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D1.4: UNCERTAINTY ANALYSIS IN THE CONTEXT OF SIM4NEXUS

LEAD AUTHOR: Florian Knobloch (RU)

OTHER AUTHORS: Dimitris Kofinas, Nikolaos Mellios, Alexandra Ioannou, Alexandra Spyropoulou, Chrysi Laspidou, Maria Blanco, Pilar Martinez, Jean-Francois Mercure

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Executive summary

The primary objective of the Deliverable is to analyse the uncertainties of modelling tools within the SIM4NEXUS project, including behavioural uncertainty in decision-making. First, we classify different sources of uncertainties in different types of models. Next, we review available methodologies for their identification, analysis and communication in different contexts. Significant uncertainties come from using different models and their different assumptions, which will be analysed at the example of three models which are used within the SIM4NEXUS project. Within this context, we also analyse the relevance of behavioural uncertainties for the modelling of technological innovation, at the example of modelling the diffusion of energy end-use technologies in the residential sector.

Uncertainty can be defined as *"any deviation from the unachievable ideal of completely deterministic knowledge of the relevant system"* (Walker et al. 2003). While models can be an important tool for enhancing the understanding of the Nexus, uncertainties will remain. They are thus an essential component of any modelling activity, and should be analysed and communicated accordingly. For the analysis of uncertainties in models, three different dimensions can be distinguished: location of uncertainty, level of uncertainty, and nature of uncertainty. Possible locations of uncertainties in models are their context, structure, parameters, and outcomes. Levels of uncertainty range from the hypothetical ideal of complete deterministic knowledge on the one end, to total ignorance on the other end. The nature of uncertainty distinguishes if uncertainties result from imperfect knowledge of a system, or from variability within a well-understood system.

Different established methodologies exist for the identification, analysis, and communication of uncertainties in models. An uncertainty matrix can help to obtain an overview of uncertainties within a given model, by classifying uncertainties along their different dimensions. Pedigree analysis can help to evaluate the plausibility of modelling assumptions. Once critical assumptions and uncertainties are identified, they can be further analysed in a quantitative way, for example by means of a sensitivity or scenario analysis. Alternative model formulations allow to analyse structural model uncertainties which go beyond the variation of pre-defined model parameters.

Finally, identified uncertainties should be clearly communicated and set the research results into perspective, without undermining their relevance. Which insights from the modelling are robust despite the presence of the identified uncertainties, and which results should be interpreted with a degree of caution? The appropriate way of communicating uncertainties depends on the context and the target audience.

Changes with respect to the DoA

Not applicable.

Dissemination and uptake

This report will be released on the project website. The Deliverable has been written to support the development of the SIM4NEXUS project and is open to all stakeholders, including the case study leaders and researchers contributing to the case studies.

Short Summary of results

Uncertainty is relevant for any kind of modelling, and in particular in the context of modelling complex interacting systems, as they are analysed in the SIM4NEXUS project. A whole range of multi-faceted uncertainties exists in models, which can be classified according to their location within the model, the level of uncertainty, and its epistemological nature. Different established methodologies exist for the identification, analysis, and communication of uncertainties in models. Quantitative methodologies, such as sensitivity and scenario analysis, are a powerful tool for analysing the uncertainties which stem from model parameters and inputs, as well as their interactions with each other. Qualitative methodologies, such as uncertainty mapping and pedigree analysis, can be particularly useful for the analysis of structural uncertainties and modelling assumptions, which go beyond the variation of model parameters. A particular case of structural uncertainty is the uncertainty regarding the behaviour of people, for example when it comes to the choice of technologies. As the real-world effectiveness of any type of policy instrument finally depends on its impact on human decisions, behavioural uncertainty is of primary importance when it comes to the model simulation of policy effectiveness.

Evidence of accomplishment

Submission of report.

Glossary / Acronyms

A priori chosen parameters	Parameters that are chosen to be fixed although they aren't, but may be too difficult to identify by calibration. Their values are thus subject to uncertainty.
Behavioural uncertainty	The uncertain behaviour by heterogeneous agents who need to make decisions under uncertainty, impacting inter alia the impact of policies.
Behavioural variability	Differences in behaviour between different people or groups of people, or changing behaviour over time, ascribed to natural variations, such as decision thresholds, preferences.
Calibrated parameters	Parameters that are unknown from previous investigations or cannot be transferred from earlier studies, because the context is too different. They are determined by calibration, i.e. By comparing model outcomes with historical data. Typically, parameters are chosen so that they minimise the difference between observed outcomes and model outcomes.
Context uncertainty	Uncertainty which arises from ambiguity in the definition of boundaries of the system to be modelled.
Determinism	(Hypothetical) absence of any uncertainty.
Ensemble simulations	Type of global sensitivity analysis in which an ensemble of models is used instead of one single model. Each member of the model ensemble is based on the same model structure, but uses a different set of input parameters.
Epistemic uncertainty	Uncertainties which result from limited or inaccurate understanding of the system to be modelled. Examples are limited data, measurement errors, uncertain relationships between variables, or a limited knowledge of the system's general structure.
Exact parameters	Universal constants, such as mathematical constants.
External driving forces	Determine the changes within a system, and are not modelled endogenously. Both their correct specification and magnitude can be uncertain.
Fixed parameters	Parameters that can be considered exact due to detailed previous investigations, such as gravity at a given location.
Global sensitivity analysis	Type of sensitivity analysis in which all parameters are varied simultaneously, thereby also considering possible interactions and joint influences of different parameters (also referred to as 'aat analysis', for all parameters at a time).
Indeterminacy	Case of recognised ignorance in which uncertainty cannot be reduced by means of additional scientific investigation.
Inherent randomness of nature	Chaotic or unpredictable processes in natural systems, such as the exact movement of particles, or the eruption of volcanoes, processes that result from uncharacterised complex systems.
Irreducible ignorance	Case of recognised ignorance in which uncertainty cannot be reduced by means of additional scientific investigation.
Level of uncertainty	Dimension for the classification of uncertainties in modelling: how can the uncertainty be classified on a spectrum from completely deterministic knowledge to total ignorance?
Local sensitivity analysis,	Type of sensitivity analysis in which changes in the model output are analysed against variations of specific model parameters or input variables around their pre-specified default or reference values, one parameter at a time.

Location of uncertainty	Dimension for the classification of uncertainties in modelling: where in the model does uncertainty manifest itself?
Model outcome uncertainty	The overall uncertainty of the model outcomes of interest.
Model structure uncertainty	Uncertainty that can result from incomplete understanding of the represented real-world system: the behaviour within a system, its relevant elements, and how they relate to each other.
Model technical uncertainty	Uncertainty which originates from errors in the hardware or software being used, from errors in implementing the algorithms, or simply from typing errors when writing the source code.
Monte Carlo analysis	A very common type of global sensitivity analysis , which represents the uncertainty around each model parameter by means of a probability distribution.
Multiple model ensemble	Form of ensemble modelling in which different models are combined into one ensemble.
Multiple model routes	Technique for addressing structural uncertainties by means of developing different alternative versions of the same initial model.
Multiple-starts perturbation methods	Type of sensitivity analysis which is methodologically similar to local sensitivity analysis, extended into the direction of global sensitivity analysis.
Nature of uncertainty	Dimension for the classification of uncertainties in modelling: what is the fundamental epistemological reason behind the uncertainty?
Normal science	Scientific paradigm which focuses on iterative experimentation, which allows to resolve testable hypothesis.
Parametric uncertainty	Uncertainty which arises from the input data and parameter calibration.
Pedigree analysis	Methodology for the (qualitative) analysis of uncertainty. It aims at systematically analysing the strengths and weaknesses behind model assumptions, by critically examining their quality and production process.
Positivism	Main epistemological position in natural science and modelling. In the tradition of Descartes, it is based on the premise that it is possible to systematically inquire reality, for example by means of mathematical and quantitative methods.
Post-modernism	Epistemological position which stresses the inherent subjectivisms of scientific enquiry. In this perspective, although science can lead to knowledge, this knowledge is never certain.
Post-normal science	Science that deals with systems that characterised by both quantifiable and unquantifiable uncertainties, and the process of reducing these uncertainties cannot be separated from attempting to solve the policy-question.
RBD	River basin district
Recognised ignorance	Situation in which the analyst has neither a sufficient understanding of the underlying mechanisms, nor of their statistical properties. Importantly, however, the analyst is aware of his own limited knowledge-base.
Reducible ignorance	Case of recognised ignorance in which uncertainty can be reduced by means of additional scientific investigation.
Risk	Situation in which we don’t yet know the future outcome of a system, but do know the probability distribution of all possible future outcomes. This requires perfect knowledge of the system, so that a known probability can be assigned to every possible realisation.

Scenario	Any plausible description of how the system and or its driving forces may develop in the future. This includes both plausible and highly implausible scenarios.
Scenario analysis	Widely used methodology for analysing uncertainty which goes beyond statistical uncertainty: the scenario uncertainty which is located in a system's input parameters or external driving forces, foremost its present or future external environment.
Scenario uncertainty	Situations in which a parameter or structural mechanism cannot adequately be described in terms of statistical terminology. Typically, such uncertainties concern future developments, but can also refer to relevant uncertain knowledge of the past or present.
SDM	System Dynamics Model
Sensitivity analysis	Methodology for the (quantitative) analysis of uncertainty. It aims at characterizing how model results respond to changes in different model inputs and parameters. It is therefore suitable for analysing statistical uncertainty, both at the location of model input and parameters.
Single model ensemble	Form of ensemble modelling in which the same single model is run multiple times, each time with different sets of parameters or structural specifications.
Societal variability	Chaotic or unpredictable processes in complex economic, social or cultural systems, such as wars, political decisions, financial crashes.
Statistical uncertainty	Any uncertainty which can be described statistically, i.e. For which it is possible to quantify a statistical distribution.
Structural uncertainty	Uncertainty which arises from the chosen structure and implementation of the model.
System data	Describes the characteristics of a modelled system as such. For models of natural systems, this may be the description of a terrain, map, geophysical properties, or the stock of chemicals in different locations.
System models	Any kind of abstraction of the system of interest, based on simplified representations of its cause-effect relationships.
Technological surprise	Unexpected scientific discoveries, technological developments or new consequences of existing technologies, such as new information technology revolutionising management practices, artificial intelligence.
Total ignorance	Uncertainties which are relevant for the model outcome, but whose very existence remains unknown to the analyst.
Uncertainty	Any deviation from the unachievable ideal of completely deterministic knowledge of the relevant system, on a spectrum from 'know' to 'not know that we do not know'
Uncertainty matrix	Methodology for the (qualitative) analysis of uncertainty, which maps the characteristics of identified uncertainties according to different classifications.
Unknown unknowns	Uncertainties which are relevant for the model outcome, but whose very existence remains unknown to the analyst.
Variability uncertainty	Uncertainty that would remain even if the analyst had a perfect understanding of the system. It does not result from limited knowledge, but from the fact that parts of the system are inherently variable: they differ over space or time.
Wicked problems	Situations in which high-stake decisions must be informed in the context of fundamental uncertainty, so that the process of solving the policy question becomes identical with the process of understanding its underlying drivers.

1 Introduction

The world is inherently uncertain - in particular so when we deal with the future, complex systems, or a combination of both. We don't know for certain what will happen in a century, in a decade, or even in a day from now. Often, we do not fully understand the underlying mechanisms, dynamics and feedbacks. In many cases, we are not even aware of what is uncertain, as it is still beyond our imagination, which is constrained by the perspective of our current knowledge base. It is a long-debated question in the philosophy of science if certainty of knowledge is even possible, and if so, to which extent and under which circumstances.

Despite its importance for all realms of life and science, there is no universally shared definition of uncertainty. Different terminologies are used for the same type of uncertainty in different scientific fields or even by different scientists within a field. At the same time, seemingly common terms might refer to different types of uncertainty. We here adopt the terminology suggested by Walker et al. (2003), who define uncertainty as *"any deviation from the unachievable ideal of completely deterministic knowledge of the relevant system"* (p. 5). This definition applies to a wide spectrum of uncertainties, ranging from 'know' to 'not know' and 'not know that we do not know'. It covers uncertainty due to a lack of information, as well as to uncertainty due to variability which is inherent to a system, and may thus persist even when plenty of information is available.

When completely deterministic knowledge is an unachievable ideal, the achievement of certainty becomes impossible. Additional research and analysis may improve our level of understanding of a given system, but can never lead to complete knowledge. Sometimes, research might even discover new, previously unknown or overseen aspects of the system, thereby increasing the known uncertainty instead of reducing it.

As there is no escape from uncertainty, decisions need to be taken in a context of incomplete knowledge. Be it a high school graduate who is contemplating what kind of career to pursue, or a politician who needs to choose between different policy proposals: Eventually, some kind of decision needs to be taken. While it is sometimes possible to wait or look for *additional* information which reduces *some* uncertainty, it is never possible to wait for *complete* information which eliminates *all* uncertainty. Rittel & Weber (1973) classify such decision situations as 'wicked problems': Due to inherent incomplete information and limited understanding of all relevant properties of the system, the process of solving the policy question becomes identical with the process of understanding its underlying drivers. As a result, all decisions are sub-optimal by definition. Knowledge and understanding continues to improve incrementally after decision were taken, after which decisions may need to be adjusted, which will lead to additional knowledge and understanding, and so forth.

In the scientific literature, situations in which high-stake decisions on 'wicked problems' must be informed in the context of fundamental uncertainty (such as long-term climate policy) are also classified as 'post-normal science'. The term is not meant to downplay the role of science in any way, and must not be mixed up by present-day discourses on 'post-truth' and 'alternative facts'. Instead, 'post-normal science' must be seen in relation to 'normal science' as defined by Kuhn, where iterative experimentation allows to resolve testable hypothesis. In 'post-normal science', experimentation as such is not possible. The system is characterised by both quantifiable and unquantifiable uncertainties, and the process of reducing these uncertainties cannot be separated from attempting to solve the policy-question. For example, the true impact of any policy decision can only be known after its implementation. While such a policy implementation may be seen as a large-scale experiment, it is never reproducible, as the context is constantly evolving. This means that the full attribution of cause-effect relationships remains uncertain.

As uncertainty is inherent to all aspects of the world, it also applies to all types of system models, which can be defined as ‘any kind of abstraction of the system of interest’ (Walker et al. 2003). As models are simplified representations of cause-effect relationships in real-world systems (either of existing or of hypothetical future systems), the modeller also needs to consider all of the underlying uncertainties. Although models themselves are typically deterministic (always yielding the same outcome for the same set of input parameters), the represented system is not. While the model can be an important tool for enhancing the understanding of a system, uncertainties will remain. They are thus an essential component of any modelling activity, and should be analysed and communicated accordingly.

Throughout this report, we will thus review and summarise possible methods for the analysis of uncertainties in complex[1] models, as they are used in Sim4Nexus. A particular focus lies on analysing the uncertain impacts of policy instruments and the underlying facets of *behavioural uncertainty,* which is of central importance for policy-making and any attempts of modelling policy impacts. We use the term to refer to the uncertain behaviour of people who need to make decisions under uncertainty. When modelling behaviour, uncertainty is thus present on two levels: On the system level (agents making decisions), and on the model level (conceptualising an abstract representation of such decisions). On the systems level, agents face uncertainty in their decision-making, which impacts the way in which they decide between alternative choices (e.g. technologies, courses of actions). On the model level, the analyst needs to formalize a structural representation of such decision-making, for example in order to estimate policy impacts. In the absence of perfectly deterministic descriptions, such modelling representations remain uncertain themselves (in their structural form and/or parameterisation). Importantly, behavioural uncertainty determines the potential impact of any kind of policy instruments, even of those that are primarily concerned with natural or technological systems: No such system can ever react to policies, which always need to be targeted at human behaviour.

1.1 Structure of the document

The report is structured as follows. Section 2 classifies the relevant types of uncertainty in a context of modelling. Section 3 reviews different methodologies for the analysis and communication of uncertainty, and suggests a pragmatic approach which is applicable to different classes of models. Section 4 applies this approach by mapping and identifying different types of uncertainty that are relevant for policy impacts in three different models which are used in SIM4NEXUS. Section 5 concludes.

[1] ‘Complex’ in the sense that the models deal with dynamic systems (such as agriculture or the economy), which are represented within the respective models by means of a large number of interacting variables.

2 What is uncertainty?

In this section, we first clarify the meaning of uncertainty from a philosophy of science perspective. We then analyse how uncertainty manifests itself from two different positions, both of which are relevant for modelling: the perspective of people who are acting within the real-world system to be modelled, and the modeller's or scientist's perspective on the system.

2.1 Uncertainty in the philosophy of science

The nature of uncertainty is deeply rooted within philosophy, and has been discussed intensively throughout the centuries: what can we know about the world in its current and future states, and what are the role and limits of science? The origin, nature, methods, and limits of human knowledge are at the heart of a whole branch of philosophy, referred to as epistemology.

The main epistemological position in natural science and modelling is *positivism* in the tradition of Descartes. It is based on the premise that it is possible to systematically inquire reality, for example by means of mathematical and quantitative methods. From this perspective, science is seen as *'the search for and prediction of empirical regularities to make universal, true statements that can be falsified in the Popperian sense'* (Van Asselt and Rotmans 2002). Accordingly, uncertainty is seen as the absence of knowledge, which can be reduced by means of further scientific enquiry. However, as argued by philosophers such as Hume and Hegel, the obtained knowledge can never be perfect and complete. There will always remain a gap between reality and observation, and this gap cannot be fully bridged by reason. In the words of Werner Heisenberg (1958): *"What we observe is not nature itself, but nature exposed to our method of questioning."*

This line of arguments leads to two rather opposite epistemological perspectives, namely *post-modernism* and *social-constructivism*. Both stress the inherent subjectivisms of scientific enquiry. From both perspectives, science is seen as *'a creative process in which social and individual values interfere with observation, analysis and interpretation'* (Van Asselt and Rotmans 2002). Taken to its extremes, scientific knowledge is seen as nothing but social 'conventions'. Therefore, although science can lead to knowledge, this knowledge is never certain. This perspective is more dominant in the social sciences. Multiple theories aiming at explaining the same phenomena can co-exist, without any one theory having a higher claim for truth. Uncertainty is not just the absence of knowledge, but can still exist in the presence of extensive information. If new enquiry reveals that something is more complex than previously known, additional information may even increase the overall level of uncertainty. In the words of Shackle (1955): *"There would be no uncertainty if a question could be answered by seeking additional knowledge. The fundamental imperfection of knowledge is the essence of uncertainty."*

While both epistemological positions seem to stand at the extreme opposite ends with regard to the nature and limits of scientific reasoning, the positivist approach to uncertainty in the tradition of Hume and Hegel is not fundamentally different from a more moderate constructivist position. Both acknowledge that scientific knowledge cannot be seen independently from the chosen means of enquiry, and stress that some forms of uncertainty will inevitably remain. Therefore, throughout the analysis in this report, we take an epistemological middle-ground: quantitative enquiry and reasoning with models can generate knowledge. However, within the context of complex systems and wicked problems, uncertainty cannot be fully eliminated, and will always play a key role.

