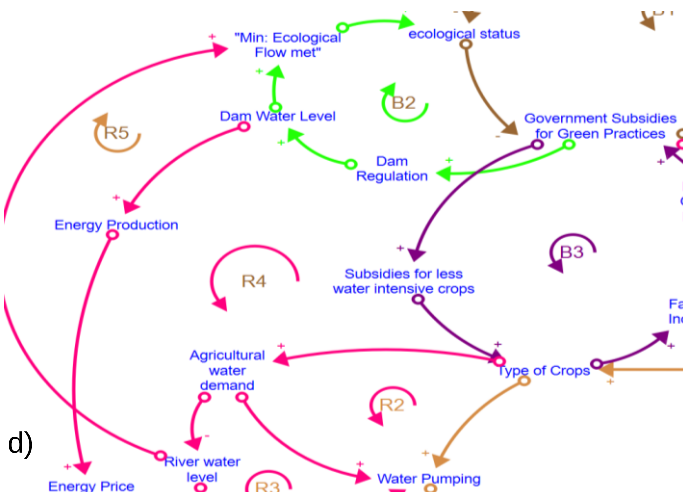
b)</td>
<td>R2: Agri WD-> Water Pumping-> Groundwater level-> Salinization-> Food Prod-> Food Availability-> % of national food needs met from nat prod-> Demand for Increased Food Resilience-> Subsidies for specific food crops-> Type of crops</td>
</tr>
<tr>
<td>

c)</td>
<td>R4: Energy Prod-> Energy Price-> Water Pumping-> Groundwater level-> Salinization-> Food Prod-> Food Availability-> % of national food needs met from nat prod-> Demand for Increased Food Resilience-> Subsidies for specific food crops-> Type of crops-> Farmer Income-> Demand for Gov Intervention-> Gov Sub for Green Practices-> Dam regulation-> Dam Water Level</td>
</tr>
</table>



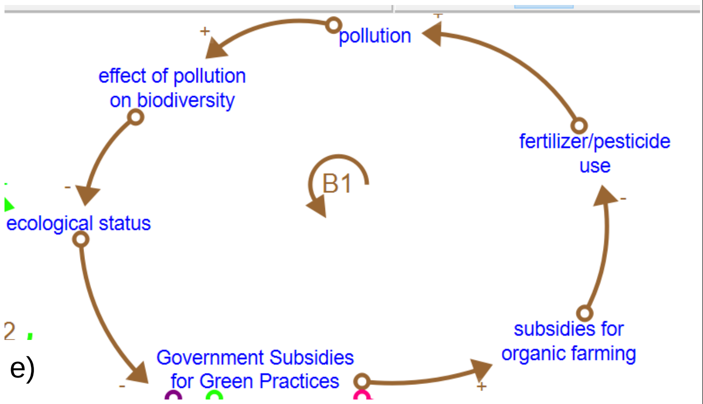
NEXOGENESIS STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881



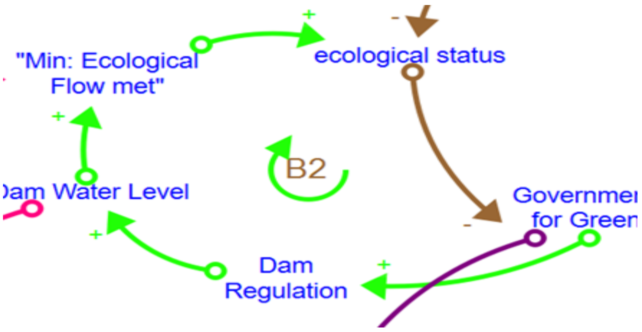

d)

R5: River Water Level-> Min Eco Flow Met-> Eco Status-> Gov Sub for Green Pract-> Sub for less Water intensive crops-> Type of Crops->Agri WD




e)

B1: Pollution-> Effect of pollution on biodiversity-> Ecological Status-> Gov Sub for Green Pract-> Subsidies for organic farming->fertilizer use



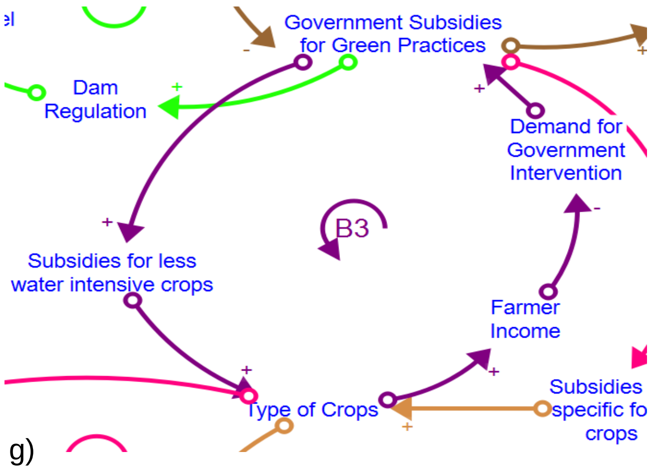

f)

B2: Ecological Status-> Gov Sub for Green Pract-> Dam Regulation-> Dam Water Level-> Min Ecol Flow met



NEXOGENESIS STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

| | |
|---|---|
| g)  | B3: Dov Sub for Green Pract-> Subsidies for less water intensive crops-> Type of Crops-> Farmer Income-> Demand for Gov Intervention |





NEXOGENESIS STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

## 4.2 Case Study #2: Lielupe River Basin (Lithuania – Latvia)

This section presents the causal loop diagram (CLD) for the water-energy-food-ecosystems (WEFE) nexus in the Lielupe River Basin (LRB). The CLD presented in Figure 5 maps the interlinkages (and polarities) of the nexus system in the basin. Beyond the WEFE systems, land and climate variables are also considered due to their relevance for the case study. Nexus sectors are identified in the diagram using a color code as described in Figure 5. The CLD shows the causal relations, and feedback loops, among the considered variables. Every causal relation has a polarity (see Section 2). Currently unknown (or not evident) relationships are marked with a question mark ("?") and orange color. These visual aids help to facilitate the inspection of the diagram.

Inspection of the CLD shows the highly intertwined nature of the nexus system in the LRB. There are no "isolated" sectors. On the contrary, activities in one sector depend and have impacts on one or more different sectors, either in a direct or indirect way. Particularly, interactions among the sectors of land, energy and food exhibit trade-offs and causal pathway of effects that may negatively impact the water and ecosystems sectors. Potential synergies in the sectors are visible in some sectoral outputs that may benefit other sectors. For example, organic fertilizers may be produced using inputs from different sectors and can be re-used for crop production (therefore reducing the need of importing synthetic fertilizers).

Despite most of the interactions being endogenous (i.e. they can be explained in relation with other variables in a common causal system), the diagram shows important exogenous drivers in the system. Examples of these are the exogenous commodities demands (e.g. for energy and food), climatic variables, or the fraction of crop production dedicated to agriculture or energy.

The CLD is a powerful system thinking tool to translate mental models of a complex system (i.e. the LRB nexus system) into a more tangible visual representation to be shared and discussed. However, complexity can escalate quickly by considering various sectors, variables and their interactions. This may make the CLD hard to read and interpret at a first glance. Yet the benefit of extensively mapping the set of relations in the system open the possibilities for exploring the likely existence of key feedback loops that previously were not evident, or even counterintuitive, for the system's stakeholders.

Further work in NEXOGENESIS may exploit potential qualitative insights derived from the CLD. Feedback loops can be characterized as reinforcing and balancing. Having this knowledge broadens the nexus system's understanding and allows to hypothesise potential policies that could take advantage of the identified feedback loops. This opens the possibility for communicating those feedback loops to other stakeholders to discuss their implications. Finally, a deep qualitative understanding of the CLD is a necessary bridge to develop further quantitative models (i.e. System Dynamics simulation) that aim to support the policy evaluation processes in the river basin.





This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

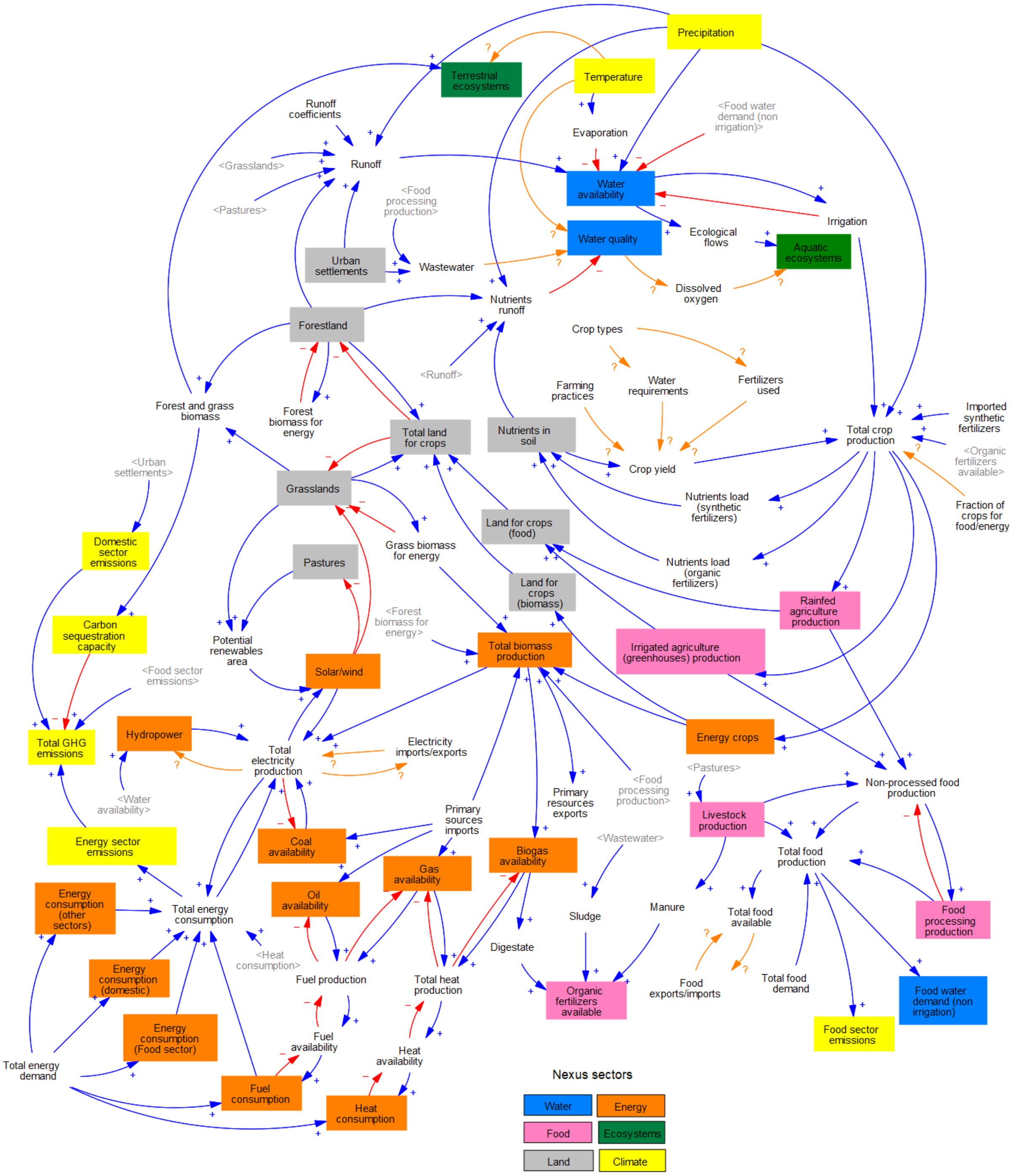



*Figure 5 .Developed CLD for the Lielupe River Basin.*



NEXOGENESIS STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

## 4.3 Case Study #3: Jiu River Basin, Lower Danube (Romania)

The Jiu River Basin CLD is shown in Figure 6. This preliminary CLD iteration will be further discussed and validated with the stakeholders. The impact of climate change on the Jiu river basin is becoming more evident and severe in the last decade. The increasing temperature and the changes in precipitation patterns are exacerbating the risk of floods and drought with an unavoidable impact on ecosystems and water quantity and quality, energy production (via hydropower) and consumption (e.g. for cooling), and agro-food resources (crop production, food demand changes).

One of the main challenges in the basin is ensuring water security that is closely related to the good status of water resources in terms of both quantity and quality. The basin's water availability is challenged by the changing climate (hydrological regime) and the increasing demand for water use in households, energy sector, irrigated agriculture, processing industry, as well as husbandry, aquaculture, and pisciculture. A good level of water in the rivers is essential for preserving the aquatic ecosystems as well as for maintaining water transport and (national) hydropower production, with a direct impact on the social and economic development of the local communities in the catchment.