2.2 Risk versus uncertainty

Importantly, following the early distinctions by Knight (1921) and Keynes (1921), uncertainty is fundamentally different from pure risk.

Risk can be defined as a situation in which we don't yet know the future outcome of a system, but do know the probability distribution of all possible future outcomes. This requires perfect knowledge of the system, so that a known probability can be assigned to every possible realisation. As this is rarely the case, risk is mostly confined to a few well-defined situations, often being artificially created. Examples are throwing a dice or playing the lottery. Although it remains unknown which number will be on top of the dice or which combination of numbers will be drawn in the lottery, the underlying probabilities are well-defined. For example, for a non-manipulated standard dice, the probability that any individual number will be on top equals 1/6. When betting on a dice, the outcome is risky, but not uncertain.

In contrast, *uncertainty* is a situation in which we neither know the future outcome of a system, nor the underlying probability distribution. We don't have perfect knowledge of the system, and hence cannot assign *objective* probabilities to all possible outcomes. In fact, we may not even be aware of all possible outcomes. The best we can do is to assign *subjective* probabilities to all considered outcomes, based on what we see as a reasonable estimate in the context of incomplete knowledge. A prominent example of uncertain outcomes are the future damages from climate change: it remains uncertain in which exact ways the climate system will dynamically react to changing greenhouse gas emissions, and how the resulting changes in the climate will dynamically interact with other natural systems, such as the Atlantic Meridional Overturning Circulation (Holden et al. 2018).

In the context of *fundamental* or *deep uncertainty*, not even all relevant outcomes are known. As it is impossible to assign probabilities to outcomes which are not even considered yet (not even subjective probabilities), in such context it is also effectively not possible to apply frequentist statistical methods which rely on well-defined probabilities of all outcomes, such as the calculation (or maximisation) of an expected value. As neither objective nor subjective probabilities can be assigned to unknown events and outcomes, fundamental uncertainty also precludes the meaningful application of Bayesian statistical approaches (which are foremost based on conditional probabilities, given subjective degrees of belief).

2.3 Uncertainty as part of decision-making

In the context of modelling socio-economic systems, agents are people who act within the system of interest - either as individuals (e.g., as consumers), or within organisations (e.g., firms or political institutions). As the world is uncertain, agents are constantly required to make decisions under uncertainty. What will the world look like in the future? What will be the impact of alternative courses of action?

It is a common finding that empirically observed decisions are often inconsistent with basic economic concepts of rationality, profit or utility maximisation (Tversky and Kahneman 1992; Kahneman 2003) as defined in standard expected utility theory. For example, decisions by individuals and firms are found empirically to be much more sensitive to upfront costs (monetary or otherwise) than to future benefits, which may be related to subjective degrees of time preferences (preferring present over future consumption), loss aversion (relatively higher impact of subjectively perceived losses on decisions), or risk aversion (Anderson and Newell 2004; Jaffe and Stavins 1994; Gillingham and Palmer 2014). Such forms of decision-making are not necessarily irrational. Instead, they can partly be interpreted as a rational strategy for making decisions under uncertainty. For example, when future benefits are uncertain, it makes sense to focus on upfront costs. If the future is uncertain, why not focus on the present?

Uncertainty is a key element not just for explaining the decisions of individuals, but also of firms. In the Keynesian theory of economics, for example, future demand for products is considered to be uncertain, and firms need to plan accordingly (Bellais 2004). Under such conditions, it is not possible to maximise profits over time. Instead, firms base their investment decisions on their subjective expectations, which may or may not turn out to be true. For example, firms may expect an increase in demand, and expand their production capacity accordingly, or maintain unused production capacity in case this happens.

In a context of uncertainty, decisions by firms and individuals are not taken in isolation. Instead, decisions by one agent may impact decisions of others. For example, new technologies are typically first adopted by a relatively small fraction of the population, which is characterised by lower risk-aversion and higher curiosity (Rogers 2010). These early adopters provide valuable information to the rest of the population: is the new technology reliable, and does it provide the promised benefits? Waiting and observing the experiences of others can thus be a strategy for reducing uncertainty. This kind of behaviour is common not just for individuals (Bikhchandani, Hirshleifer, and Welch 1998; Bala and Goyal 1998; Young 2009; Abrahamse and Steg 2013) and firms (Kapur 1995; Jochem and Gruber 2007), but has also been observed in primates (Van De Waal, Borgeaud, and Whiten 2013) and whales (Kawamura et al. 2013).

The modeller must decide how to represent human decision-making under uncertainty in a stylised and mathematically tractable way. As such representations are always imperfect, they lead to uncertainty within the model – be it uncertainty about the appropriate functional form, or uncertainty regarding the input data for a given functional form. There is thus *behavioural uncertainty* in any descriptive (positive) model that attempts to represent how social systems and decision-making operate and evolve in the real world.

2.4 Uncertainty within models

Within models, the representation of human behaviour is just one of many possible uncertainties. This section analyses the whole range of multi-faceted uncertainties in models from the perspective of the analyst. For this purpose, we distinguish between three different dimensions of uncertainty, adapted from the framework by Walker et al. (2003):

- **Location of uncertainty:** where in the model does uncertainty manifest itself?
- **Level of uncertainty:** how can the uncertainty be classified on a spectrum from completely deterministic knowledge to total ignorance?
- **Nature of uncertainty:** what is the fundamental epistemological reason behind the uncertainty?

These three dimensions are also at the heart of the uncertainty matrix, an analytical methodology for classifying multi-faceted uncertainties within a model (see section 3.1.1).

2.4.1 Location of uncertainty in models

The first dimension is the *location of uncertainty.* Where exactly does uncertainty manifest itself in the model? While the exact terminology may differ from model to model, possible locations of uncertainty may be summarised under the following generic classifications:

- **Context uncertainty:** ambiguity in the definition of boundaries of the system to be modelled
- **Structural uncertainty:** arising from the chosen structure and implementation of the model
- **Parametric uncertainty:** arising from the input data and parameter calibration
- **Model outcome uncertainty:** the overall uncertainty of the model outcomes of interest

2.4.1.1 Context uncertainty

The context of a model determines which aspects of the real-world system are represented within the model, and which parts are treated as exogenous to it. Within this process, *context uncertainty* originates from *"the conditions and circumstances (and even the stakeholder values and interests) that underlie the choice of the boundaries of the system, and the framing of the issues and formulation of the problems to be addressed within the confines of those boundaries."* (Walker et al. 2003). Different people (modellers, policy-makers, stakeholders) can have different perceptions of the real-world system that should be modelled, possibly being related to different world views, framings and prior knowledge. This may translate into different choices of the modelling context and the framing of the research question: what should be included into the model, what are its boundaries, and what are the variables of interest? Such decisions can be explicit or implicit, resulting from tacit values.

2.4.1.2 Structural uncertainty

Once the system boundaries are defined, a model representation must be formalised and implemented, leading to two different types of *structural uncertainty*: *model structure uncertainty* (about the conceptual model formulation), and *model technical uncertainty* (arising from the technical implementation of a given model formulation).

Model structure uncertainty refers to the uncertainty that can result from incomplete understanding of the represented real-world system: the behaviour within a system, its relevant elements, and how they relate to each other. If the true structure and dynamics are not fully known, there is uncertainty about the most appropriate model representation of the system of interest. Possible locations of such structural uncertainties are the definitions of variables and parameters, the relationships between inputs and variables, between variables and output, functional forms, equations, assumptions and mathematical algorithms. Depending on the available knowledge, but also on the context and framing of the modelling, there can be multiple alternative model formulations, and more than one such formulation may be plausible. For the same reasons, no proposed model structure may be adequate, for example because the system is not understood well-enough, or it is too complex to be represented in a model. The modeller may or may not be aware of such uncertainties. Also, it depends on the context and purpose of a modelling exercise what kind of model formulation is considered as being adequate.

Should a given model structure be implemented as a computer code, there is an additional level of *model technical uncertainty*. It can originate from errors in the hardware or software being used, from errors in implementing the algorithms, or simply from typing errors when writing the source code.

2.4.1.3 Input uncertainty

Input uncertainty refers to the uncertainty arising from the input data, which either (i) describe the characteristics of the system to be modelled, or (ii) the external drivers of this system.

The *system data* describes the characteristics of the modelled system as such. For models of natural systems, this may be the description of a terrain, map, geophysical properties, or the stock of chemicals in different locations. For socio-economic models, the system data may describe the stock of technologies in different economic sectors (such as power plants or cars), or the existing infrastructure (such as transmission lines).

External driving forces determine the changes within a system, and are not modelled endogenously. Both their correct specification and magnitude can be uncertain. For socio-economic models, examples for external driving forces may be the population in different world regions, economic growth, or energy demand. For models of natural systems, driving forces may be the level of emissions or pollutants in different regions, or demand for water.

2.4.1.4 Parametric uncertainty

Parametric uncertainty originates from uncertainty regarding the choice and calibration of model parameters, which are then typically fixed within a model run or scenario. It is useful to distinguish between different types of parameters, which are subject to different levels of uncertainty, as shown in Table 1.

Table 1: Different types of parameters within system models (adapted based on Walker et al. 2003).

Exact parameters	Universal constants, such as the mathematical constants π and *e*.
Fixed parameters	Parameters that can be considered exact due to detailed previous investigations, such as gravity at a given location.
A priori chosen parameters	Parameters that are chosen to be fixed although they aren't, but may be too difficult to identify by calibration. Their values are thus subject to uncertainty.
Calibrated parameters	Parameters that are unknown from previous investigations or cannot be transferred from earlier studies, because the context is too different. They are determined by calibration, i.e. by comparing model outcomes with historical data. Typically, parameters are chosen so that they minimise the difference between observed outcomes and model outcomes.

Importantly, parametric uncertainty cannot always clearly be separated from structural uncertainty. Depending on the model formulation, the same system may either be represented as (i) a model with a very simple structure and only few parameters, or as (ii) a very complex model with many parameters. Model uncertainty would then likely be dominated by structural uncertainty in case of the simple model, and parametric uncertainty in case of the more complex model. However, in principle it is always possible to formulate any model in a more general way, which includes both the simpler and the more complex model as two of its many possible sub-cases, nested within its mathematical formulation. Different model structures would then be represented by means of different parameterisations, and model structure uncertainty would be re-classified as parametric uncertainty.

For example, let the simple model (i) be a linear function, $f(x)=x$, and the complex model (ii) a quadratic function, $f(x)=x^2$. We can then define a more general model as $f(x)=x^a$. The general model will be equal to the simple linear model for *a=1*, and equal to the quadratic function for *a=2*. This way, it is often possible to transform structural into parametric uncertainty.[2]

2.4.2 Levels of uncertainty within models

As discussed in the introduction, there is no single definition of uncertainty. Instead, many different levels of uncertainty are possible, which can be ordered along a linear spectrum – ranging from the hypothetical ideal of complete deterministic knowledge on the one end, to total ignorance on the other end. Along this spectrum, Walker et al. (2003) differentiate between *determinism, statistical uncertainty, scenario uncertainty, recognised ignorance* and *total ignorance.*

Determinism without any degree of uncertainty is only possible in case of exact parameters, which are fixed and constant by definition (e.g., equations with only natural constants, such as π). As soon as a parameter is not such a constant, but results from measurements in any form, it is not deterministic in a strict sense. As an example, consider fixed parameters: even when they can be classified as exact, this exactness is never absolute, as any kind of measurement still involves some measurement error (for example, the speed of light, which is fixed but subject to measurement error).

As soon as a parameter needs to (and can) be measured, it is subject to *statistical uncertainty:* any uncertainty which can be described statistically, i.e. for which it is possible to quantify a statistical distribution. Such measurement uncertainty may result from the inaccuracy of individual measurements (e.g., the *true* body size of one person may deviate from the *measured* size), or from sampling error when considering multiple measurements (e.g., the average body size within a sample of people may not be representative of the average body size in the whole population). This is the type of uncertainty which is most commonly analysed in the natural sciences or most types of modelling.

Scenario uncertainty describes situations in which a parameter or structural mechanism cannot adequately be described in terms of statistical terminology. Typically, such uncertainties concern future developments, but can also refer to relevant uncertain knowledge of the past or present. Although the analyst is aware that different manifestations are possible and relevant for the model outcome, it is impossible to objectively quantify the statistical probabilities of such manifestations. For example, this may be the case when the underlying mechanisms are uncertain, or are so complex that they cannot easily be represented in mathematical form. In such situations, the analyst needs to make subjective assumptions on uncertain model structures or parameters. As soon as such assumptions are made, models no longer address the question what *will most likely happen* (probabilistically), but instead indicate what *could happen*, given that chosen assumptions are reliable. A self-consistent set of modelling assumptions is often referred to as a *scenario*. In its most common form, a scenario includes a set of assumptions on the future development of model input parameters and exogenous drivers – such as population growth or economic development throughout the next decades. Scenarios may also involve different assumptions on model structure, such as on the characteristics and structure of human behaviour.

[2] Note that this is not always possible. For instance, if a model contains some forms of differential equations, radically different model outcomes might result from seemingly small changes in parameter values, such as in an exponent. In non-linear models, it is therefore possible that bifurcations occur at specific parameter values, on each side of which a very different system emerges, for the 'same' mathematical expression.

In the case of *recognised ignorance*, the model structure itself is uncertain. The analyst has a sufficient understanding of neither the underlying mechanisms, nor of their statistical properties. Importantly, however, the analyst is aware of his own limited knowledge-base. If the uncertainty can be reduced by means of additional scientific investigation, recognised ignorance is in fact *reducible ignorance*. If this is not possible, the analyst needs to deal with *irreducible ignorance*, also referred to as *indeterminacy*.

Last but not least, *total ignorance* describes all uncertainties beyond recognised ignorance – uncertainties which are relevant for the model outcome, but whose very existence remains unknown to the analyst. This is a situation of deep uncertainty, in which we don't know what we don't know. The former US defence secretary Donald Rumsfeld has famously described such uncertainties as the 'unknown unknowns'.

2.4.3 Nature of uncertainty within models

The third dimension of uncertainty is its nature: Does it result from imperfect knowledge of the mechanisms embedded in a real-world system, or from variability within a well-understood system? The former can be classified as *epistemic uncertainty*, the latter as *variability uncertainty* (inherent in sampling from a known frequency distribution). Despite some level of ambiguity, this distinction can serve as a useful classification for analysing uncertainty, and for identifying possible strategies how to characterise and analyse it.

Epistemic uncertainty refers to the uncertainties which result from limited or inaccurate understanding of the system to be modelled. Examples are limited data, measurement errors, uncertain relationships between variables, or a limited knowledge of the system's general structure. Such epistemic uncertainty can sometimes be reduced by means of additional research, given that it generates the knowledge that is needed for improving the model's accuracy (which would be a case of reducible ignorance). According to this definition, measurement error is also a type of epistemic uncertainty, given that it can be reduced by further research (if not, measurement error is a case of variability uncertainty, see next paragraph).

Variability uncertainty is uncertainty that would remain even if the analyst had a perfect understanding of the system. It does not result from limited knowledge, but from the fact that parts of the system are inherently variable: they differ over space or time. Possible reasons are summarised in Table 2.

Table 2: Different sources of variability uncertainty (adapted based on Walker et al. 2003).

Inherent randomness of nature	Chaotic or unpredictable processes in natural systems, such as the exact movement of particles, or the eruption of volcanoes, processes that result from uncharacterised complex systems.
Behavioural variability	Differences in behaviour between different people or groups of people, or changing behaviour over time, ascribed to natural variations, such as decision thresholds, preferences.
Societal variability	Chaotic or unpredictable processes in complex economic, social or cultural systems, such as wars, political decisions, financial crashes.
Technological surprise	Unexpected scientific discoveries, technological developments or new consequences of existing technologies, such as new information technology revolutionising management practices, artificial intelligence.

If *variability uncertainty* is present at the level of statistical uncertainty, it can sometimes be described (and modelled) in statistical terms, for example by using probability distributions. In some cases, the parameters of the distribution are highly certain (such as for the variability of body sizes within the *current* population). In other cases, the statistical distribution parameters itself are uncertain (such as for the variability of body sizes within the *future* population). It may then be possible to define distributions of the uncertain statistical parameters itself.

The distinction between epistemic and variability uncertainty is not necessarily straightforward in all cases. The classification often depends on the model formulation or subjective judgements by the modeller. Furthermore, the classification of the nature of uncertainty may change over time. For example, there may be high confidence in the level of understanding of a functional relationship within the modelled system, and deviations of the model outcome from observations may be treated as variability uncertainty. If then knowledge reveals that the true level of understanding of a system was lower than previously thought, the uncertainty may be re-classified as epistemic uncertainty.

2.5 Uncertainty in different types of models

Different types of uncertainty may either be more or less prevalent in different types of system models – depending on the context and purpose of the modelling activity. Especially when dealing with the nexus, models from many different domains of science are used, often coming from different epistemological traditions. On the most basic level, nexus models may be grouped based on the *type of system* they are meant to analyse, into the following two categories:

- Models of natural systems: climate models, hydrological models
- Models of socio-economic systems: economic models, land-use models, engineering models

Integrated or coupled models sometimes represent aspects of natural and socio-economic systems, combining elements of both categories within one larger model. In such cases, the classification can still be applied to the individual sub-models.

As a second dimension, we find that nexus models may be grouped according to their *epistemological purpose*, i.e. based on the research questions they are supposed to answer[3]:

- Normative models: what *should* ideally happen (such that the outcome is consistent with a pre-determined set of human values, e.g. efficiency or equality)?
- Positive models: what *would* happen or *can* happen (in principle, i.e. what are all the possible states we can find the system in)?
- Forecasting models: what *is likely* to happen?

[3] Note that there is only limited agreement on this classification of epistemology. Because research questions are often framed based on the researchers' subjective perspectives and worldview, different fields of research, and different researchers within a field, can have different interpretations of what they consider to be normative and what not, and whether something is a value judgment or not.

Table 3 summarises the classification of models according to the two different dimensions. Depending on the research question and the system to be modelled, different types of uncertainty may unfold differently. In the table, this is illustrated for the case of behavioural uncertainty.