The ecosystem, their services, and local biodiversity depend on the amount of water ensured to preserve the ecological functions (via the ecological flow) in the Jiu river basin and on the quality and timing of that water. Education (i.e. citizen awareness) and digital instruments (monitoring) are currently prioritized to increase and improve knowledge about the multiple uses of water resources and the importance of integrated resources management for the environmental and socio-economic system of the basin, helping to define the links between ecosystems and the other WEF sectors.

Agriculture is not only one of the main users of water resources but also a potential contributor to significant water pollution. The increasing crop production (both for food crops and energy crop production) is the main driver of chemical load into water bodies. In addition to nutrients and pesticides used for enhancing the yield (a positive benefit in terms of food security), livestock production, aquaculture and pisciculture are contributing to polluting water resources (although they also lead to food production benefits). Although agricultural activities currently require a significant amount of water, the main priority in the basin is to ensure water for domestic and industrial purposes. In order to achieve this goal, an extension of the water supply and sanitation network is currently in place. This network aims to increase water quantity and quality, thus increasing water availability and minimizing potential conflicts among sectors for its use. Recently, aquatic plants have been tested and introduced as nature-based solutions with the aim of cleaning polluted water without recourse to engineering solutions demanding more energy.

Food and energy demand are driving a rapid land use change leading to a potential conflict for land use for growing crops for both food and biomass production, as well as land for ecosystems. The expansion of arable land is currently leading to increased deforestation with an unavoidable impact on climate change, ecosystems, and biodiversity, forming a link between these sectors.



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

Hydro, biomass, and solar production are the main renewable sources for energy production. Coal completes the energy mix in the Jiu river basin. The sector is currently under transition towards clean energy and reduced impact on climate in terms of greenhouse gas emissions. Energy demand is driven by population and socio-economic drivers.

The energy in the basin holds a major importance in the national energy mix as well as for providing water services for population (water supply and water treatment), industry, agriculture, and transport in the region.



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

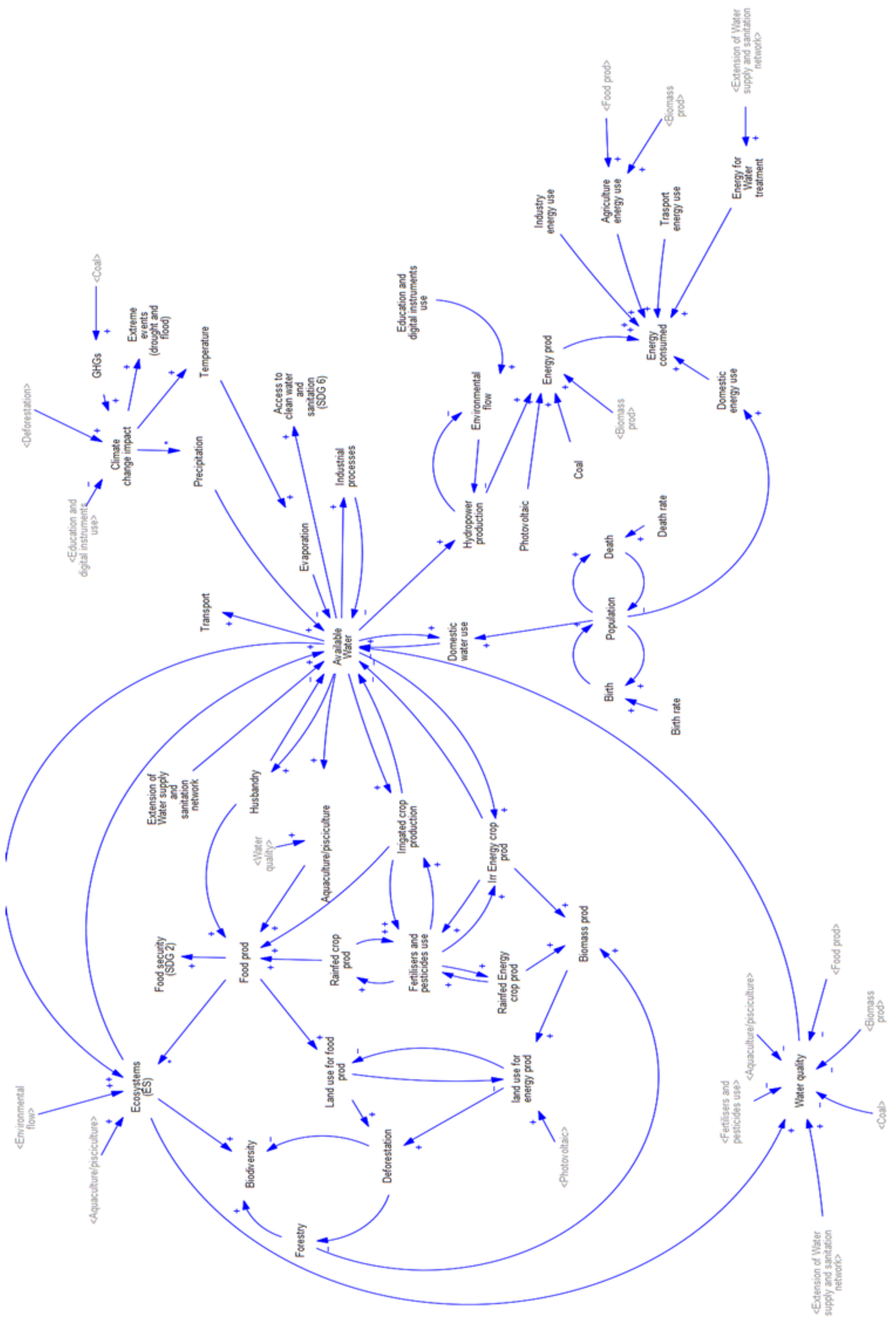



*Figure 6. Jiu River Basin CLD.*



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# 4.4 Case Study #4: Adige River Basin (Italy)

The CLD for the Adige case study is shown in Figure 7. Climate change has significantly impacted the Adige river basin in the last decade. The increasing temperature and the changes in frequency and intensity of precipitation threaten water availability with a cascade effect on other sectors such as food, energy, and ecosystems. The water supply instability might lead to increase conflicts among water use sectors, especially as demand is set to increase. Climate change, especially leading to increasing snowpack melting, is expected to directly impact the basin’s economy which is driven by the tourism sector strongly influenced by the recreational activities offered (skiing, hiking, kayaking).

Surface water, groundwater, and treated wastewater are the three main water sources. The available water in the Adige river basin is used mainly in industries, households, tourism, and especially in agriculture (irrigated crop and livestock production). In addition to supplying water to these economic sectors, it is essential to guarantee that environmental water needs are met by ensuring a minimum environmental flow. The amount of water allocated to the ecosystem is essential to preserve and increase its good and services, but is itself affected by the impacts of climate change and water demand in the other sectors.

The pressure on the water resource is not only in terms of quantity but also quality, especially due to the increasing agricultural activities driven by food demand, and temperature changes driven by climate change. Fertilisers and pesticides are used to achieve higher and more reliable crop yields. The runoff of these substances in addition to livestock farming effluents are the main causes of soil and water pollution. Ensuring good quality of water bodies is essential to preserving aquatic ecosystem functioning that, together with terrestrial ecosystem, is at the basis of supporting, regulation, and provisioning services.

The Adige river basin is characterised by heterogeneous landscapes and ecosystems. The role of the ecosystems is crucial in the basin to i) ensure climate and water regulation (regulating ecosystem services), ii) preserve biodiversity by ensuring the good status of water bodies (supporting ecosystem services), iii) provide water, energy, and food resources (provisioning ecosystem services); vi) support the tourism and preserve the natural parks in the basin (cultural ecosystem services). These functions are affected by impacts and activities all the other nexus sectors, leading to close nexus relationships.

Good water quality is fundamental for aquaculture and fishery that, with livestock, irrigated and rainfed crops production, characterise the main food supply sources as well as majority water users in the basin. The residues of crop production and manure are used to produce biogas, representing a link between food production and energy sources. Biogas and solar and wind power energy contribute to increasing the renewable energy sources in the basin’s energy mix. The energy produced is used in different sectors, such as industry, domestic, transport, water treatment, and agriculture (especially for irrigation).

Land use is expected to change due to the food and energy priorities outlined in the basin, as well as due to the influence of climate change (over a longer time period). In this regard, a potential trade-off between land use for food crop production and for energy production (e.g., installation of wind farms and solar plants) needs to be considered in the coming decades.



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 101003881

To mitigate greenhouse gas emissions from the different sectors, it is crucial to ensure the ecosystem regulating services whose functionality is directly impacted by the health of both terrestrial and aquatic ecosystems, as well as considering how to transition towards a more renewably-based energy mix in the basin.



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

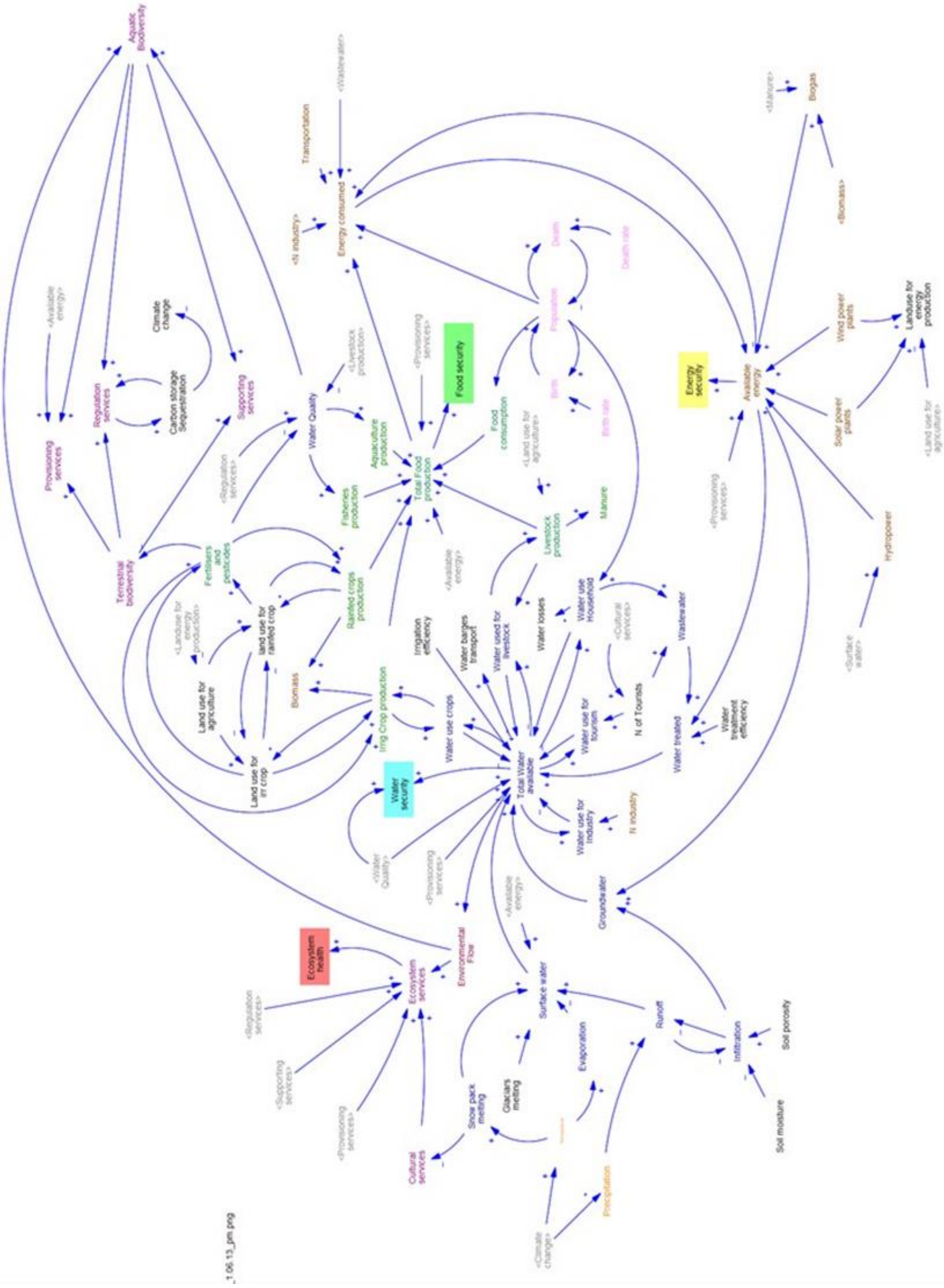


*Figure 7. CLD for the Adige case study.*



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

## 4.5 Case Study #5: Inkomati-Usuthu (South Africa)

The Inkomati-Usuthu CLD is shown in Figure 8. Starting from the left, climate change impacts on rainfall, temperature, and evaporation. On these links, no polarity is given as it is still unclear precisely how climate change will impact on these variables. Increases in rainfall would lead to increased water resources and vice-versa. Conversely, increasing temperatures and evaporation would lead to decreases in water availability. An increase in water available could potentially lead to an expansion in irrigated agriculture, so long as land availability allows.