Behaviour and the associated uncertainty are most obviously relevant in case of socio-economic models with positive research focus (what *would* happen?). Here, the model outcome directly depends on the question of how people make decisions, given a scenario of contextual factors. For example, how would firms and consumers react to different climate policy instruments, such as carbon taxes or subsidies?

Table 3: Uncertainty for different classes of system models and research questions within the nexus.

		Normative *What should happen?*	Positive *What would happen?*	Forecast *What will happen?*
Natural systems	*Examples*	---	Climate models (if run in scenario 'what if' mode)	Weather models
	Role of behaviour		Natural science laws derived from prior experiment directly determines model drivers; possible feedback effects	No dependence on behaviour in the short term
Socio-economic systems	*Examples*	Optimisation models	Simulation models	---
	Role of behaviour	Assumed behaviour determines optimal or feasible model outcomes under assumption of perfect knowledge	Real behaviour determines endogenous model outcomes in the 'what if' mode, usually based on imperfect knowledge	

The relevance of behavioural uncertainty is less clear-cut for socio-economic optimisation models. If such a model is aimed at identifying a feasible or optimal system configuration (such as the allocation of scarce resources, or a long-term energy scenario), behaviour is typically not simulated under a positive philosophy, but assumed, given that moral philosophy research questions generally concern what the behaviour itself should be. For example, identifying the optimal energy system configuration and development, that reach certain objectives, if firms and consumers are assumed to behave consistently following a hypothetical benchmark of perfectly rational and forward-looking decision-making that allows them to 'make the appropriate decisions'. For determining a hypothetical optimum, it is then less important how people actually behave in reality, since the question concerns what ideally they should do, not whether it is likely that agents behave in this particular way. Importantly, such a hypothetical optimum is only well-defined under the assumption that people have perfect knowledge of the current and possible future states of the system (either of all future outcomes itself, or at least of their probabilities). Under conditions of fundamental uncertainty, there are by definition possible future outcomes that people (and also the modeller) do not know about, so that any optimisation (of behaviour or system configurations) becomes effectively impossible (see section 2.2). In short, one might say that optimal behaviour is only possible if all possible consequences of any possible action are known to the decision-maker (Mercure et al. 2019).

The distinction between positive and normative modelling is more ambiguous when the research focus is on policy design – such as determining the optimal level of a carbon tax. For example, a perfectly rational agent may make a hypothetically 'optimal' (under certain criteria) investment decision at a tax level of 20 Euro/tCO_2, while in reality, it could be found that it takes a higher tax rate of 40 Euro/tCO_2 for incentivising such a decision to be made by boundedly rational humans. In such a situation, a question arises whether a policy should be considered optimal when it leads to the desired outcomes under hypothetical decision-making, or under real-world decision-making.

For models of natural systems, behavioural uncertainty is, by convention, mostly constrained to exogenous model drivers. In case of climate models, for example, human behaviour impacts the total level of greenhouse gas emissions, which is traditionally taken as an exogenous model input for estimating future changes in the climate. However, there is also the possibility of feedback effects: given rising temperatures or a higher frequency of natural disasters, people may adapt their behaviour accordingly, and decide to devote larger effort to the reduction of greenhouse gas emissions (Beckage et al. 2018). Natural and social systems are in principle inseparable, as they are connected by a web of reciprocal influence, and we separate them for reasons of scientific tractability and areas of competence.

3 Methodologies and strategies

In this section, we review different methodologies for the identification, analysis, and communication of uncertainties in model-based decision-support.

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Overview: A pragmatic approach for uncertainty analysis in large and complex models

(1) **Choose a focus for the uncertainty analysis**
In many complex models, the list of variables and assumptions is so large that a complete analysis remains unfeasible. It is then necessary to focus the analysis – for example, on a specific model component, the relevance of behavioural uncertainties, or the uncertain effect of policies. (Obviously, there is always the risk that focusing too much could lead to missing something important that is out of the focus.)

(2) **Identification and qualitative analysis of relevant uncertainties**
As a first step, relevant uncertainties need to be identified within the model, and within individual modelling assumptions.

- **Mapping relevant uncertainties: uncertainty matrix**
  What kind of uncertainties are located in which parts of the model? An uncertainty matrix can help to obtain an overview, by classifying uncertainties along different dimensions (location, level, and nature of uncertainties).
- **Analysing important modelling assumptions: pedigree analysis**
  Assumptions are part of every model. How plausible are they, and how important are they for the model outcome of interest? This can be analysed by performing a qualitative pedigree analysis, which assigns subjective pedigree scores to each individual assumption. Ideally, this is done by more than one person. The impact of assumptions on model results can either be estimated subjectively at this stage, or can be obtained from prior sensitivity analysis (if available or easy to perform). Finally, the most critical assumptions are identified in a diagnostic diagram: Which assumptions have a low pedigree score, but a (potentially) high impact on results?

(3) **Quantitative analysis of uncertainties where possible**
Once critical assumptions and uncertainties were identified, some of them can be further analysed in a quantitative way, depending on the nature and level of uncertainties.

- **Sensitivity analysis**
  In case of parametric uncertainties, the respective model parameters can be varied in systematic ways, in order to estimate their quantitative impact on model results. This may be done in the form of local or global sensitivity analysis (e.g., in form of a Monte Carlo simulation).
- **Alternative model formulations**
  Structural uncertainties may be critical, but cannot easily be altered within a sensitivity analysis. Instead, the model structure itself needs to be changed. This is rarely feasible, but if it is, it can allow to get a better understanding of how important a structural uncertainty is for the model outcome.

(4) **Communication of uncertainty results**
Finally, it needs to be decided how the results of the uncertainty analysis should be communicated. Which insights are relevant for which target audience, and how should they be included within different forms of publications? At this stage, it is important to strike a delicate balance: Uncertainties should be clearly communicated and set the research results into perspective, without undermining their relevance. Which insights from the modelling are robust despite the presence of the identified uncertainties, and which results should be interpreted with a degree of caution?

We suggest a new ‘pragmatic approach for uncertainty analysis in large and complex models’ (see text box above), which combines aspects of the reviewed methodologies. We focus on the approaches which are most relevant for interdisciplinary modelling in the context of the nexus, and which can be implemented for large and complex models, even with only limited resources at hand. For this purpose, we recommend the following procedure for multi-faceted uncertainty analysis (summarised in the box above):

1. Identification of relevant uncertainties within the model
2. Quantitative analysis of uncertainties where possible
3. Communication of uncertainties and their relevance for model results

In principle, if sufficient resources are available, the analyst can perform an exhaustive analysis of all possible uncertainties within the model. In practice, the available time will usually be constrained. In such cases, the analyst can focus on a particular type of uncertainty – such as behavioural uncertainty or the uncertain effects of policy instruments.

Practical examples of uncertainty analysis for three different types of models which are used in Sim4Nexus are presented in section 4. Other useful examples of analysing and communicating uncertainty can be found in Wardekker et al. (2012) (on uncertain health risks of climate change), Benessia and De Marchi (2017) (on uncertainty management for earthquake projections), Elahi (2011) (on uncertainty communication in Greek and Roman times), Stirling (2010) (on uncertainty communication to policy-makers), Butler et al. (2014) (on global sensitivity analysis in integrated assessment models), Pye et al. (2018) (on qualitative and quantitative uncertainty analysis in energy modelling), Bankes (2002) (on policy-making under deep uncertainty), van der Sluijs (2005) (on coping strategies for uncertainty communication), van Asselt and Rotmans (2002) (on pluralist uncertainty analysis in modelling), Kloprogge et al. (2011) (on the analysis of uncertain assumptions in models), Refsgaard et al. (2006) (on analysing model structure uncertainty), and Kok et al. (2011) (on participative scenario development).

3.1 Identification of key uncertainties

As a first step, relevant uncertainties need to be identified - both within the model, and for individual assumptions. We here present two methodologies which are suitable for this purpose: the mapping of uncertainties within an uncertainty matrix, and a further analysis of uncertainties within individual assumptions by means of a pedigree analysis. While both methods could also be used independently from each other, we recommend a stepwise procedure as a more consistent approach for multi-faceted uncertainty analysis.

First, the uncertainty matrix is used for obtaining a better overview of relevant uncertainties. As a second step, the analyst needs to pick a set of uncertain assumptions which seem to be most relevant. A pedigree analysis can then be performed for each of these assumptions, which combines two elements: the pedigree of assumptions and their impact on the model results. How appropriate are the assumptions, which alternative assumptions could be made, and how relevant are they for the model outcome?

3.1.1 Uncertainty within the model: uncertainty matrix

The uncertainty matrix (Table 4) conceptualises the three dimensions of uncertainty within models, as they are described in section 2.4: the location, level and nature of different uncertainties. The three main locations of uncertainty within models (context, structural uncertainty, input uncertainty, parametric uncertainty) are shown in the left column of the table. The level of uncertainty (statistical uncertainty, scenario uncertainty, ignorance) is shown in the top row.

Within this two-dimensional structure, different model assumptions can be classified according to both their location and level, by writing them into the respective cell of the table. The nature of uncertainty is incorporated as a third dimension, shown in the second row of the table: within each cell, an uncertainty may be classified as being of epistemic or variability nature. When it is not possible to clearly distinguish between both, the assumption can be written down anywhere along this spectrum, or can simply be put into the middle. Also, uncertainty may manifest itself in more than one place of the matrix, in which case the assumption would also need to be included in different cells.

The uncertainty matrix serves as the starting point of the analysis, as it allows the analyst to gain a better overview of the different uncertainties within the model.

Table 4: Uncertainty matrix for the location of key uncertainties within a model.

Nature / Location	**Level**					
	Statistical uncertainty		Scenario uncertainty		Recognised ignorance	
	Epistemic	*Variability*	*Epistemic*	*Variability*	*Epistemic*	*Variability*
Context						
Structure						
Input						
Parametric						

3.1.2 Uncertainty within assumptions: pedigree analysis

Every part of the model which was identified as being uncertain contains a *modelling assumption*: a value or structure which has been chosen as an approximation of the real world, in the absence of perfect knowledge. For each single assumption within the model, a so called *pedigree analyses* can be performed, which focuses on two key characteristics: an assumption's overall 'pedigree' (similar to its overall quality, see further below), and its estimated impact on model results.

Pedigree analysis aims at systematically analysing the strengths and weaknesses behind model assumptions, by critically examining their quality and production process. It originates in the so called 'NUSAP approach' (short for 'numeral, unit, spread, assessment, and pedigree'), which was developed as a broad approach for uncertainty analysis in the 1990s, in reaction to strong criticism of models and assumptions used by the Netherlands Environmental Assessment Agency (Van Der Sluijs et al. 2005; Rotmans et al. 2003). NUSAP aims at going beyond a purely statistical analysis of uncertainty, by also including epistemological and methodological considerations. In addition to established quantitative measures (sensitivity of results to spread in the numbers used in a calculation), the quality of the underlying knowledge base and assumptions are assessed (their pedigree). This way, the robustness of model results and conclusions can be evaluated more transparently by model users, policy-makers or members of the public.

The overall degree of pedigree is a composite measure, resulting from a multi-criteria evaluation of different aspects of uncertainty, which is performed for each analysed model assumption. Typically, these criteria are qualitative in nature, and are based on subjective expert judgement. However, to make them comparable and more transparent, a subjective score can be assigned. For each criterion, a discrete numeral scale is defined (e.g., from 0 to 3), with linguistic descriptions (modes) of each level on the scale. The overall pedigree of an assumption can then be calculated as the mean score over all considered criteria. Pedigree analysis is facilitated by the creation of a pedigree matrix for each analysed assumption, which contains all the selected criteria and the assigned scores.

Table 5 shows an example of a pedigree matrix (based on Kloprogge, Van der Sluijs, and Petersen 2011), which contains the following criteria: influence of situational limitations, (im)plausibility, choice space, (dis)agreement among peers, (dis)agreement among stakeholders, and sensitivity to view and interests of the analyst. Depending on the specific requirements in a given model analysis, this set of criteria may be extended or restricted, according to individual needs.

Table 5: Pedigree matrix for the analysis of individual modelling assumptions (adapted from Kloprogge, Van der Sluijs, and Petersen 2011).

Type	*Practical*	*Epistemic*			*Socio-political*	
Criteria / **Score**	**Influence of situational limitations**	**(Im)plausibility**	**Choice space**	**(Dis)agreement among peers**	**(Dis)agreement among stakeholders**	**Sensitivity to view and interests of analyst**
2	Choice assumption hardly influenced	The assumption is plausible	Hardly any alternative assumptions available	Many would have made the same assumption	Many would have made the same assumption	Choice assumption hardly sensitive
1	Choice assumption moderately influenced	The assumption is acceptable	Limited choice from alternative assumptions	Several would have made the same assumption	Several would have made the same assumption	Choice assumption moderately sensitive
0	Totally different assumption had there not been limitations	The assumption is fictive or speculative	Ample choice from alternative assumptions	Few would have made the same assumption	Few would have made the same assumption	Choice assumption sensitive

The second key characteristic is the assumption's estimated impact on model results, which can be evaluated on a similar numerical scale, based on either subjective expert judgement or a prior quantitative analysis:

- 2 - The assumption has only local influence
- 1 - The assumption greatly determines the results of the modelling step
- 0 - The assumption greatly determines the results of the model

Both key characteristics (pedigree and impact) can then be combined, in order to identify *critical assumptions*: such assumptions that have weak pedigree, but a high impact on model results. A diagnostic diagram may be used to illustrate both characteristics for multiple assumptions at the same time, as shown in Figure 1. Here, critical assumptions would be located in the 'danger zone' (Q4). Uncritical assumptions (strong pedigree and low impact) would be located in the 'safe zone' (Q1).

In principal, it would be possible to analyse the pedigree of all elements listed in the uncertainty matrix. In practise, time constraints imply that the analyst can only consider a sub-set of uncertainties for further analysis. If available, a sensitivity analysis can indicate which variables are most important. However, such a sensitivity analysis is time-consuming in itself, and is only applicable to modelling assumptions which can be changed easily (e.g., parametric uncertainty), thereby being relatively unsuitable for structural uncertainties. Therefore, we suggest the following step-wise, iterative procedure:

1. For all elements within the uncertainty matric, the analyst estimates their potential relative impact on model results, and ranks them accordingly.
2. From this ranking, the analyst chooses a set of the most impactful assumptions, based on available time and resources.
3. A pedigree analysis is performed for the chosen assumptions.
4. Based on their pedigree and estimated impact, the most critical assumptions are identified.
5. The most critical assumptions are further analysed, e.g. by means of sensitivity analysis, scenario analysis, or the formulation of alternative model specifications.
6. Based on this analysis, the initial selection of uncertain assumptions is re-evaluated.

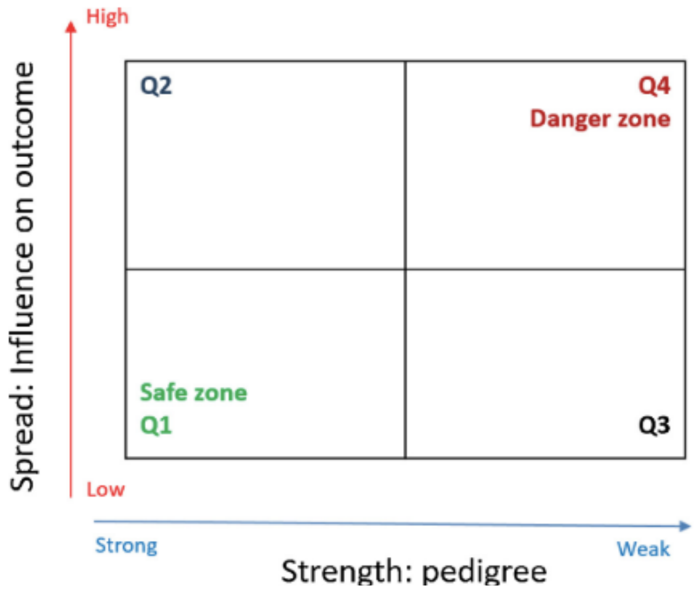

Figure 1: Diagnostic diagram for the combined analysis of pedigree and impact of modelling assumptions (source: Pye et al. 2018).

3.2 Quantitative analysis of key uncertainties

Once a set of uncertain assumptions and variables has been identified, several methods exist for their quantitative analysis. There is no single methodology that is superior in all cases. Instead, different methods are adequate in different situations, depending both on the type of uncertainty and the purpose of the analysis. Here, we discuss the application of local and global sensitivity analysis, scenario analysis, and the use of alternative model formulations. Table 6 gives an overview which of these methodologies can be used for which kind of uncertainty. For each methodology, we present a summary of its key characteristics in the respective sub-chapter. More detailed explanations of all possible variants of each methodology, as well as all the necessary steps for their practical implantation, are available in the referenced literature.

Table 6: Methodologies for the quantitative analysis of uncertainty on different levels and locations.

Methodology	Level of Uncertainty	Location of Uncertainty
Sensitivity analysis	Statistical uncertainty	Input; parameter
Scenario analysis	Scenario uncertainty	Input
Alternative model formulations	Recognised ignorance	Structure; context

3.2.1 Sensitivity analysis

Sensitivity analysis is the probably most widely used methodology for uncertainty analysis. Fundamentally, it aims at characterizing how model results respond to changes in different model inputs and parameters. It is therefore suitable for analysing statistical uncertainty, both at the location of model input and parameters. The method cannot be used for the analysis of uncertainty in non-parametric locations, such as the uncertainty with regard to model structure and context.

From a modelling perspective, possible insights from a sensitivity analysis are the relationships between the model inputs and outputs, an improved understanding of the model structure, and an increased transparency of its architecture and dynamics. From a policy perspective, sensitivity analysis may also provide additional insights into the likelihood of reaching some policy target, on the robustness of policies or the suitability of technologies under conditions of uncertainty, and for the identification of robust policy choices (which would realise the desired policy target under a wide range of model outcomes).

Various types of sensitivity analysis exist, which allow for different degrees of detail in the analysis, and which have different computational burdens for their implementation. Broadly, they can be grouped into two sub-classes: local sensitivity analysis, and global sensitivity analysis.

Independent of its type, any sensitivity analysis requires three basic choices, which need to be made ahead of the actual analysis:

- Which model parameters will be subject to sensitivity analysis?
- The sensitivity of which model output shall be analysed?
- Which values are chosen for all other parameters, and which are kept constant?

In addition, for the choice of methodology, it should be considered in which form the model outcome is expected to change for variations on one parameter:

(1) sub-linear,
(2) linear or
(3) super-linear.