Water demand increases with increases in the population and socio-economic drivers, energy consumption, energy generation, mining activities, land use, livestock production, irrigated agriculture, and ecosystem water requirements. An increase in demand would lead to a decrease in water resources availability. A change in water demand will impact on ecosystems by potentially impacting on water quality, quantity, and timing, but the nature of this connection is not yet known. Increasing water demand will lead to an increase in untreated wastewater, with impacts to water quality if not properly treated.

Energy consumption will increase with population and socio-economic drivers, water demand (forming a feedback loop between these two variables), food production (another feedback), and mining activities. Energy generated increases as diesel, coal, and renewable energy production is increased, and as mining activities increase in scale. Renewables, coal production, mining, livestock production, irrigated agriculture, and rainfed agriculture do impact land use, but the causal relationship is not clearly known.

Food production increases with livestock production, and more land is utilised for food production, with food demand (driven by socio-economic considerations), food imports, rainfed agriculture, and as more fertilisers are used and more land is given over to agricultural production. Food demand is controlled by population and socio-economic factors, and with food imports and exports.

Water quality will improve as ecosystems quality improves, but will deteriorate with increasing mining activities, increasing food production, increasing fertiliser use, and increasing volumes of untreated wastewater. There are therefore important policy considerations here. Finally, ecosystem health/quality will be impacted by water demand (forming another feedback loop) in an unknown manner, will improve with improving water quality, but will deteriorate with increasing food production, mining activities, and energy generation. Therefore, all nexus sectors are connected to and through ecosystems. Coal and diesel energy generation will exacerbate climate change impacts, as will food production, especially via the livestock sector which is responsible for considerable methane emissions to the atmosphere. These links to climate change thus close the WEFE nexus feedback cycle in the CLD.



NEXOGENESIS STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

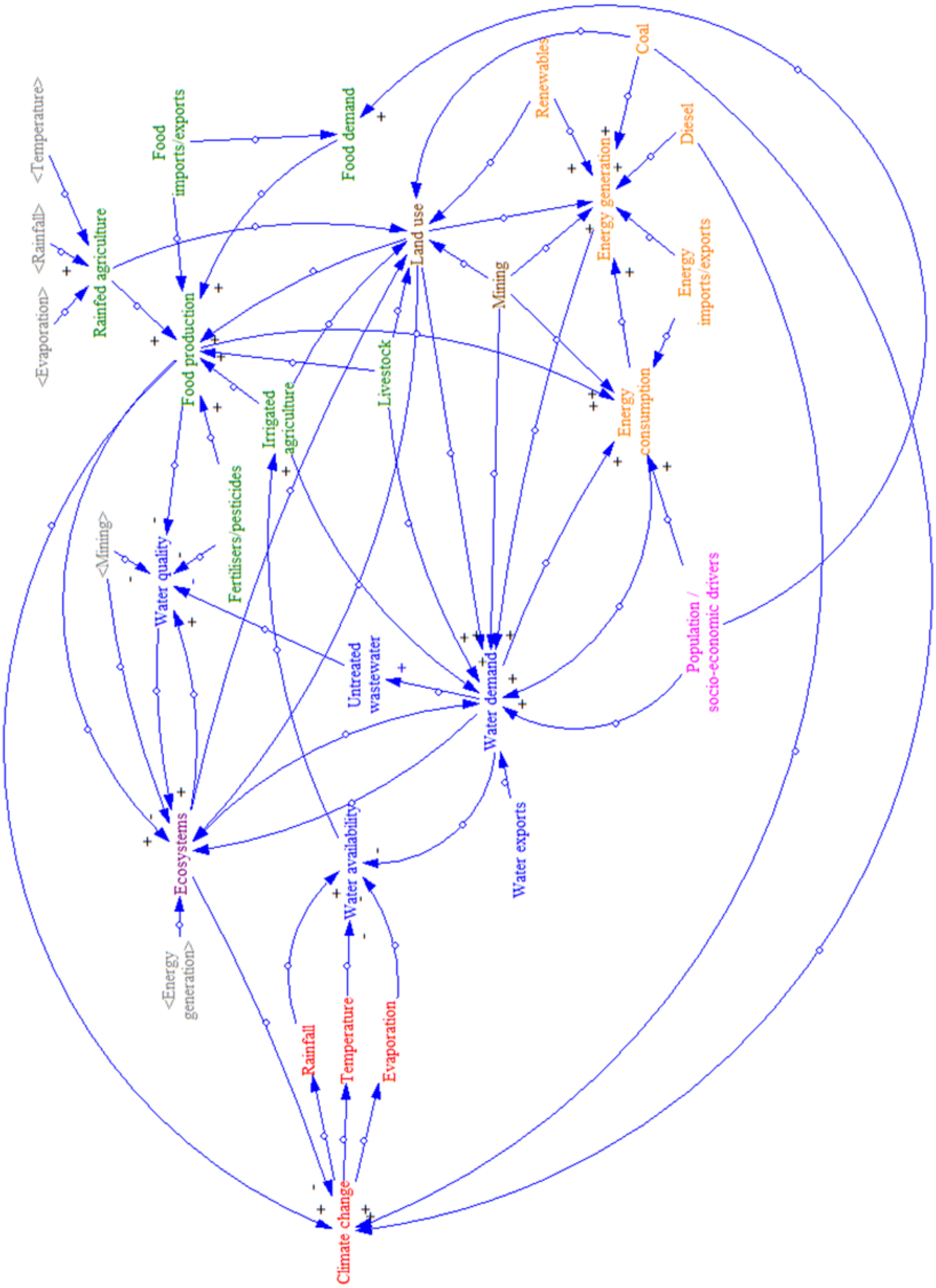



*Figure 8. The Inkomati-Usuthu CLD.*



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# 5. Contribution to the next steps in the NEXOGENESIS modelling chain

The CLDs in NEXOGENESIS form an early part of the whole modelling process, complementing the conceptual maps developed and presented in detail in Deliverable 3.1. As they are developed in close cooperation with local stakeholder groups (via the work of the Case Study leads and through the local stakeholder workshops), the intention is that the quantitative models and the results from the SLNAE will have more relevance for these stakeholder groups.

The next stage in the modelling process is to develop the quantitative system dynamics models (SDMs; Sterman, 2000; Ford, 2009). The case study SDMs will be developed to mimic, as closely as possible, the conceptual maps in order to account for all relevant nexus connections and integration of policies identified. This work will be carried out in close cooperation with WP2 to identify data availability reported in Deliverable 3.3 (Final report on the application of biophysical models and stakeholder recommendations) (M21). Connections and/or variables for which no data exist, or which cannot be quantitatively represented may be omitted or amended from the conceptual map representation. This will be done on a case-by-case basis. It will be crucial to integrate as many identified policies as possible to assess their nexus-wide impacts upon potential implementation. The policies have already been identified by the case study leads based on a thorough policy inventory and coherence analysis and are being validated with stakeholders via workshops. The integration of these policies in the SDSs will depend on data availability to be discussed with WP2. Adjustments will be made case by case and explained to stakeholders accordingly. The SDM prototypes will be reported in Deliverable D3.4 (Complexity science models implemented for all the Case Studies-Prototypes and explanatory report/manual for each CS) (M23). The SDMs form the basis for the development of the SLNAE to be implemented by WP4.

The CLDs are a key part of the whole NEXOGENESIS modelling process. It is important therefore that considerable effort was put into this stage in the project, and the wide stakeholder groups were involved in their development so as to capture pertinent issues, relevant policies to include, and to promote the eventual uptake of NEXOGENESIS policy recommendations emanating from the models. This Deliverable therefore serves to demonstrate the development of the CLDs, which will be taken forward through the rest of NEXOGENESIS, and aims to contribute to the successful implementation of the SLNAE and the development of sound policy advice in all Case Studies.



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

# 6. Conclusions

This Deliverable (D3.2) is the output of Task 3.1, which describes the methodology to be used in WP3. For all of the project's Case Studies, it presents the conceptual level of the Complexity Science integration models. STELLA (isee systems) environment has been successfully used to implement System Dynamics Modelling (SDM) in multiple occasions, and was therefore chosen for NEXOGENESIS's application of complexity science.

The conceptual models were co-created with the stakeholders at each Case Study workshop and delivered in D3.1 (Conceptual Models completed for all case studies, M16). CLDs where designed with respect to the conceptual maps delivered in MS11 (Complexity science tools progress report for all case studies), and have been presented in detail in this report for all the Case Studies.

The CLDs will feed the SDMs that will be delivered in D3.4 (Complexity science models implemented for all the Case Studies-Prototypes and explanatory report/manual for each CS, M23).

The sensitivity/uncertainty analysis is an ongoing process (M12 to M30) that is carried out on each of the implemented complexity science model developed to assess the WEFE nexus system behavior and response to likely changes (e.g. climate, socio-economic futures) as well as hypothetic changes (e.g. what-if scenarios, model stress tests). The sensitivity analysis procedure is related to the Tasks 3.4 (Sensitivity/Uncertainty analysis, Monte Carlo Stochastic analysis), and will be reported in D3.6 (Sensitivity/Uncertainty Analysis, M30).





This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 101003881

# 7. References


Acampora, G., & Loia, V. (2009, August). A dynamical cognitive multi-agent system for enhancing ambient intelligence scenarios. In 2009 IEEE International Conference on Fuzzy Systems (pp. 770-777). IEEE.

Allesch, A., & Brunner, P. H. (2015). Material flow analysis as a decision support tool for waste management: A literature review. Journal of Industrial Ecology, 19(5), 753-764.

Andersson, C., Frenken, K., & Hellervik, A. (2006). A complex network approach to urban growth. Environment and Planning A, 38(10), 1941-1964.

Andreou, A. S., Mateou, N. H., & Zombanakis, G. A. (2003). The Cyprus puzzle and the Greek-Turkish arms race: Forecasting developments using genetically evolved fuzzy cognitive maps. Defence and Peace Economics, 14(4), 293-310.

Azar, A. T. (2012). System dynamics as a useful technique for complex systems. International Journal of Industrial and Systems Engineering, 10(4), 377-410.

Batty, M. (2000). Geocomputation using cellular automata. In Geocomputation (pp. 95-126). New York: Taylor & Francis.

Bakhshianlamouki E., Masia S., Karimi P., van der Zaag P., Sušnik J. 2020. A system dynamics model to quantify the impacts of restoration measures on the water-energy-food nexus in the Urmia Lake Basin, Iran. Science of the Total Environment. 708: 134874. DOI: 10.1016/j.scitotenv.2019.134874

Barles, S. (2011, November). L'écologie territoriale: qu'est-ce que c'est. In Ecotech&tool Conference (Vol. 30).

Bayer, S. (2004). Sterman, John. 2000. Business dynamics: Systems thinking and modeling for a complex world. Interfaces, 34(4), 324-327.

Baynes, T. M., & Wiedmann, T. (2012). General approaches for assessing urban environmental sustainability. Current Opinion in Environmental Sustainability, 4(4), 458-464.

Benenson, I., Hatna, E., & Or, E. (2009). From Schelling to spatially explicit modeling of urban ethnic and economic residential dynamics. Sociological Methods & Research, 37(4), 463-497.

Bithell, M., Brasington, J., & Richards, K. (2008). Discrete-element, individual-based and agent-based models: Tools for interdisciplinary enquiry in geography?.Geoforum, 39(2), 625-642.

Buclet, N. (Ed.). (2019). Essai d'écologie territoriale: l'exemple d'Aussois en Savoie. CNRS Éditions via OpenEdition.

Chen, P. C., Su, H. J., & Ma, H. W. (2013). Trace anthropogenic arsenic in Taiwan—substance flow analysis as a tool for environmental risk management. Journal of Cleaner Production, 53, 13-21.

Clifford, N. J. (2008). Models in geography revisited. Geoforum, 39(2), 675-686.