In (1), the sensitivity of the model output to parameter changes is smaller than one, so that the uncertainty decreases with propagation through the model. In case of (2), the change in model outcomes is proportional to changes in the input parameter (e.g. uncertainty on future energy demand gives proportional uncertainty on resulting emissions), which implies that a linear analysis in form of local sensitivity analysis is sufficient. In case of (3), the uncertainty of the model outcome grows with the degree of uncertainty propagation. An example is path-dependence, where differences in the model outcome grow with the increasing difference in trajectories. Therefore, one parameter can drive most of the model uncertainty (especially if the other parameters are of type (1) or (2)), which implies that a global sensitivity analysis may be necessary.

3.2.1.1 Local sensitivity analysis

In *local sensitivity analysis*, changes in the model output are analysed against variations of specific model parameters or input variables around their pre-specified default or reference values, one parameter at a time. While the parameter of interest is varied along a specified range, all other model parameters are held constant. Therefore, local sensitivity analysis is sometimes also referred to as 'OAT analysis' (one parameter at a time). This is in contrast to *global sensitivity analysis*, where all parameters are varied simultaneously, thereby also considering possible interactions and joint influences of different parameters (also referred to as 'AAT analysis', for all parameters at a time).

The impacts of parameter variations on the model results can be analysed visually (e.g., by comparing time series of the model output under default and perturbed values) and quantitatively, by calculating the output sensitivity to changes in a given input. Formally, this type of sensitivity equals the partial derivative of the model with respect to the parameter, evaluated at its reference value. Importantly, such a partial derivative cannot capture the model's sensitivity to changes in parameter combinations and non-linear interactions. For such effects, it is necessary to perform a (computationally much more expensive) global sensitivity analysis.

Multiple-starts perturbation methods are methodologically similar to local sensitivity analysis, extended into the direction of global sensitivity analysis. Such a global extension is realised by combining multiple local sensitivities, each of which starts from a different reference value (or 'perturbation') of the analysed variable. The perturbed reference values are different from the default value of the parameter in a normal model run, but still located within the feasible input space. Global sensitivity can then be estimated by aggregating all such individual local sensitivities. While there are different methods for doing so, the most established one is the 'Morris method' (Morris 1991), later refined into the 'Elementary Effect Test' (Saltelli et al. 2008). The basic idea is to take the mean of a finite set of local sensitivities at different perturbations as a measure of global sensitivity.

3.2.1.2 Global sensitivity analysis

In contrast to its local counterpart, *global sensitivity analysis* does not only capture the sensitivity of model outcomes to single separate model parameters around their default value, but also considers their co-variations within the entire space of feasible combinations of input parameters. However, the methodology does require the specification of a feasible input space for each analysed variable. If the input space itself is uncertain, results from global sensitivity analysis are constrained in their validity, as it remains unclear if the considered input space is indeed representative of the real input space. This may also arise if the task is too large and focus on a subset of the system is chosen, in which case the boundaries of the analysis may remain uncertain.

The most common type of global sensitivity analysis is *Monte Carlo Analysis*, which represents the uncertainty around each model parameter by means of a probability distribution. For each model run, a value is drawn from the respective distributions for each uncertain parameter, so that multiple input parameters are varied simultaneously. The resulting model outputs can then be analysed statistically, for example by means of regression analysis or the computation of partial correlation coefficients. This not only allows to estimate the sensitivity of model outputs with respect to different parameters, but also to apportion variations in the model outcome to different sources of uncertainty in the model input. The following steps are generally required for a Monte Carlo analysis:

1. A probability distribution is assigned to each considered model parameter.
2. For each considered parameter, a sample of random values is drawn from its respective probability distribution.

3. One single value is drawn from the random sample of each parameter, and the model is run with these input values.
4. Step 3 is repeated multiple times, where each model run uses a different set of input parameters.
5. The resulting sample of model outputs is analysed statistically.

For the sampling of parameter values, any random or quasi-random technique can be used in principle, and computational efficiency is the main difference between them. Some sampling techniques allow to reduce the total number of runs which is required for statistically significant results, such as 'Latin-Hypercube sampling' and 'Sobol quasi-random sampling' (for an introduction to sampling methods, see Forrester, Sobester, and Keane 2008). In Latin Hypercube Sampling, for example, values are sampled evenly from each parameter's probability distribution, so that a relatively small sample set is sufficient for representing the parameter's real variability.

The sufficient number of model runs is typically between hundred to several hundred, depending on the number of parameters and the desired level of statistical significance. In addition to the choice of efficient sampling techniques, the number of model runs can be further reduced by means of a preliminary local sensitivity analysis: Based on its results, a global sensitivity analysis is then only performed for variables which show a relatively stronger effect on the model outcome, or a coarser set of input values is defined for less influential variables. One well-established method for such an initial screening of variables was presented by Morris (1991), and has been subsequently improved by Campolongo et al. (2007).

A particular type of global sensitivity analysis is the use of *ensemble simulations* (e.g. Stephenson and Doblas-Reyes 2000; Monier et al. 2015). In this methodology, an ensemble of models is used instead of one single model. Each member of the model ensemble is based on the same model structure, but uses a different set of input parameters. N simulations are performed with N choices of model parameter values, all starting from different initial model states. For example, this approach is used in weather and climate modelling, where the sensitivity of simulations to model parameters is captured by using perturbed physics ensembles.

Global sensitivity analysis has the advantage that is does not require any modifications of the model structure, and can thus be performed within the existing modelling infrastructure. At the same time, this is one of the main limitations of the approach: Global sensitivity analysis cannot be applied for analysing structural model uncertainties, for which the mathematical model formulation itself would need to be changed. Furthermore, global sensitivity analysis tends to be computationally expensive. In particular in case of complex models, it can be unfeasible to perform the required number of iterations, which typically are several hundreds. Last but not least, often it is not possible to get reliable estimates of the necessary probability distributions of uncertain model parameters. In reality, parameters and the shape of probability distributions often remain unknown, in particular with regard to future parameters realisations. Even with the same mean and standard deviation, different shapes of the distribution can lead to substantially different results of the sensitivity analysis.

3.2.2 Scenario analysis

Scenario analysis is a widely used methodology for analysing uncertainty which goes beyond statistical uncertainty: the scenario uncertainty which is located in a system's input parameters or external driving forces, foremost its present or future external environment. Generally, a scenario is any *"plausible description of how the system and or its driving forces may develop in the future"* (Walker et al. 2003). This includes both plausible and highly implausible scenarios. Plausible scenarios are those scenarios which are built on a set of assumptions about input parameters and key relationships which is coherent and internally consistent. Each plausible scenario can then be seen as one plausible indication of how the system *might* develop in the future. However, due to the presence of scenario uncertainty, no single scenario can forecast what actually *will* happen in the future.

In modelling, scenarios are used to answer *what if* questions: How would the system develop, given a spread of different scenarios? Such scenarios may explore model variations which result from any type of variation in model assumptions, such as:

- Different policy instruments (e.g., the effect of a carbon tax or of subsidies)
- Different driving forces (e.g., energy demand, food demand)
- Different technological assumptions (e.g., future fuel costs, investment costs)
- Different behavioural assumptions (e.g., different discount rates, degrees of risk aversion)
- Different model constraints (e.g., a different resource potential, trade barriers)

However, scenarios as such always remain deterministic, and are constrained by the model's structure. Scenarios can be insufficient for anticipating relevant developments in the real world, and may underestimate the possible range of relevant scenarios and model outcomes. In the end, the modelled scenario space is only as broad as the modeller's imagination, which can lead to cognitive bias in the process of scenario design: Some scenarios may be seen as more probable than they really are, while some probable scenarios might be ignored altogether (Trutnevyte et al. 2016; Morgan and Keith 2008). The bias remains with the interest and choices of the researcher as opposed to likelihood.

3.2.3 Alternative model formulations

Both sensitivity and scenario analysis depend on the variation of existing input or other model parameters, and can therefore only be used for the analysis of parametric uncertainties. However, nexus models typically attempt to model a highly complex system in a context of deep uncertainty. Therefore, structural uncertainties will always be relevant. One obvious strategy for dealing with structural uncertainties is the development of more complex and detailed models, which have a more accurate representation of all relevant dynamics. However, structural uncertainties will always remain, even for highly sophisticated model formulations: Simplifications and assumptions about functional relationships are always made when building a model. Does the chosen structure indeed appropriately represent the system of interest, and its potential reaction to policy instruments? Here, we provide a short overview of two common methodologies for the quantitative analysis of structural uncertainties: Multiple model routes, and ensemble modelling (or the use of multiple models).

Multiple model routes were proposed by Van Asselt and Rotmans (2002) as a technique for addressing structural uncertainties by means of developing different alternative versions of the same initial model. Each version of the model is hereby referred to as a model route. Each model route constitutes an experiment, which can explicitly consider and represent different perspectives on the modelled system. Model routes may either differ with respect to model parameters, or with respect to functional relationships within the model. In the first case, the focus is on the quantification of alternative values for existing model parameters, similar to a sensitivity analysis. In the second case, the modeller also modifies the relationships between model parameters - for example by choosing a different functional form, or by considering additional types of functional relationships within the model. No probabilities are assigned to different model routes, which are meant to span the space of possible futures, constrained by what is known. The implementation of multiple model routes is therefore similar to scenario analysis, being applied to model structures instead of future states of exogenous model drivers.

In a next step, the modeller can evaluate to which extent the resulting model outcomes differ from previous model runs, and explore possible reasons behind these differences (van Asselt 2000). In the end, the analysis of different model routes can help to identify policy strategies which are robust, i.e. modelling insights that are largely independent of the chosen model formulation.

Different variants of the same model (i.e., the model routes) can be combined by means of **ensemble modelling.** In a **single model ensemble**, the same single model is run multiple times, each time with different sets of parameters or structural specifications. The methodology can either be used to produce a probability distribution of model estimates and identify one 'best' model estimate (e.g. Kronvang et al. 2009; Trolle et al. 2014), or to analyse the uncertainty which underlies the ensemble (e.g. Georgakakos et al. 2004). The results of the various ensemble members (i.e., the different model specifications) are either converted into a simple average (implicitly assuming equal probabilities for each model route), or by aggregating the respective estimates based on further weighting (i.e., assigning different probabilities to different model routes).

If more than one model is available for describing the same system, it is also possible to design a **multiple model ensemble**. The method might offer a wider range of diversity compared to the reliance on a single model ensemble, given that the underlying assumptions were made independently for each model (Viney et al. 2009; Exbrayat et al. 2014; Kriegler et al. 2015). Most processes are not straightforward to model, and different researchers may follow different approaches. This does not mean that all models are unreliable or even wrong. Instead, the combination of diverse modelling approaches can be helpful, as it allows to compare the outcomes of different models, which can help to quantify their uncertainty. If different models produce very different outcomes for the same scenario under a consistent parameterization, it may be concluded that the model estimate is subject to large structural uncertainty. The opposite conclusion is more difficult to make, however: Even if the results of different models are very similar to each other, this does not necessarily mean that the structural uncertainty is small. It is always possible that the small range of model outcomes results from the fact that different models have all been fitted to the same data, which then naturally leads to similar model outcomes, depending on the chosen scenario. Alternatively, many different models within an ensemble may be based on very similar structural assumptions. This can then lead to a relatively small range of model outcomes within the ensemble, and a false sense of robustness, without considering the potentially much larger range of model outcomes if different model structures and assumptions were to be considered. One prominent example are the scenarios of climate change mitigation pathways reviewed by the IPCC in its latest assessment reports (Clarke et al. 2014; Rogelj et al. 2018): the integrated assessment models used for generating these scenarios are very close to each other in their basic structural assumptions (optimisation), which limits the range of model outcomes by construction, and may lead to the wrong impression that structural model uncertainty is not of primary importance (as claimed by Gillingham et al. 2015).

Models (individually or as ensembles) can also be used as part of a **Delphi Method analysis**, in the context of which they might help to gain a better quantitative understanding of the uncertainties involved in a given situation. The Delphi Method was developed by RAND in the 1950s, initially for the purpose of forecasting technological developments and their potential impacts on warfare (Linstone and Turoff 1975). The method is based on a selected group of experts who anonymously respond to questionnaires on a given topic, and are then given the chance to adjust their initial forecasts based on the aggregated responses of the rest of the group. The goal of this iterative process is to reduce the range of responses and forecasts given by experts, so that eventually a consensus forecast will be reached. Quantitative models can be used to supplement and inform this procedure, for example by projecting different scenarios, based on the expert responses.

3.3 Communication of uncertainties

Once the various facets of uncertainty within a model have been analysed, the modellers need to decide on an appropriate communication strategy: Which results of the uncertainty analysis should be communicated, to whom, and in which form? The communication strategy should be tailored to the individual situation, considering the primary purpose and audience of the modelling study. For example, different types of uncertainty communication may be required in the context of a scientific publication in form of a journal article, a policy brief, or within a serious game.

We structure the following sections based on the checklist which is recommended in the 'Guide for Uncertainty Communication' of the PBL Netherlands Environmental Assessment Agency (Wardekker et al. 2013). We only aim here at providing a brief overview, focusing on the aspects which are most relevant in the context of the Sim4Nexus project. For further details, please refer to the original publication.

- **Target audience (who?) and relevance (what and when?):** to whom should the communication be directed, what is relevant to them, and when?
- **Uncertainty communication (where?):** how could uncertainty information be incorporated into the story and where?
- **Presentation (how?):** how could uncertainty information be presented?

3.3.1 Target audience and relevance

Who is the target audience of the communication?

It can make a crucial difference if the target audience of the uncertainty communication are scientists from the modeller's own field, from other scientific disciplines, policy-makers, other stakeholders, or the general public. As a first step, it must therefore be clarified who is going to be addressed by the respective publication.

What information on uncertainty are required for the target audience, and which information is most relevant?

Different audiences can have different requirements, expectations and needs with regard to the content, type and form of uncertainty communications – depending on their interests, prior expertise, or concerns. Possible requirements are (but are not restricted to):

- None.
- Discuss the robustness of the modelling results with respect to identified uncertainties.
- Reflect on the identified uncertainties, and how they impact the results.
- Determine the main sources and causes of uncertainty.
- Identify possible policy implications which could stem from the uncertainty.

Sometimes, it may be possible to identify the requirements based on previous experience and interactions with the target audience, for example during stakeholder workshops. Furthermore, it may also be the case that the requirements are not only determined by the expectations of the target audience, but also by other stakeholders (e.g., the funding agency). Last but not least, a lack of interest on part of the target audience does not imply that there is no need for the communication of uncertainties to them.

In general, the need for uncertainty communication for a given audience may be estimated by answering the following question:

What questions, problems, tasks and (policy) challenges does the target audience face? On the basis of this, which uncertainties are significant or of interest to them?

What are possible implications of uncertainty for the modelling results and for policy-making?

Identified uncertainties may have various implications, such as:

- How robust are the modelling results and derived recommendations for policy-making?
- What are the main assumptions behind the results?
- How representative are the results (e.g., outside the modelled region, timeframe)?
- How could the identified uncertainties be reduced, and for which uncertainties would this be impossible or infeasible?
- What are possible implications for policy-implementation (e.g., is there a need for adaptive evaluations and policy adjustments)?

The target audience and its needs determine which possible implications are relevant and should be communicated.

3.3.2 Uncertainty communication

At the communication stage, the modeller should be clear about the main messages. Furthermore, it should be considered how the target audience might react to the main message and the communication of underlying uncertainties.

What are the main results/messages of the modelling study?

It is of primary importance to be clear about the main messages. In the process of uncertainty analysis, the modellers themselves might increasingly focus on the uncertain part of their results. However, they should always bear in mind the initial purpose of their modelling study: What key results were obtained, despite the inevitable presence of uncertainty on various levels of the modelling? The communication of uncertainties should always be seen in this context, and framed accordingly.

In particular, it can be helpful to formulate conclusions and policy recommendations which are robust, even when considering the analysed uncertainties. The degree of robustness should be clear from the phrasing, and all conclusions should have a consistent level of precision (e.g., when the direction of change is relatively certain while its exact extent remains uncertain, it would be misleading to quantify the range with overly precise numbers).

How will the communication of uncertainties be interpreted and digested by the target audience?

Importantly, while uncertainty is an integral part of any scientific research activity, it can have rather negative connotations in non-scientific language, where it might be understood as meaning that results are unreliable, arbitrary or useless. In the guide “Making Sense of Uncertainty” (Sense about

Science 2013), a multi-disciplinary group of researchers summarises the resulting challenge in the communication of uncertainty in the following way:

"Uncertainty is normal currency in scientific research. Research goes on because we don't know everything. Researchers then have to estimate how much of the picture is known and how confident we can all be that their findings tell us what's happening or what's going to happen. This is uncertainty. But in public discussion scientific uncertainty is presented as a deficiency of research. (…) Uncertainty is seen as worrying, and even a reason to be cynical about scientific research – particularly on subjects such as climate science, the threat of disease or the prediction of natural disasters. In some discussions, uncertainty is taken by commentators to mean that anything could be true, including things that are highly unlikely or discredited, or that nothing is known."

However, the presence of uncertainty does not imply that modelling results are wrong or useless, or that that anything could be true. Decisions can be made in the presence of uncertainty, and waiting for increased certainty might not necessarily lead to better decisions. Normally, the most relevant question for decision-making based on scientific evidence is not 'do we know everything?', but 'do we know enough?' or 'how can we best make a decision based on the available knowledge?'.

In the case of climate change, for example, many details of the underlying processes in climate science remain extremely uncertain. However, there is only very little uncertainty over the main finding of global warming in reaction to increased levels of greenhouse gas emissions. This can be seen in analogy to someone dropping a ball: There will always remain substantial uncertainty about the question where the ball might come to a final stop (e.g., depending on the exact conditions of the ball and the environment), so that its final position can only be approximated within some range. Still, due to the presence of gravity, we can be virtually certain that the ball is going to fall towards the ground.

What layers of communication are available, and how should uncertainty communication be incorporated in them?

Results and the underlying uncertainty of modelling studies can be communicated in various formats (e.g., journal article, report, press release), each of which may consist of different parts (e.g., abstract, executive summary, appendix). It must thus be decided which kind of uncertainty information should be communicated in which format, and where.

"*A summary containing many pages of uncertainty information does not invite reading and may quickly disappear into a drawer. Placing all the uncertainty information in an appendix will ensure that hardly anyone will read it – except for readers specifically searching for such information. Few people read a report from cover to cover or consult all publications resulting from a study. The crucial question, therefore, is: What to mention where?"* (Wardekker et al. 2013, 14)

For any possible format and location within a respective publication, it should be considered: What is its main purpose and target audience? What is the purpose of the uncertainty communication within this context? What are the informational needs and expectations?