Clarke, K. C. (2014). Cellular automata and agent-based models. Handbook of regional science, 1217-1233.




NEXOGENESIS STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

Clift, R., Druckman, A., Christie, I., Kennedy, C., & Keirstead, J. (2015). Urban metabolism: a review in the UK context. Foresight future of cities project.

Coyle, G. (2000). Qualitative and quantitative modelling in system dynamics: some research questions. System Dynamics Review: The Journal of the System Dynamics Society, 16(3), 225-244.

De Meester, S., Nachtergaele, P., Debaveye, S., Vos, P., & Dewulf, J. (2019). Using material flow analysis and life cycle assessment in decision support: A case study on WEEE valorization in Belgium. Resources, Conservation and Recycling, 142, 1-9.

Drew, D. R. (1995). System dynamics: Modeling and applications. ENGR 5104 Study Notes.

Eckelman, M. J., & Daigo, I. (2008). Markov chain modeling of the global technological lifetime of copper. Ecological Economics, 67(2), 265-273.

European Academies Science Advisory Council. Circular Economy: A Commentary from the Perspectives of the Natural and Social Sciences; European Academies Science Advisory Council: Halle (Saale), Germany, 2015.

Eurostat. (2001). Economy-wide material flow accounts and derived indicators: A methodological guide. Office for official publications of the European Communities.

Fischer-Kowalski, M. (2011). Methodology and Indicators of Economy-wide Material Flow Accounting/[Fischer-Kowalski M., Krausmann F., Giljum S., Lutter S. and others]. Journal of Industrial Ecology, 15, 855-876.

Ford A. 2009. Modeling the Environment (2nd Edition). 488pp. Island Press, Washington DC, USA. ISBN: 9781597264730.

Forrester, J. W. (1992). Policies, decisions and information sources for modeling. European Journal of Operational Research, 59(1), 42-63.

Froelich, W., & Wakulicz-Deja, A. (2009, May). Mining temporal medical data using adaptive fuzzy cognitive maps. In 2009 2nd Conference on Human System Interactions (pp. 16-23). IEEE.

Forrester, J. W. (1997). Industrial dynamics. Journal of the Operational Research Society, 48(10), 1037-1041.

Forrester, J. W. (2009). Some basic concepts in system dynamics. Sloan School of Management, 1-17.

Geng, Y., Fu, J., Sarkis, J., & Xue, B. (2012). Towards a national circular economy indicator system in China: an evaluation and critical analysis. Journal of cleaner production, 23(1), 216-224.

Georgopoulos, V. C., Malandraki, G. A., & Stylios, C. D. (2003). A fuzzy cognitive map approach to differential diagnosis of specific language impairment. Artificial intelligence in Medicine, 29(3), 261-278.

Ghisellini, P., Cialani, C., & Ulgiati, S. (2016). A review on circular economy: the expected transition to a balanced interplay of environmental and economic systems. Journal of Cleaner production, 114, 11-32.



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

Gimblett, H. R. (Ed.). (2002). Integrating geographic information systems and agent-based modeling techniques for simulating social and ecological processes. Oxford University Press.

Habib, K., Schibye, P. K., Vestbø, A. P., Dall, O., & Wenzel, H. (2014). Material flow analysis of NdFeB magnets for Denmark: a comprehensive waste flow sampling and analysis approach. Environmental science & technology, 48(20), 12229-12237.

Ioannou, A. E., & Laspidou, C. S. (2022). Resilience analysis framework for a water–energy–food nexus system under climate change. Frontiers in Environmental Science, 342.

Ioannou, A. E., & Laspidou, C. S. (2023). Cross-mapping important interactions between Water-Energy-Food nexusindices and the SDGs. Sustainability, 15 (accepted on publication).

Kalmykova, Y., Sadagopan, M., & Rosado, L. (2018). Circular economy–From review of theories and practices to development of implementation tools. Resources, conservation and recycling, 135, 190-201.

Kennedy, C., & Hoornweg, D. (2012). Mainstreaming urban metabolism. Journal of Industrial Ecology, 16(6), 780-782.

Kosko, B. (1992) Neural Networks and Fuzzy Systems: A Dynamical Systems Approach to Machine Intelligence. Prentice-Hall International, Upper Saddle River, 23-27.

Laspidou, C. S., Mellios, N., & Kofinas, D. (2019). Towards ranking the water–energy–food–land use–climate nexus interlinkages for building a nexus conceptual model with a heuristic algorithm. Water, 11(2), 306.

Laspidou, C. S., Mellios, N. K., Spyropoulou, A. E., Kofinas, D. T., & Papadopoulou, M. P. (2020). Systems thinking on the resource nexus: Modeling and visualisation tools to identify critical interlinkages for resilient and sustainable societies and institutions. Science of the Total Environment, 717, 137264.

Laspidou, C., & Ziliaskopoulos, K. (2022). Using System Dynamics Modelling to visualize the effects of resource management and policy interventions on biodiversity at a regional scale. Ecological Indicators, 145, 109630.

Lu, W., Yang, J., & Li, Y. (2010, August). Control method based on fuzzy cognitive map and its application on district heating network. In 2010 International Conference on Intelligent Control and Information Processing (pp. 295-299). IEEE.

Matthews, E., Amann, C., Bringezu, S., Fischer-Kowalski, M., Hüttler, W., Kleijn, R., ... & Weisz, H. (2000). The weight of nations. Material outflows from industrial economies World Resources Institute, Washington.

McDonnell, S., & Zellner, M. (2011). Exploring the effectiveness of bus rapid transit a prototype agent-based model of commuting behavior. Transport Policy, 18(6), 825-835

Miller, H. J. (2009). Geocomputation. The SAGE handbook of spatial analysis. Sage, London, 397-418.

Mirchi A., Madani K., Watkins D., Ahmad S. 2012. Synthesis of System Dynamics Tools for Holistic Conceptualization of Water Resources Problems. Water Resources Management. 26: 2421–2442. DOI: 10.1007/s11269-012-0024-2.



NEXOGENESIS
STREAMLINING WATER RELATED POLICIES
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

Neutens, T., Witlox, F., Van De Weghe, N., & De Maeyer, P. H. (2007). Space–time opportunities for multiple agents: a constraint-based approach. International Journal of Geographical Information Science, 21(10), 1061-107

Niazi, M., & Hussain, A. (2011). Agent-based computing from multi-agent systems to agent-based models: a visual survey. Scientometrics, 89(2), 479-499.