As a general rule, very important information on the relevance of uncertainty for the presented results should be communicated in very prominent parts of the publication (e.g. summary, recommendations). For less crucial analysis of uncertainty, it may be sufficient to include them into separate sub-chapters or as supplementary information.

What kind of information should be provided on uncertainty?

Depending on the target audience and type of publication, the following may be useful starting points for the consideration what kind of information on uncertainty should be communicated:

- Which methods were used by the modellers/analysts for the analysis of uncertainty. (May be included as an appendix.)
- In which ways are uncertainties communicated within the publication (e.g., definitions of uncertainty, employed terminology, reference to additional information on uncertainty analysis).
- What kind of scenarios were used, and why their use was necessary.
- Which 'knowledge gaps' still remain.
- In how far the conclusions would significantly change in reaction to improved knowledge, or if they would likely remain the same.
- How different views and controversies were dealt with/included in the analysis.
- In case of quantitative uncertainty analysis: Which uncertainties were included in the analysis, which were not, and why.
- Additional 'educational information' on uncertainty (e.g., information on the different types of uncertainty, and that some uncertainty will always remain).

3.3.3 Presentation

Finally, it needs to be decided in which way the uncertainty information is presented in each case: verbally, numerically, graphically, or as a combination thereof.

Verbal presentation

The verbal presentation of information is often easier and more intuitive to understand and remember for many people, especially when they are not trained in statistics or any quantitative science. Verbal presentation is often more adequate when numerical indicators are only of secondary importance, or not available at all. Verbal presentation can play a central role when information needs to be presented in very concise ways, such as within summaries.

Table 7: Linguistic indicators for the verbal presentation of uncertainty information (adapted from Wardekker et al. 2013).

Linguistic indicators	Examples
uncertainty terms	'likely', 'not certain'
auxiliary verbs	'can', 'may', 'appear'
remarks that indicate preliminary status of a finding	'initial conclusions', 'initial approach', 'preliminary estimate', 'more research needed', 'based on current insight'
remarks that imply (scientific) consensus	'people have considerable confidence in [claim]'
'if–then' constructions	'if we can assume that [assumption], then [claim]'
combined constructions	'as far as is currently known [claim], however [uncertainty], which implies that [implications/consequences of uncertainty]'.

Table 7 presents a selection of linguistic indicators which can be used for the verbal presentation of uncertainty information, together with some specific examples. However, different people use different terms for referring to different kinds of uncertainty or statistical information (such as 'certain', 'very unlikely'), so that the specific meaning of verbal uncertainty presentations can remain unclear. If linguistic indicators are used, they should therefore be clearly defined, and used consistently throughout the whole publication.

A prominent example of a clearly calibrated range of linguistic uncertainty indicators are the verbal uncertainty scales used in the 5th assessment report of the Intergovernmental Panel on Climate Change (IPCC) (Mastrandrea et al. 2010). Importantly, the IPCC distinguishes between two separate kinds of uncertainty:

1. The uncertainty of scientific evidence (level of confidence in the scientific understanding, expressed through verbal scales of qualitative judgement, see Figure 2).
2. The uncertainty of something occurring (the likelihood of occurrence of a single event or of an outcome, expressed as a verbal equivalent of numeric ranges, see Table 8).

For the first type of uncertainty, scientific evidence is qualitatively evaluated along two dimensions (see Figure 2):

1. Confidence in the validity of a finding, based on the type, amount, quality, and consistency of evidence (e.g., mechanistic understanding, theory, data, models, expert judgment) (summary terms: “limited,” “medium,” or “robust”).
2. Degree of agreement among experts on a finding (summary terms: “low,” “medium,” or “high”).

Confidence should not be interpreted probabilistically, and it is distinct from “statistical confidence.” A finding is seen as most robust when there are multiple, consistent independent lines of high-quality evidence.

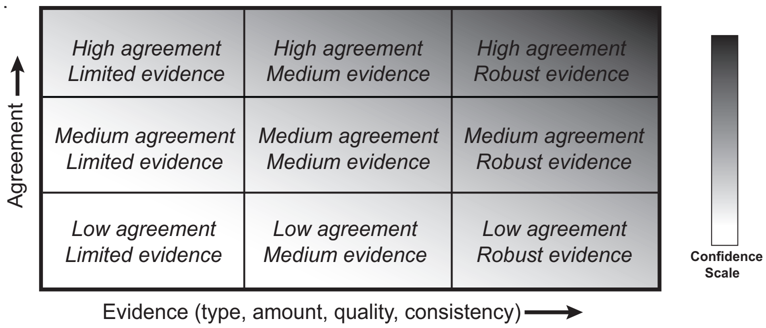

Figure 2: A depiction of evidence and agreement statements and their relationship to confidence, as used in the 5th assessment report of the IPCC (source: Mastrandrea et al. 2010). Confidence increases towards the top-right corner as suggested by the increasing strength of shading.

Table 8: Scale of linguistic likelihood indicators used in the 5th assessment report of the IPCC (source: Mastrandrea et al. 2010)

Linguistic indicators	Likelihood of the outcome
Virtually certain	99-100% probability
Very likely	90-100% probability
Likely	66-100% probability
About as likely as not	33-66% probability
Unlikely	0-33% probability
Very unlikely	0-10% probability
Exceptionally unlikely	0-1% probability

For the second type of uncertainty, the likelihood of something occurring is expressed on a verbal scale, where each expression corresponds to a likelihood range of the outcome (with 'fuzzy' boundaries between the ranges, see Table 8). Likelihood may be based on statistical or modelling analyses, elicitation of expert views, or other quantitative analyses. However, such a quantitative evaluation of uncertainty is only recommended for findings with high confidence. In case that a finding or variable is ambiguous, the underlying processes poorly known or not measurable, confidence should only be expressed based on the summary terms as shown in Figure 2.

Numerical presentation

Compared to verbal expressions, a numerical presentation of uncertainty has the advantage of being more specific, and potentially more detailed. At the same time, numbers can easily evoke the false impression of precision, and can also be more difficult to interpret. When using numbers (e.g., in form of a likelihood range or a confidence interval), it must be unambiguous what the number refers to:

(4) What does the numerical uncertainty information indicate (e.g., a 95% confidence interval)?
(5) What kind of uncertainties are included in the data?
(6) How these uncertainties were analysed?
(7) What has been omitted in this quantitative analysis (and why)?

Importantly, as pointed out by the IPCC recommendations (Wardekker et al. 2013), uncertainty should only be quantified if it is actually possible to do so. In case of unquantifiable uncertainties, any number would be misleading. Instead, it should be clearly indicated what the limitations and uncertainties are, and what the researchers do not know (such as 'unknown unknowns' or recognised ignorance, both of which cannot be quantified by definition).

Graphical presentation

A graphical presentation in form of figures has the advantages that it can summarise a large amount of information. At the same time, such as a figure may not be very intuitive to understand, and may lead to misinterpretations. In general, figures are better suited for directing the attention towards a particular point. When designing a graphical presentation of uncertainty, the following points should be considered:

- Figures should be easy to understand.
- The represented type of uncertainty should be clearly indicated.
- Suggestiveness and risk of misinterpretation should be avoided.

Some forms of uncertainty information are easier to communicate graphically than others. For example, it is quite common to have graphical representations of uncertainty ranges (such as a 95% confidence interval), which are thus more likely to be understood by a wide audience. In contrast, more abstract concepts, such as probability density functions, may be more difficult to understand, and require more careful explanation. The same holds for more specialised figures (such as a diagnostic diagram), even if they are not very complex per se.

4 Mapping of uncertainty in nexus-related models

In this section, we exemplarily apply the proposed guideline for multifaceted uncertainty analysis to three different types of models, all of which are used within the SIM4NEXUS project:

- System-dynamics model: The case study of Greece (section 4.1)
- Agroeconomic model: CAPRI (section 4.2)
- Simulation model of technology uptake: E3ME-FTT (section 4.3)

Each of the following sub-sections presents the uncertainty analysis for one of the respective models, which each focus on different types of uncertainty, and apply different methodologies for their analysis. In case of the newly developed system-dynamics model for the case study of Greece, the structural uncertainties of model assumptions are analysed along with parametric uncertainties, based on the methodology which was introduced in section 3. In case of the agroeconomic model CAPRI, the focus is on a quantitative analysis of scenario and parametric uncertainties, at the example of the Andalusia case study. In case of E3ME-FTT, the focus is on the analysis of structural model uncertainties with regard to the assumed technology choice behaviour of humans, and the resulting uncertain effectiveness of different policy instruments. For this purpose, a qualitative uncertainty is combined with a development of alternative model formulations, which replace the original assumptions on choice behaviour with an alternative description of human decision-making.

4.1 System-dynamics model: The case study of Greece

4.1.1 Short description of the Greek System Dynamics Model

The developed System Dynamics Model (SDM) for the Greek case study relies upon a detailed framework concerning the mapping and quantification of the interrelations of the five Nexus dimensions along with the detailed analysis behind each component. The analysis is characterized by a high spatio-temporal resolution, justified by the expansion of the relevant information from national scale to River Basin District (RBD) level and by elongating the time scale on a monthly basis. Greece is a Mediterranean country with high spatial variability in terms of climate conditions, resources' availability, and demographic dynamics; thus, the disaggregation of national data to RBD level—14 RBDs—is deemed necessary to conduct a thorough and sufficiently precise Nexus analysis.

Land use comprises the basic Nexus dimension in the SDM, containing the areas occupied by natural resources—forests, wetlands, grasslands—and by human-related activities such as cropland, livestock, and artificial areas. Cropland areas are connected to water, food, energy, and climate components through irrigation water demand, food production, energy demand, and Greenhouse Gas Emissions (GHGs), respectively. On the other hand, forests, wetlands, and grasslands operate as relievers to climate GHGs increasing carbon sequestration. ELSTAT, the Greek Statistical Authority, provided all the relative information concerning crop areas, crop types, irrigated crops or not, livestock areas, animal types, and animal heads in each RBD. Forest, wetland and grassland areas were provided by the Corine database. The SDM provides the ability to apply changes to land use and consequently it returns the impact on other dimensions through the aforementioned interlinkages; thus, one can realize the multi-dimension effects of adopting different land use policies.

The water dimension of the SDM involves surface and groundwater dynamic availability as a result of the balance between precipitation, water losses though evapotranspiration, runoff to the sea and several anthropogenic water stressing activities (agriculture, industry, household/commercial, power generation, and livestock). Especially for irrigation water, which consists the highest water consumer in Greece, matching crop types with precise seasonal irrigation needs and water losses with irrigation technologies renders it feasible to dynamically map irrigation demand. Population and tourism distribution on RBDs determine the household/commercial water demand, while industrial, power generation and livestock water demand are distinguished according to each RBD's potential in each subsector. Water is interlinked to energy and climate dimensions of the Nexus through several cause and effect pathways. Irrigation technologies used in the agricultural sector are mapped in the SDM, providing the ability to estimate the real irrigation needs while switching between the technologies results in different water demands. Pumping water is straightly connected to energy demand and consequently to GHG emissions. Additionally, wastewater resulting from wastewater treatment plants and industry, contributes to GHG emissions. Population and tourism dynamics pose the main regulator of wastewater, meaning that a possible change can induce different GHG emissions regimes. Eurostat, through the European open data portal, provided all the relevant datasets of the water subsectors in the SDM.

Food is treated as the product of crops and livestock activities mapped in the land dimension of the SDM. According to the crop type and the area it occupies in each RBD, food, feed, and industrial products arise as a function of surface unit multiplied by a crop type-oriented yield coefficient. Livestock products—meat, milk, eggs, and honey—arise as a function of animal heads multiplied by a yield coefficient customized according to the product type. In this way, agricultural products are quantified and distributed in each RBD, constituting an inventory map of agricultural products downscaled from national to RBD level. The food dimension apart from the quantities produced, contains the value of crop and livestock products as a function of production units multiplied by customized value coefficients, respectively. Both production quantities and corresponding value data, are provided by ELSTAT. Possible changes in food production are linked to different GHG emissions and different water demand regimes which lead to alterations in energy consumption.

The energy sector is modelled in the SDM both from the perspective of demand and generation. Oil, gas, coal, heat, biomass and electricity demands are quantified and mapped in all RBDs. These energy demand categories are divided in several subsectors such as the industrial, the household/commercial, the transportation, the agricultural, the power generation and other. Regarding power generation, all the electricity producing plants according to the fuel type they use (oil, coal, gas, biomass, renewables: solar, wind, hydropower) are mapped in each RBD. E3ME, a global, macro-economic model designed to address major economic and economy-environment policy challenges, provided all the relative data used in the SDM. Possible changes in energy demand are connected to climate through interlinkages with the GHG emissions, while other energy-related sectors such as water and food, play a decisive role both in energy demand and in GHG emissions.

Climate is a sector which is dealt as Greenhouse Gas Emissions (GHGs) coming mainly from fuel emissions and secondly from agriculture, livestock, Land Use, Land-Use Change and Forestry (LULUCF), and wastewater treatment. Eurostat, provided all the relevant GHG information on a national level, forming the basis on which disaggregation to RBD level relied. The SDM relates GHG emissions to every aforementioned source through several pathways that are mapped and quantified. Since climate can be affected by all other dimensions in the SDM, possible policy interventions on current land use, water, food, and energy components will affect GHG emissions.

The whole Nexus concept is underpinned by the interaction of the five components as well as the scale of information detail in each one, highlighting the SDM potential and effectiveness in depicting and valuating the flows among the Nexus dimensions. The outcome of the SDM indicates which components strongly affect others and which interlinkages are comparatively and relatively weak. Concluding, the SDM is a powerful tool that can be used to model complex systems. The resource Nexus for Water-Energy-Food-Land Use-Climate has been modelled for the national case study of Greece and the interlinkages among all Nexus dimensions are quantified in a user-friendly environment that is intended for use by policy-makers and stakeholders in a participatory process.

4.1.2Mapping the major uncertainties within the Greek SDM

The major assumptions made while building the Greek SDM are listed in Table 9, as in Table 10 they are mapped according to the three dimensions of the related uncertainty (as described in section 3.1.1). Following the mapping, the strength and level of impact for all assumptions are assessed, while for the ones that give out high risk, short descriptions are given on how these risks are retained to acceptable levels by fine tuning the assumption or by inserting a stochastic approach for key outputs. The detailed pedigree analysis of all model assumptions can be found in the Appendix (section 0).

As SDM is an accounting rather than a behavioural framework, the discussion on how the agents in the framework view uncertainty is not of primary relevance. Predictions in the model are based on modelling outputs provided by E3ME, so any agent-relevant assumptions included in the model are the ones "inherited" by E3ME (which are discussed in section 4.3). The role of agents (policy-makers) is addressed in one instant in Model assumption 14 (presented in section 4.1.3), in which the issue of implementation of decarbonization policies in Greece is discussed. Based on the recent history, it is highly uncertain that the targets proposed by the EU will actually be achieved without delay, since the timing of policy instruments and the corresponding vote by the Hellenic Parliament lags behind. Therefore, in this case that the agents' willingness to act plays a role, we chose to model the most conservative scenario, turning off all policies, as described in the assumption.

Model assumptions 1, 2 and 3 state that some variables are "not modelled", essentially describing approaches internal to the modelling effort. In reality, the assumption used instead is that the variables that are not modelled do change, but the changes they bring about occur at an "endpoint" of the model and do not have important feedback effects, so they do not significantly alter overall model results of the system; therefore, they can be ignored.

Table 9: List of major model assumptions which were made while building the Greek SDM.

Model assumption 1: The Nexus components that are interlinked to depict a holistic view of the sustainability status of a case study are Water, Land, Energy, Food, and Climate.
Model assumption 2: The food consumption subsystem is not modelled.
Model assumption 3: The urban land use proportioning is not modelled.
Model assumption 4: The GHG emissions model is simplified to be incorporated in the SDM, with yields that are calibrated to give out the forecasted GHG emissions.
Model assumption 5: The uniform distribution of water demand, water sources, energy demand, energy production and food production throughout space.
Model assumption 6: The temporally uniform distribution of water demand, water sources, energy demand, energy production and food production on a yearly basis.
Model assumption 7: Freshwater resources modelled as a whole, without the distinction between surface water and groundwater.
Model assumption 8: Classification of crops in 14 distinct crop categories.
Model assumption 9: Different yield coefficients of each crop type in each RBD were used as provided by the Hellenic Statistical Authority (ELSTAT) for base year 2010. Yield coefficients remain constant in time.

Model assumption 10: Different meat, milk, eggs, and honey yield coefficients per type of animal per head in each RBD were used as provided by the Hellenic Statistical Authority (ELSTAT) for base year 2010. Animal production yield coefficients remain constant in time.
Model assumption 11: Agricultural value of crop and livestock products is determined per unit of produced goods according to ELSTAT values for the base year 2010. The values per unit of agricultural products (crop, livestock) are kept constant through time.
Model assumption 12: The values of water losses coefficients for different irrigation technologies were set according to the suggested literature value ranges and calibrated to fit Greek reported agricultural water demand data.
Model assumption 13: The values of per capita residential and touristic water consumption were set according to suggested literature ranges and calibrated to fit reported urban water demands.
Model assumption 14: The definition of a base line scenario holds the assumption that de-carbonization policy cannot be taken for granted. Instead, a business as usual scenario is defined as the base line scenario.
Model assumption 15: The values of National Factors Power Plant were taken from E3ME model and are the same values for the whole Greece. These factors were categorized in 8 groups (Coal, Oil, Gas, Solar, Wind, Hydro and Biomass) and these values were used to estimate the electricity generated in GWh of each RBD of Greece by multiplying each factor with the corresponding value of each group.
Model assumption 16: The initial values of areas of land uses were taken by ELSTAT which was assumed to be the most trustworthy data source. The land uses were categorized into the following groups according to crop or livestock: fruits, rice, fodder permanent, fodder temporary, tobacco, cotton, sugar beet, pulses, potatoes, vegetables, olives, other cereals, citrus, maize and beehives, cattle heads, sheep heads, buffalos heads, goats heads, swine heads, horses/donkeys heads, rabbits heads, poultry heads respectively.
Model assumption 17: The monthly water demand for each crop was set according the literature based on data for Cyprus with the assumption that the water crops needs are the same in all the RBDs. The data were calibrated to fit the Greek water irrigation demand recorded by ELSTAT.
Model assumption 18: The values of Emission Factors were taken from E3ME model and are the same values for the whole Greece. The Emission Factors were categorized in 6 groups and each group was divided in more subgroups: Coal Emission Factors (Power Generation, ETS Industry), Gas Emission Factors (ETS Industry, non-ETS Industry, non-ETS Transportation, Household, Other), Oil Emission Factors (Power Generation, ETS Industry, non-ETS Industry, Other, Construction, Agricultural, Household, ETS Transportation, non-ETS Transportation), Biomass Emission Factors (Power Generation), Agricultural Factors (Cattle, Sheep/Goats, Swine, Horses/Donkeys, Manure, Rice, Managed Agricultural Soil, Field Burning, Urea) and LULUCF Factors (Cropland, Grassland, Forest, Wetlands).

Table 10. Mapping the assumptions of the Greek SDM according to the three dimensions of the related uncertainties.

Location/ Nature	**Level**					
	Statistical uncertainty		Scenario uncertainty		Recognized ignorance	
	Epistemic	Variability	Epistemic	Variability	Epistemic	Variability
Context		7			1, 2, 3	
Structure		5, 6		8, 14		4
Input		16, 17			9, 10	11
Parametric		12, 13, 15, 18				

Model assumption 1: Even though some Nexus literature is available on extending the list of Nexus components to include more elements such as ecosystems (European Commission 2019), or include soil and waste instead of energy and food (UNU-FLORES approach, see United Nations University 2019), we decided to assess the sustainability of resource use in the Greek case study using the five-element Nexus comprising Water, Energy, Food, Land Use and Climate, since it is holistic and captures the effects of sectors that are identified as important for Greece, namely water scarcity and antagonistic uses with tourism and agriculture, droughts and desertification, intense coal use and large Renewable Energy Source (RES) potential, etc. When assessing the Pedigree score criteria, Methodological rigour, Validation and Choice space are scored low since there is still a lot of ambiguity in the scientific community on how to assess nexus coherence and how to validate methodologies. To date, the resource Nexus has not been critically and systematically assessed in operational and well-defined terms and an implementable process for integration of the Nexus elements has not been proposed. Our list of five Nexus elements is intended to cover most interlinkages, relevant to a national case study, such as that of Greece.

Model assumption 2 mainly lies within the need to restrict the work effort and model complexity respectively to the project targets. Food consumption is speculated or known to have links with the rest of the processes modelled, however, it is a process that can be located at the end of its supply chain. The process itself might not be modelled, however its links to the rest of the processes exist in the SDM agnostically. For example, the energy and water demand for food consumption are inherent to the respective urban demands. This means that the SDM is capable of catching the trends of these demands as linked to population and tourism, but will not catch any change related to a potential dietary shift.

Model assumption 3 is made to keep the complexity of the SDM to a relatively manageable level. The land uses in Greece are considered settled when talking about high level categorization. This means that agricultural land is not expected to shift into urban, neither is (or at least to a very small extend) forests. The linked energy and water demands and GHGs emissions that are linked to the urban and industrial activities are not modelled as linked to the actual geographical extent of these land uses, but as linked to the activities taking place (such as transportation) and the population. The land use simulation was decided to instead be focused in increased detail regarding the agriculture, wetlands, forests, where dynamics are much more intense and policy making is expected to cause domino effects within the Nexus components

Model assumptions 4: The GHG emissions are currently estimated by a rather sophisticated and complex set of models. The incorporation of these models into the SDM would unjustifiably multiply the overall SDM complexity, taking into account that the purpose of this approach is to highlight the overall sustainability and sources efficiency and not accurately and exhaustively estimate every single component, parameter, and variable or sub system. Instead the links of GHG emissions to the related activities were assumed linear throughout, and were calibrated to yield the expected outputs as estimated and forecasted by specific climate models.

Model assumption 5 is one of the unacceptable assumptions that create risk in the danger zone. Greece is intensively variable – spatially and temporally — in water and energy demand, energy production, water resources availability, etc. Resources consumers such as agriculture, urban, industry and tourism are localized in different regions of Greece, thus assuming uniform distribution of the Nexus components and relevant processes, would insert very high uncertainty and very high impact across the model results. For this reason, in order to deal with such a high risk, the Greek case study increased modelling granularity to Water District level in regard of space and month time step in regard of time.

Model assumption 6: The seasonal variability in Greece regarding demand and consumption patterns and availability patterns of resources is intense. Two main drivers of the seasonal variability are the touristic activity which massively determines energy, and water consumption and the weather witch directly determines water availability, food production and land uses, thus water and energy demand. The assumption of annually uniform distributions of demands and availability inserts an unacceptable level of risk in the model as it dominantly determines all the model outputs. For this reason, it is decided that the model time step is monthly and not annually, which offers a more precise temporal granularity and is capable of catching the temporal variability in resources efficiency, such as the summer water scarcity danger, especially in Greek islands region, the danger of energy black outs the over exploitation of water during the irrigation periods etc.

Model assumption 7: The initial assumption of not distinguishing groundwater and surface freshwater resources and modelling them as a whole inserts an unacceptable error in the estimation of the related energy consumption for transferring and pumping the water. Groundwater needs pumping which is energy consuming, while the amount of energy demand is related to the level of the aquifer. On top of that the level of groundwater is also related to the quality of water since very low levels in regions where groundwater resources are overexploited allow sea intrusion and increase of salinity which deteriorates the quality of water and increases the treatment needs. For retaining the risk that holds within these uncertainties among others, it is decided to simulate distinctively surface and groundwater, through a water cycle chain that incorporates surface water, groundwater, the communication of these two, run-off to the sea, withdrawals for all uses and return, and precipitation.

Model assumption 9: Yield coefficients for the calculation of agricultural production are well documented in the literature, so proxy is scored high. It is also clear that yields might be affected by improved agricultural conditions, so theoretical understanding, justification, and agreement among peers are scored relatively high. Not much specific information is available on how yields will be affected by new technologies and/or other conditions and what these conditions might be in the coming decades. Thus, methodological rigour and validation are scored with 2, while empirical basis and choice space are scored relatively low, since no distinct methodology for yield evolution in time currently exists. An added level of complication is the fact that yield coefficients vary spatially among RBDs. Besides, keeping yield coefficients constant remains a relatively safe assumption and does not greatly affect model results, as it is not expected to change dramatically in the coming decades.

Model assumption 10: Livestock yield coefficients for the calculation of meat, milk, eggs, and honey production are well documented in the literature, so proxy is scored high. It is also clear that livestock yields might be affected by future conditions including improved animal feeding, animal dietary supplements, slaughtering practices to meet market demands, etc., so theoretical understanding, justification, and agreement among peers are scored relatively high. Not much specific information is available on how livestock yields will be affected by more effective feeding regimes, new technologies and/or other conditions and what these conditions might be in the coming decades. Thus, methodological rigor and validation are scored with a 2, while empirical basis and choice space are scored relatively low, since no distinct methodology for livestock yield evolution in time currently exists. Besides, keeping livestock yield coefficients constant remains a relatively safe assumption and does not greatly affect model results, as it is not expected to change dramatically in the coming decades.

Model assumption 11: Agricultural value per crop/livestock unit for the calculation of total agricultural value in the Greek case study is assumed to stay constant throughout the modelling period and the corresponding values of base year 2010 are used. There is no uncertainty in the representation of the variable, so proxy is scored high; the same is true for theoretical understanding, since there is no ambiguity on the fact that values will fluctuate in the coming years. There is however a lot of speculation on how the global market might influence agricultural product prices, so empirical basis is found relatively speculative. All other pedigree scoring criteria are set to 2, since such economic models are based on market equilibrium, they are enormously complex, they are influenced by a large number of factors including geo-political conditions that are difficult to predict and often fail to give accurate predictions. Without a doubt, our SDM will greatly improve with a layer that includes forecasts of agricultural values based on different SSPs, but this is not the type of analysis that we can conduct with given resources. MAGNET is the thematic model that may be able to address this shortcoming and provide future agricultural product pricing trends, so this maybe something that we will include in the SDM in the future.

For the **model assumption 12**, 100 Monte Carlo simulation runs were executed for the sensitivity and uncertainty analysis. For the sensitivity analysis the “Sensitivity Index” of the three water loss coefficients was calculated which indicated that Sprinkler loss coefficient affects the agricultural water demand of Thessaly the most (Table 11). Furthermore, a tornado diagram was plotted showing the 5% and 95% of agricultural water demand range while the three loss coefficients (Drip, furrow and Sprinkler) are changing (Figure 3 and Figure 4).

Table 11: Sensitivity Index of Water Loss Coefficients of Thessaly (model assumption 12).

Loss coefficients	Sensitivity index
SPRINKLER	0.199
FURROW	0.074
DRIP	0.061

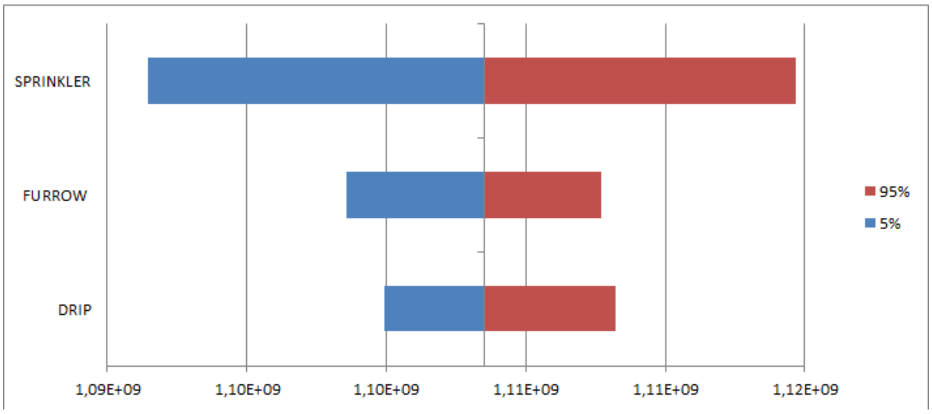

Figure 3: Tornado plot for the influence of the 3 loss coefficients of Thessaly (for a tested range of +/- 10% of the assumed value) in the respective agricultural water demand in m^3, expressed by bars from 5% to 95% percentiles of the distributions (model assumption 12).

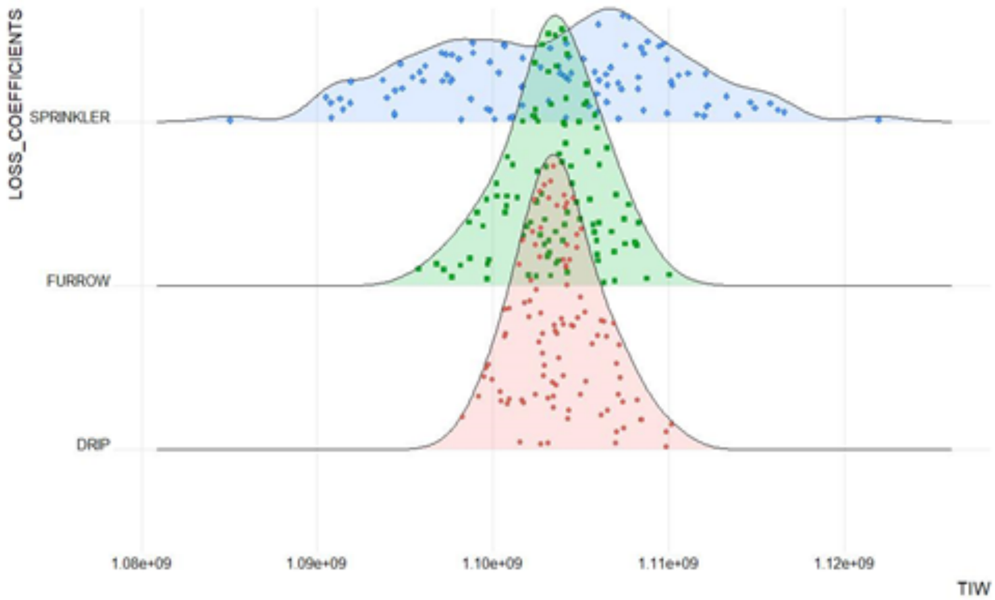

Figure 4: The influence of the three loss coefficients for River Basin District of Thessaly GR08 (for a tested range of +/- 10% of the assumed value) in the respective Total Irrigated Water (TIW) in m^3, expressed by the equivalent distributions (model assumption 12).

For **model assumption 13** the calculated Sensitivity Index revealed that touristic water consumption per capita has much less impact on the total household/commercial water consumption of GR08 (Thessaly) than the residential one (Table 12). The results are reinforced after the analysis of using 5% and 95% percentiles in order to get the impact of the parameter variables into the total household/commercial water consumption of GR08 - the output (Figure 5 and Figure 6).

Table 12: Sensitivity Index of per capita household and touristic household/commercial water consumption of Thessaly (model assumption 13).

Per capita household and tourist household/commercial water consumption	Sensitivity Index
Per capita household water consumption	0.991
Per capita tourist water consumption	0.009

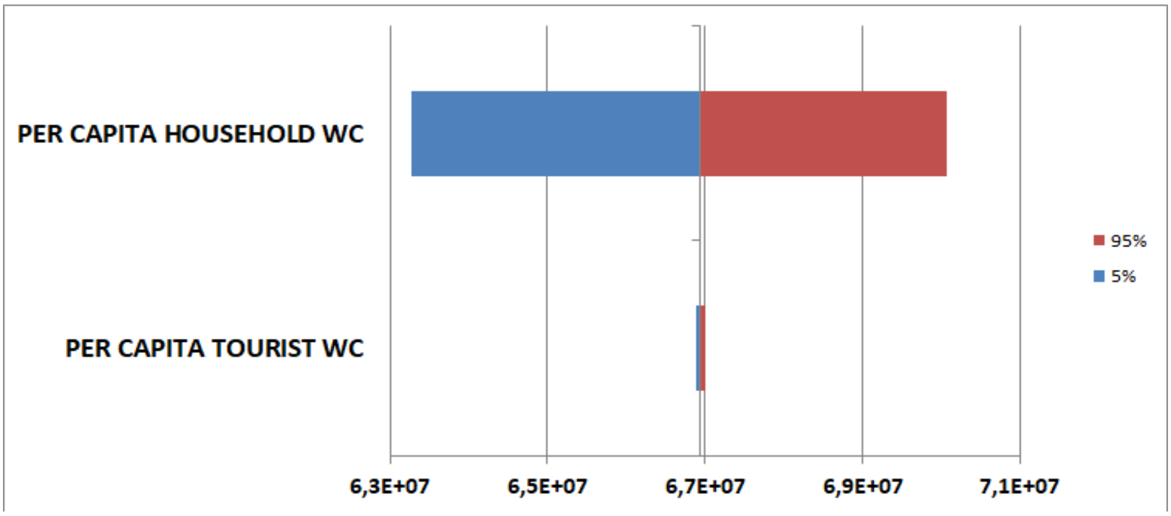

Figure 5: Tornado plot for the influence of the per capita household/commercial and tourist water consumption (for a tested range of +/- 10% of the assumed value) in the respective total household/commercial and tourist water consumption in m^3, expressed by bars from 5% to 95% percentiles of the distributions (model assumption 13).

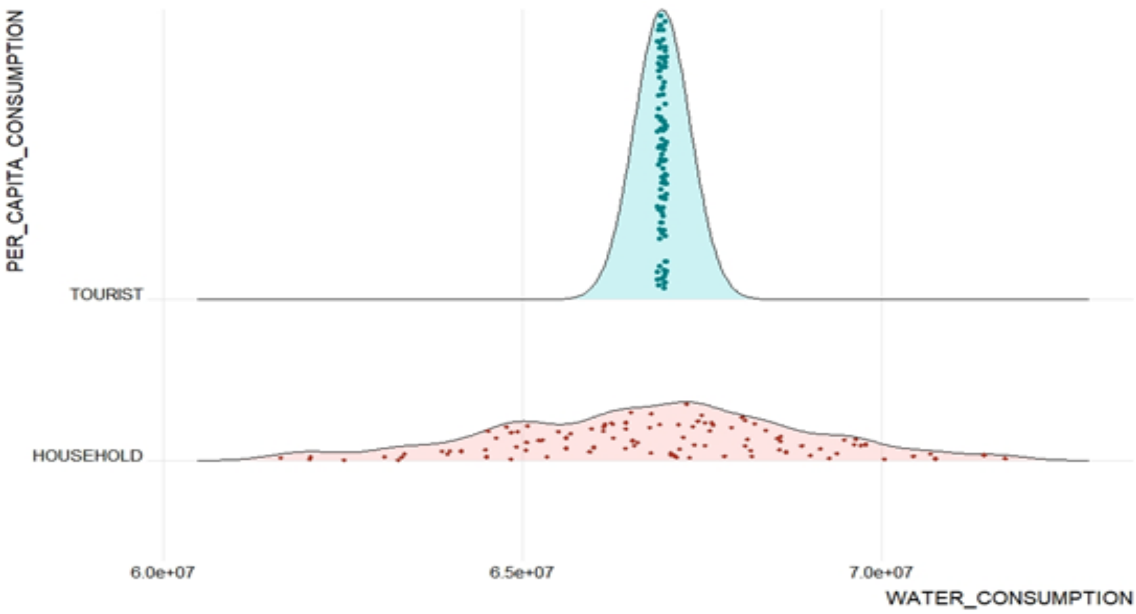

Figure 6: The influence of per capita household/commercial and tourist water consumption (for a tested range of +/- 10% of the assumed value) in the respective total household/commercial water consumption in m^3, expressed by the equivalent distributions (model assumption 13).

Model assumption 14: The uncertainty that lies within the forecasting regarding the implementation of the decarbonisation policies in the future, as well as to what extend and how successfully creates high risk for the outputs of the SDM. The choice of defining business as usual as a baseline scenario and not a de-carbonization one is speculated to be more realistic by all, peers and stakeholders, while on top of that it gives outputs that are on the safe side, rather than overoptimistic. However, other scenario will also be modelled, including the de-carbonization policies, so that the outputs are more indicative of the whole picture and constitute a tool for helping policy makers understand the benefits and drawbacks of alternative future policy scenarios.

For **model assumption 15** the calculated Sensitivity Index revealed that Hydro and Wind affect the total electricity generated in GWh of GR08 more than Gas, Solar, Oil (Table 13). Biomass and Coal have 0 values so they are not part of this analysis. The results are reinforced after the analysis of using 5% and 95% percentiles in order to get the impact of the parameter variables into the total household/commercial water consumption of GR08 - the output (Figure 7 and Figure 8).