Odum, H. T., & Odum, E. C. (2000). Modeling for all scales: an introduction to system simulation. Elsevier.

O'Sullivan, D., & Haklay, M. (2000). Agent-based models and individualism: is the world agent-based?. Environment and Planning A, 32(8), 1409-1425.

Parker DC, Berger T, Manson SM (2002) Agent-based models of land-use and land-cover change.

LUCC Report Series No. 6, Indiana University

Papageorgiou, E. I. (2011, June). Review study on fuzzy cognitive maps and their applications during the last decade. In 2011 IEEE international conference on fuzzy systems (FUZZ-IEEE 2011) (pp. 828-835). IEEE.

Papageorgiou, E., Stylios, C., & Groumpos, P. (2008). The soft computing technique of fuzzy cognitive maps for decision making in radiotherapy. In Intelligent and adaptive systems in medicine (pp. 191-230). CRC Press.

Papageorgiou, E. I., Stylios, C., & Groumpos, P. P. (2006). Unsupervised learning techniques for fine-tuning fuzzy cognitive map causal links. International Journal of Human-Computer Studies, 64(8), 727-743.

Papakostas, G. A., Boutalis, Y. S., Koulouriotis, D. E., & Mertzios, B. G. (2008). Fuzzy cognitive maps for pattern recognition applications. International Journal of Pattern Recognition and Artificial Intelligence, 22(08), 1461-1486.

Pauliuk, S. (2018). Critical appraisal of the circular economy standard BS 8001: 2017 and a dashboard of quantitative system indicators for its implementation in organizations. Resources, Conservation and Recycling, 129, 81-92.

Purwanto A., Sušnik J., Suryadi F.X., de Fraiture C. 2019. The use of a group model building approach to develop causal loop diagrams of the WEF security nexus in a local context: A case study in Karawang Regency, Indonesia. Journal of Cleaner Production. 240: 118170. DOI: 10.1016/j.jclepro.2019.118170.

Purwanto A., Sušnik J., Suryadi F.X., de Fraiture C. 2021. Quantitative simulation of the water-energy-food (WEF) security nexus in a local planning context in Indonesia. Sustainable Production and Consumption. 25: 198-216. DOI: 10.1016/j.spc.2020.08.009

Ramos, E. P., Kofinas, D., Sundin, C., Brouwer, F., & Laspidou, C. (2022). Operationalizing the Nexus Approach: Insights From the SIM4NEXUS Project. Front. Water-energy-food-health solutions & innovations for low-carbon, climate-resilient drylands, 10, 101.

Read, D. (2010). Agent-based and multi-agent simulations: coming of age or in search of an identity?. Computational and Mathematical Organization Theory, 16, 329-347.

Richardson, G. P. (1996). Problems for the future of system dynamics. System Dynamics Review: The Journal of the System Dynamics Society, 12(2), 141-157.





This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881

Rodin, V., Querrec, G., Ballet, P., Bataille, F. R., Desmeulles, G., Abgrall, J. F., & Tisseau, J. (2009, June). Multi-agents system to model cell signalling by using fuzzy cognitive maps. Application to computer simulation of multiple myeloma. In 2009 Ninth IEEE International Conference on Bioinformatics and BioEngineering (pp. 236-241). IEEE.

Rodrigues, A., & Bowers, J. (1996). System dynamics in project management: a comparative analysis with traditional methods. System Dynamics Review: The Journal of the System Dynamics Society, 12(2), 121-139.

Schelling T (1971) Dynamic models of segregation. J Math Sociol 1(2):143–186

Schwaninger, M., & Ríos, J. P. (2008). System dynamics and cybernetics: a synergetic pair. System Dynamics Review: The Journal of the System Dynamics Society, 24(2), 145-174.

Spencer, G. M. (2012). Creative economies of scale: An agent-based model of creativity and agglomeration. Journal of Economic Geography, 12(1), 247-271.

Sterman JD. 2000. Business Dynamics: Systems Thinking and Modeling for a Complex.

Stylios, C. D., & Groumpos, P. P. (2004). Modeling complex systems using fuzzy cognitive maps. IEEE Transactions on Systems, Man, and Cybernetics-Part A: Systems and Humans, 34(1), 155-162.

Sultan, Fareena, John U. Farley, and Donald R. Lehmann. “A Meta-Analysis of Applications of Diffusion Models.” Journal of Marketing Research 27, no. 1 (1990): 70–77. https://doi.org/10.2307/3172552.

Sušnik J., Vamvakeridou-Lyroudia L.S., Savić D.A., Kapelan Z. 2012. Integrated System Dynamics Modelling for water scarcity assessment: Case study of the Kairouan region. Science of the Total Environment. 440: 290-306. DOI: 10.1016/j.scitotenv.2012.050.085.

Sušnik J., Vamvakeridou-Lyroudia L.S., Savić D.A., Kapelan Z., 2013. Integrated modelling of a coupled water-agricultural system using system dynamics. Journal of Water and Climate Change. 4(3): 209-231. DOI: 10.2166/wcc.2013.069

Sušnik J., Masia S., Indriksone D., Brēmere I., Vamvakeridou-Lyroudia L.S. 2021. System dynamics modelling to explore the impacts of policies on the water-energy-food-land-climate nexus in Latvia. Science of the Total Environment. 775: 145827. DOI: 10.1016/j.scitotenv.2021.145827.

Torrens, P. M. (2012). Moving agent pedestrians through space and time. Annals of the Association of American Geographers, 102(1), 35-66.

Vennix JAM. 1996. Group Model Building: Facilitating Team Learning Using System

Wang X., Dong Z., Sušnik J. 2023. System dynamics modelling to simulate regional water-energy-food nexus combined with the society-economy-environment system in Hunan Province, China. Science of the Total Environment. 863: 160993. DOI: 10.1016/j.scitotenv.2022.160993.

Wolfram, S. (1986). Theory and applications of cellular automata. World Scientific.

Wolfram, S. (2002). A new kind of science (Vol. 5, p. 130). Champaign: Wolfram media.

Wolstenholme EF. 1999. Qualitative vs quantitative modelling: the evolving balance. Journal of the Operational Research Society. 50: 422–428. DOI: 10.1057/palgrave.jors.2600700.





This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 101003881

World. 6th edn. Mc Graw Hill India, New Delhi.



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101003881