Table 13: Sensitivity Index of National Factors Power Plants for RBD GR08 (Thessaly) (model assumption 15).

National factors power plant	Sensitivity index
HYDRO	0.689
WIND	0.178
GAS	0.051
SOLAR	0.049
OIL	0.034

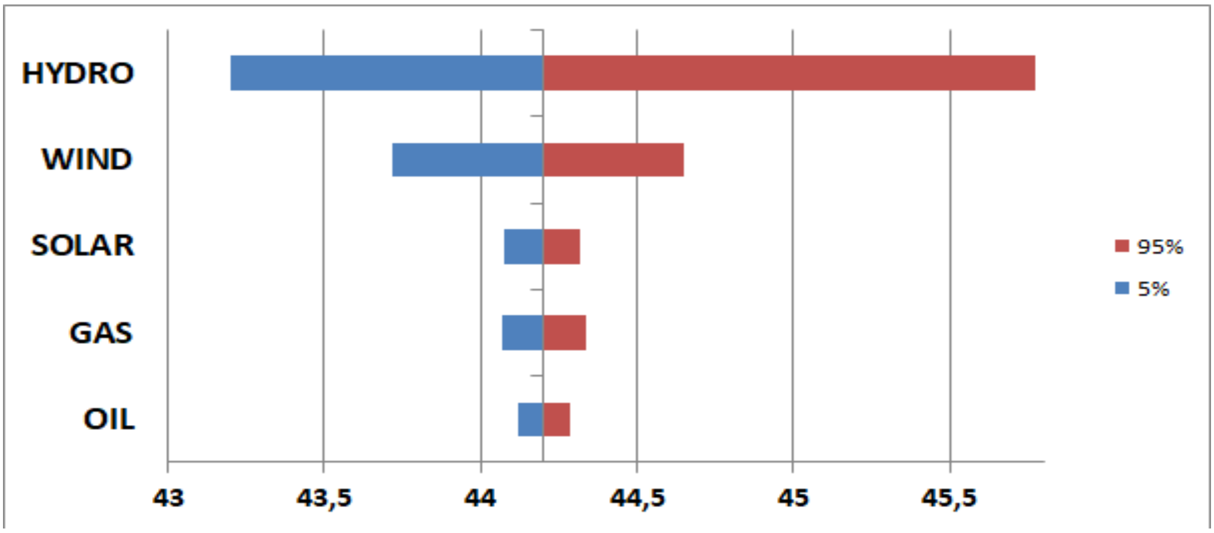

Figure 7: Tornado plot for the influence of the 5 National Factors Power Plant (for a tested range of +/- 10% of the assumed value) in the respective total electricity generated in GWh for GR08 (Thessaly), expressed by bars from 5% to 95% percentiles of the distributions (model assumption 15).

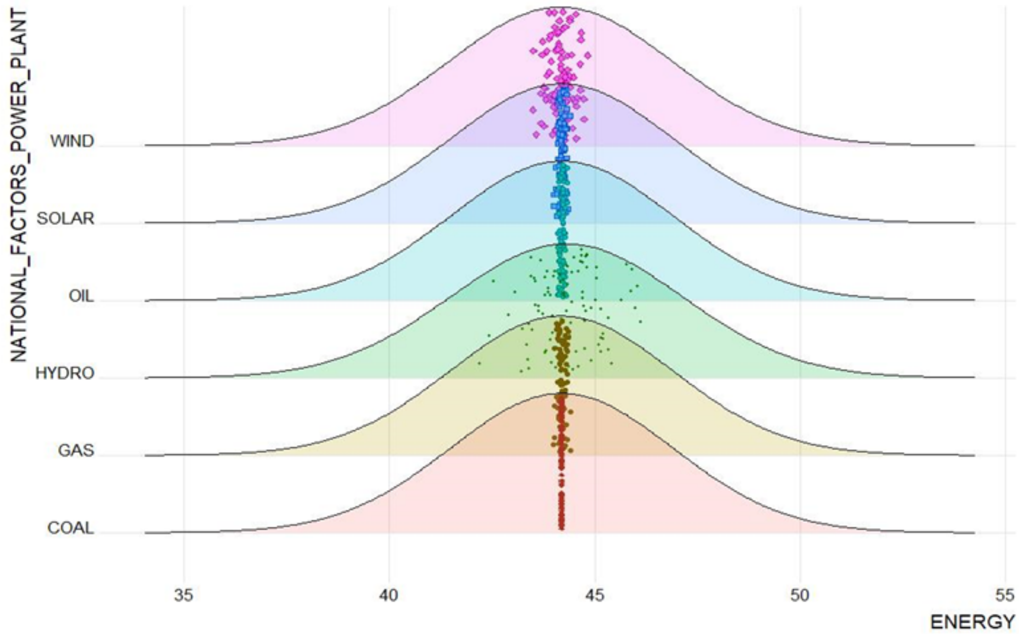

Figure 8: The influence of the 5 National Factors Power Plant (for a tested range of +/- 10% of the assumed value) in the respective total electricity generated in GWh for GR08 (Thessaly), expressed by the equivalent distributions (model assumption 15).

Model assumption 16: To quantify the uncertainty of this assumption, 100 Monte Carlo simulation runs were executed and a sensitivity analysis was conducted at first level. For the sensitivity analysis the "Sensitivity Index" of both categories was calculated which indicated the most sensitive inputs (Table 40 and Table 41 in the Appendix). For the first category (14 crop areas of Greece) we had a national analysis and we concluded that the most sensitive inputs are cotton and fodder permanent (Figure 9 and Figure 10). On the other hand, we had an analysis for GR08 (Thessaly) in order to get the most sensitive inputs of nine livestock and the results indicated that sheep heads, cattle heads and swine heads were the most sensitive ones (Figure 11 and Figure 12).

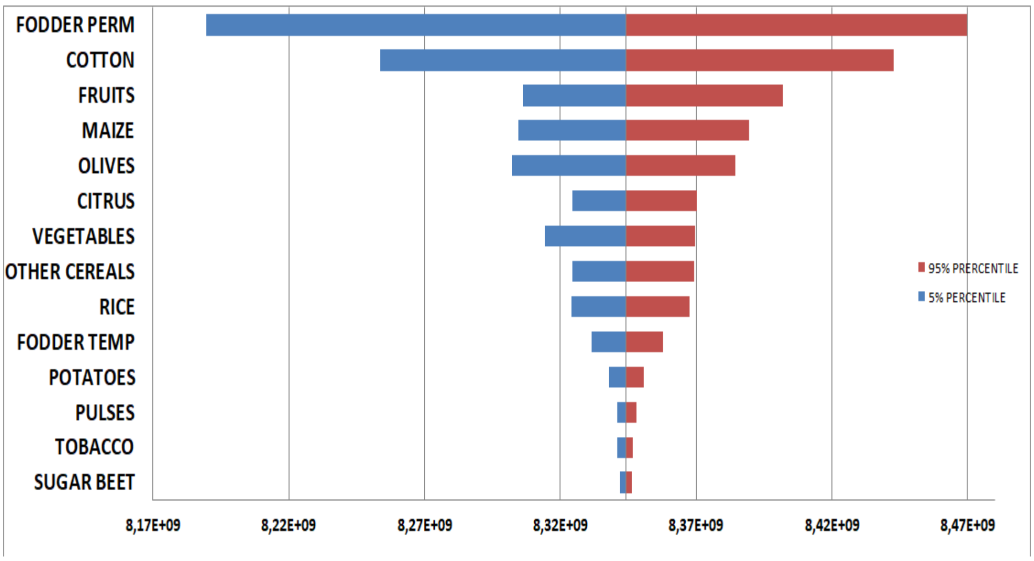

Figure 9: Tornado plot for the influence of cropland area for 14 different crops in Greece—national level (for a tested range of +/- 10% of the assumed value) in the respective agricultural water demand in m^3, expressed by bars from 5% to 95% percentiles of the distributions (model assumption 16).

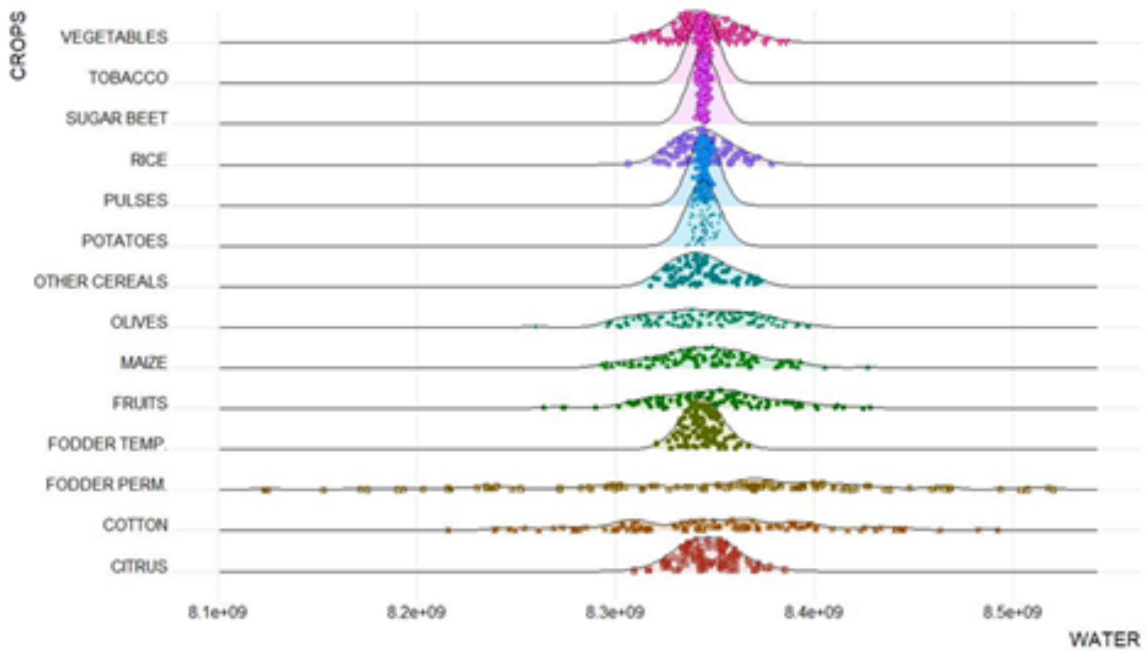

Figure 10: The influence of cropland area for 14 different crops in Greece—national level (for a tested range of +/- 10% of the assumed value) in the respective agricultural water demand in m^3, expressed by bars from 5% to 95% percentiles of the distributions (model assumption 16).

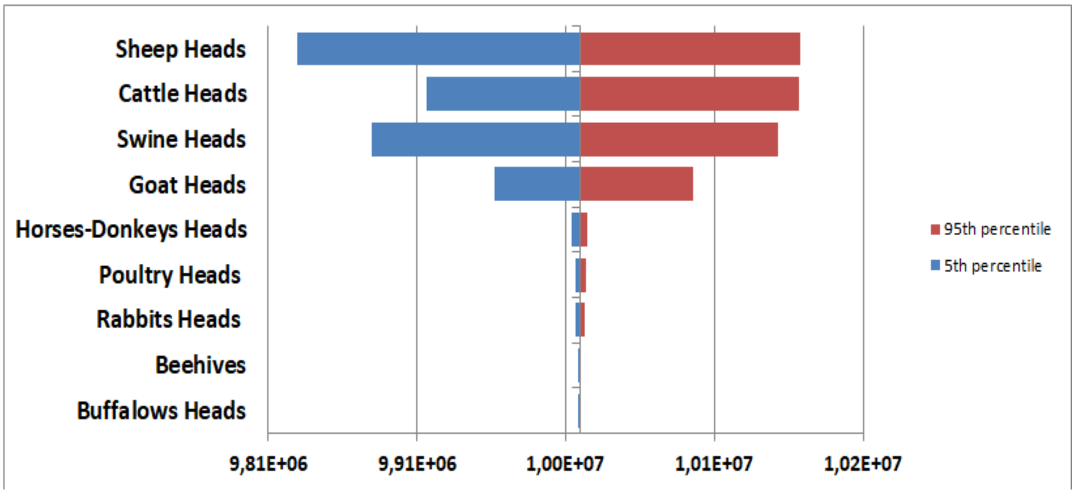

Figure 11: Tornado plot for the influence of the nine livestock of Thessaly (for a tested range of +/- 10% of the assumed value) in the respective livestock water demand in m^3, expressed by bars from 5% to 95% percentiles of the distributions (model assumption 16).

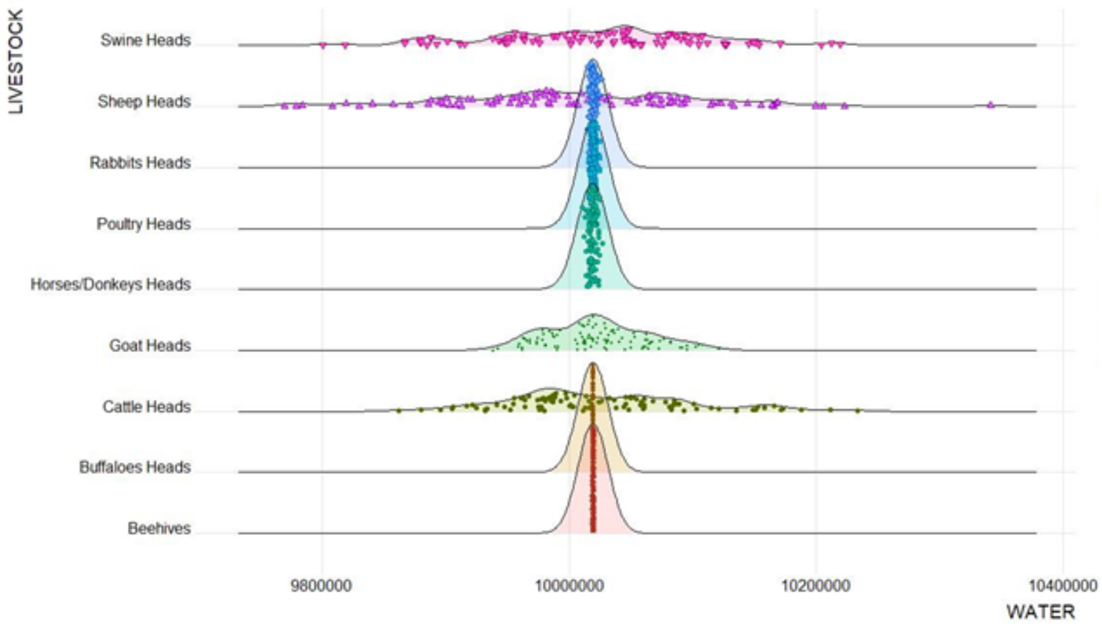

Figure 12: Distributions of total Greek agricultural water demand in m^3 for the respective distributions of the two more influential crop areas input variables for the Greek water district (model assumption 16).

For **model assumption 18** the calculated Sensitivity Index revealed that non-ETS Transportation (Oil), Managed Agricultural Soil (Agri), Household (Oil), ETS-Industry (Oil) affect the total emissions of GR08 more than emission factors (Table 42 in the Appendix). Also we calculated 5% and 95% percentiles in order to get the impact of the parameter variables into the total emissions of GR08—the output (Figure 13 and Figure 14).

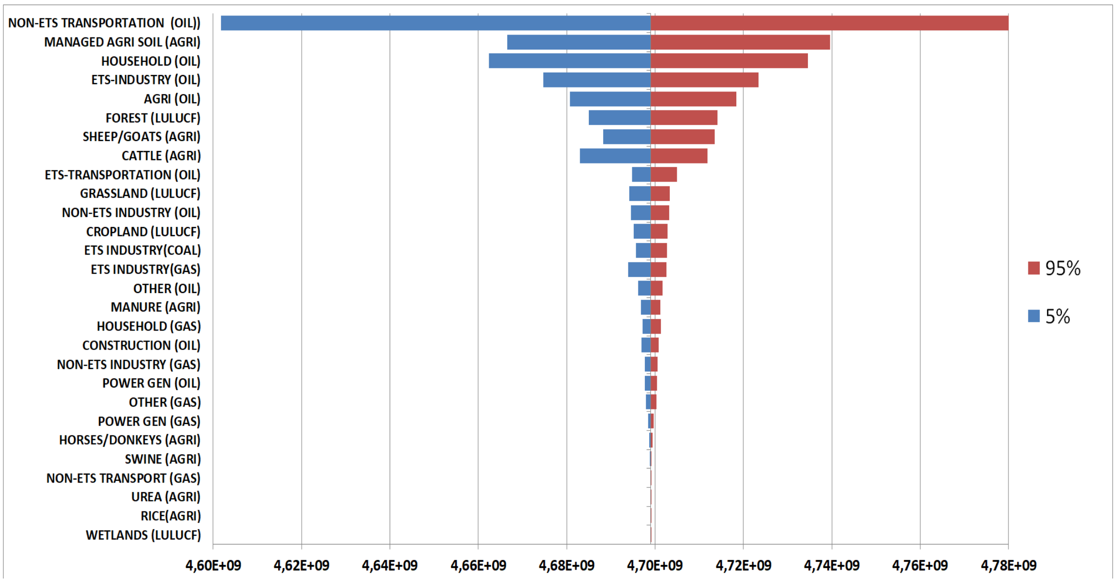

Figure 13: Tornado plot for the influence of the 28 subgroups of Emission Factors (for a tested range of +/-10% of the assumed value) in the respective total Emissions of GR08 (Thessaly) in kg, expressed by bars from 5% to 95% percentiles of the distributions (model assumption 18).

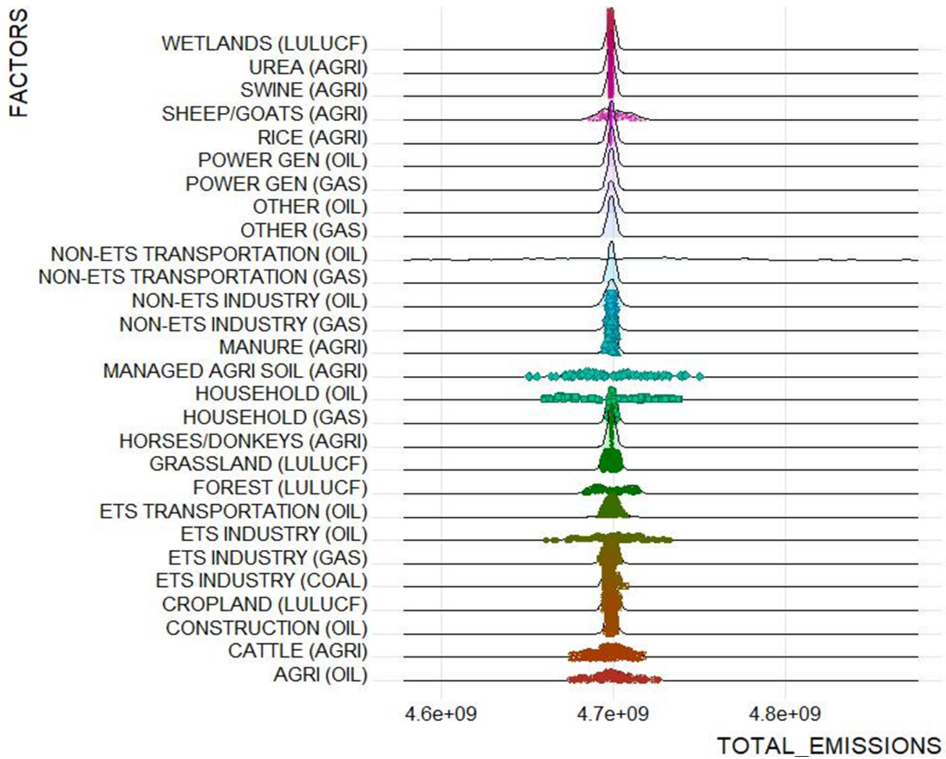

Figure 14: The influence of the 28 subgroups of Emission Factors (for a tested range of +/- 10% of the assumed value) in the respective total Emissions of GR08 (Thessaly) in kg, expressed by the equivalent distributions (model assumption 18).

4.2 Agroeconomic model: CAPRI

CAPRI is a comparative-static global spatial partial-equilibrium model for the agricultural sector built for ex-ante impact assessment of agricultural, environmental and trade policies with a focus on the European Union (Britz and Witzke 2014). The model is solved by iteration of supply and market modules.

The supply module draws on regional agricultural nonlinear programming models for the EU-28, Norway, Turkey and Western Balkans, which captures farming decisions in detail at sub-national level (NUTS 2 level). The market module is a deterministic global spatial model that simulates supply, demand, and price changes in global markets considering bilateral trade flows and trade policies. The module covers a wide range of primary and secondary agricultural products (i.e. around 60 commodities) and 40 trade blocks.

Model results cover crop areas, herd sizes, production, consumption, trade, income indicators and environmental indicators (NPK balances, greenhouse gas emissions, water use). Agricultural GHG emissions are calculated in CAPRI following the Intergovernmental Panel on Climate Change (IPCC) guidelines. For EU regions, emissions per activity are calculated endogenously in the supply module, whereas for non-EU regions emissions are estimated per product for marketable agricultural commodities. Irrigated and livestock water use are computed at the NUTS 2 level in the CAPRI water module, which is part of the supply module (Blanco et al. 2015, 2018).

To account for food-water interactions, the water module simulates irrigation and livestock water use at the NUTS 2 level within the EU (Blanco et al. 2015, 2018). The land balance in CAPRI distinguishes between irrigable and non-irrigable land. Crop activities are divided into rain-fed and irrigated variants, and corresponding input-output coefficients are estimated for each variant. Water is considered a production factor both for rain-fed and irrigated agriculture. Livestock water use is computed based on data on water requirements per livestock category and per head (drinking water and services water) from different sources and length of the production period.

CAPRI can be viewed as a deterministic model and, therefore, uncertainty is not considered in an explicit way. Nevertheless, CAPRI reproduces observed behaviour of the agents through calibration of the model to observed data and external projections (from other models or institutions, i.e. the EU), which implicitly consider uncertainty on agent decisions. Therefore, while CAPRI is an optimization and equilibrium model, it is used in a positive way (and not in a normative way). The application of calibration techniques ensures perfect calibration to current and projected agricultural market situations.

4.2.1 CAPRI and its application to the Andalusia case study

Within Sim4Nexus, the CAPRI model is applied to the Andalusia case study to assess the effects of agricultural and environmental policies on agricultural production, prices and income, and environmental indicators including water use. Those effects are analysed in a comparative-static framework, where the simulated results are compared to a baseline scenario.

The CAPRI baseline scenario depicts the projected agricultural situation up to 2050 under a policy status quo. The baseline builds on the medium-term outlook for EU agricultural markets and income for mid-term projections. In terms of policies, it represents in detail the CAP 2014-2020 and the commitments under the Uruguay Round Agreement on Agriculture regarding market access and subsidies. For long-term projections, the baseline assumes SSP2 developments and accounts for climate change impacts on agriculture under RCP 6.0.

4.2.2 Focus of the uncertainty analysis

The application of the CAPRI model for the evaluation of the water-food nexus in Andalusia entails a degree of uncertainty. Various sources of uncertainty can be identified, including model formulation, input data and parameters and scenario definition. The analysis of uncertainty is an essential step in model development (Walker et al. 2003) and systematic sensitivity analysis is recommended not only to evaluate the uncertainty in model results, but also to identify its key drivers (Saltelli et al. 2008)

However, performing uncertainty analysis in large-scale economic models, such as CAPRI, which covers many parameters and different methodological solutions, is far from trivial. A global sensitivity analysis that considers cross-effects between parameters will involve a large number of simulations and, therefore, might be unrealistic. Many sensitivity analyses relating to parameter uncertainty rely on Monte Carlo methods. One of the problems with this probabilistic approach is the curse of dimensionality if we have multi-variate distributions, where the number of simulations increases exponentially. Applying a Monte Carlo approach to a large-scale modelling system such as CAPRI is very demanding in terms of time and computing capacity. In addition, economic models comprise sets of parameters that are not independently distributed (i.e., supply and demand systems must satisfy certain conditions) and, therefore, random draws may lead to implausible parameter distributions.

To date, very few systematic sensitivity analyses have been performed with CAPRI. The difficulty to define the appropriate random draws, the extremely high computation time and the correlation between the results, are some of the reasons behind.

Given the complexity and size of the model, only a focused sensitivity analysis is reasonable for most applied research purposes. As an alternative to the probabilistic approach, here we therefore demonstrate the application of local sensitivity analysis to CAPRI. Under this approach, instead of assuming probability distributions for the parameters, we assume a set of plausible values, and then change one parameter at a time. The aim of the analysis is to measure how sensitive the results are with respect to the changes in parameter values. We therefore simulate perturbations around the parameters' values to derive the quantitative impact on the results. By means of this sensitivity analysis, we can identify those parameters with a larger impact on model results. Alternatively, we can investigate the effects on model results of changes in the values of those parameters assumed to be more uncertain.

4.2.3 Local sensitivity analysis for future water scenarios

As mentioned above, CAPRI is a large economic model involving thousands of input and output parameters. The sensitivity of each model output to the input factors may be very different. Therefore, we will focus the analysis on a reduced set of parameters, which were identified as being relevant for the application of the CAPRI model to the Andalusia case study.

The first step to undertake the sensitivity analysis was to identify the parameters that, being surrounded by uncertainty, could have a high impact on model results.

Since the CAPRI model simulates the agricultural situation until 2050, uncertainty about future scenarios is prominent. For defining the baseline scenario up to 2050, we use assumptions on future developments for a large variety of scenario parameters, including macroeconomic drivers, technological developments, food demand, input and output prices, etc. In addition, we assume a climate scenario, which is defined by the shared socioeconomic pathway “middle of the road” (SSP 2) and the representative concentration pathway 6.0 (RCP 6.0). Projections of model parameters related to all those scenario assumptions are subject to scenario uncertainty.

Since applying the sensitivity analysis to thousands of parameters would exceed the scope of this study, we decided to focus at a limited set of parameters, selecting those crucial for the analysis of the water-energy-food nexus in Andalusia.

The close interconnection between water use and food production is one of the main social concerns in this region. Limited water availability influences food production, and climate change is likely to increase competition for the limited water resources of the region. As a result, irrigation water prices will likely increase in the future. These two interconnected drivers, irrigation water availability and irrigation water price, are therefore selected for the sensitivity analysis.

While many other parameters are also relevant, there are some more reasons to focus at water parameters. First, projections for water parameters are not easily available from other models/institutions, as it is the case for food prices or macroeconomic developments. Second, uncertainties about climate projections and socioeconomic pathways have already been analysed in previous studies (Araujo-Enciso et al. 2016;Blanco et al. 2017). Last, while the need of integrating water considerations in climate impact studies is widely recognized, applications to date are scarce.

Therefore, in this study, we will focus on uncertainties related to future water developments. While it is generally acknowledged that climate change will very likely have an impact on water availability and price, information on future trends is scarce.

In Andalusia, high uncertainty exists on the future development of water availability and water prices. To what extent would a change in these parameters influences the results of the model?

To address this question, we defined two sets of scenarios. In the first one, we implemented a decrease in irrigation water availability compared to the baseline specification, ranging from 2% to 12% in equal steps. In the second set of scenarios, we simulated an increase in irrigation water prices, ranging from 0.02 €/m3 to 0.12 €/m3 in equal steps. Table 14 summarizes the scenario framework.

Table 14: Sensitivity analysis framework for the analysis of CAPRI.

Scenario name	Parameter: Irrigation water availability (m^3)	Scenario name	Parameter: Irrigation water price (€/m^3)
base	Baseline assumption	base	Baseline assumption
wa02	2% reduction from baseline	wp02	0.02 €/m^3 increase from baseline
wa04	4% reduction from baseline	wp04	0.04 €/m^3 increase from baseline
wa06	6% reduction from baseline	wp06	0.06 €/m^3 increase from baseline
wa08	8% reduction from baseline	wp08	0.08 €/m^3 increase from baseline
wa10	10% reduction from baseline	wp10	0.10 €/m^3 increase from baseline
wa12	10% reduction from baseline	wp12	0.12 €/m^3 increase from baseline

As the model parameters for water availability and water prices were only changed for Andalusia, we run the CAPRI model assuming no changes in food prices. We are thus assuming no changes in all other regions in CAPRI, and we are also assuming that changes in Andalusia will have no effect on other regions. Hence, it is important to keep in mind that the aim of this exercise is to perform a sensitivity analysis, and that the results must be interpreted in that way. If we were executing a water scenario, then we would have to consider that future water developments will have consequences for many regions and, therefore, we would have to account for cross-effects.

Looking first at model results with reduced water availability, we observe that irrigation water use decreases accordingly (Figure 15). However, not all crops are equally affected. While cereals and olive groves reduce the use of water, fruits and vegetables continue to use almost the same water volume.

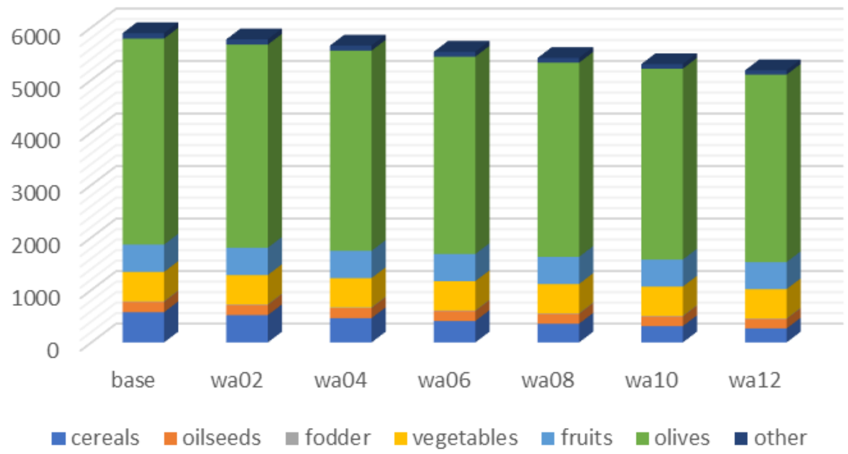

Figure 15: Sensitivity of irrigation water use (in Hm3) to changes in water availability. Source: own elaboration from CAPRI simulations for Andalusia in 2030.

The decrease in water use leads to a decrease in the irrigated area at the expense of the rainfed area (Figure 16).

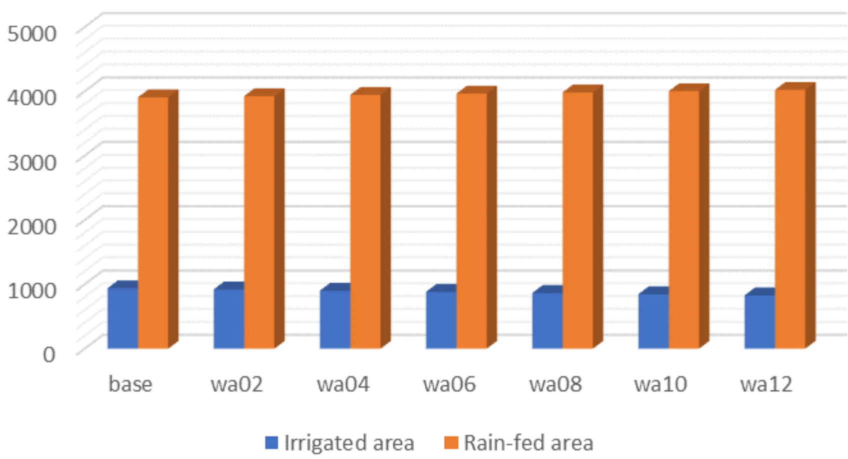

Figure 16: Sensitivity of irrigated and rainfed area (in thousand hectares) to changes in water availability. Source: own elaboration from CAPRI simulations for Andalusia in 2030.

Again, not all crops are equally affected. The irrigated area of fruits and vegetables remains almost constant. In contrast, cereals and olive groves shift from irrigated to rainfed production systems (Figure 17).

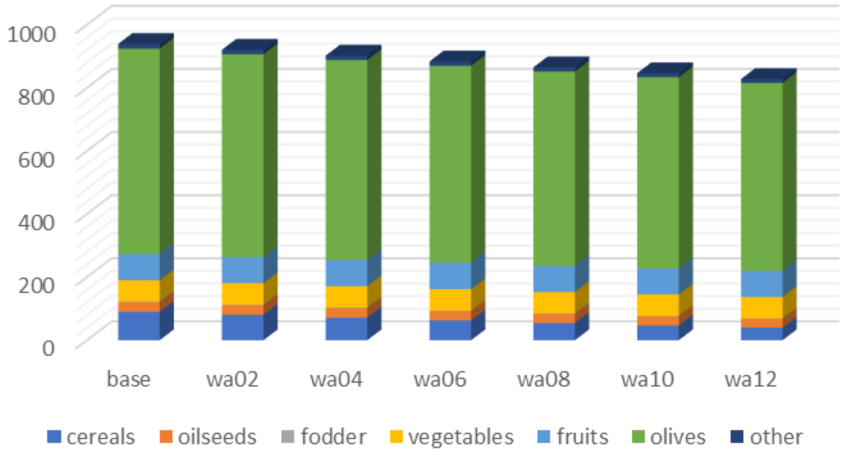

Figure 17: Sensitivity of irrigated area (in thousand hectares) to changes in water availability. Source: own elaboration from CAPRI simulations for Andalusia in 2030.

Looking now at model results with increasing water price, we observe more drastic model changes (Figure 18). As the water price increases, irrigation water use decreases noticeably. The decrease is more prominent for cereals and olive groves, but other crops such as oilseeds are also significantly affected. In contrast, water use hardly decreases for fruits and vegetables.

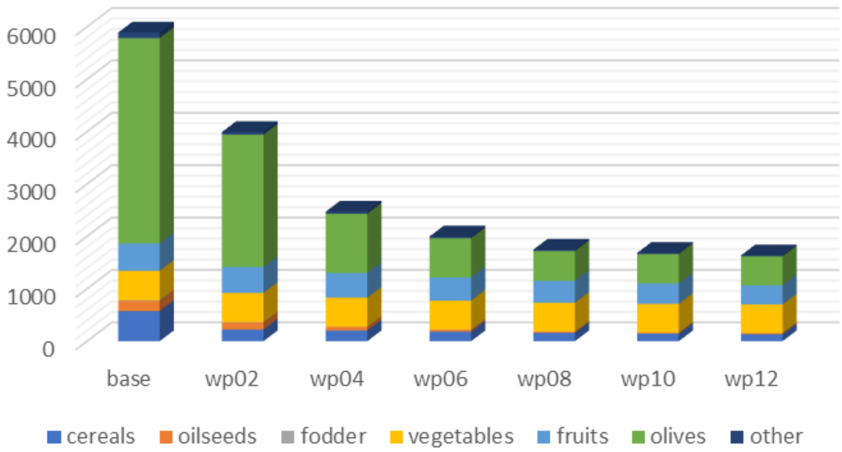

Figure 18: Sensitivity of irrigation water use (in Hm3) to changes in water price. Source: own elaboration from CAPRI simulations for Andalusia in 2030.

As a consequence of the increase in water price, the irrigated area decreases significantly at the expense of the rainfed area (Figure 19).

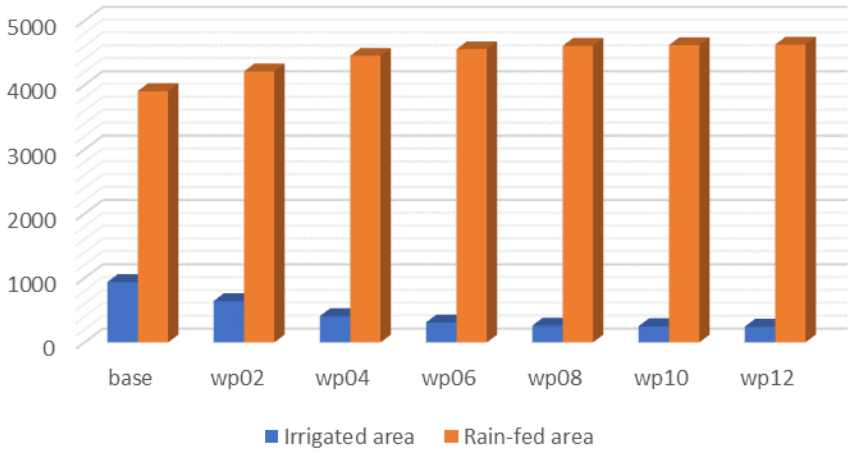

Figure 19: Sensitivity of irrigated and rainfed area (in thousand hectares) to changes in water price. Source: own elaboration from CAPRI simulations for Andalusia in 2030.

Olive groves, which account for the largest irrigated area in Andalusia, are affected the most. Cereals also experience a large shift from irrigated to rainfed production systems. Fruits and vegetables can afford higher water prices (and cannot survive without irrigation) and, therefore, are not significantly affected (Figure 20).

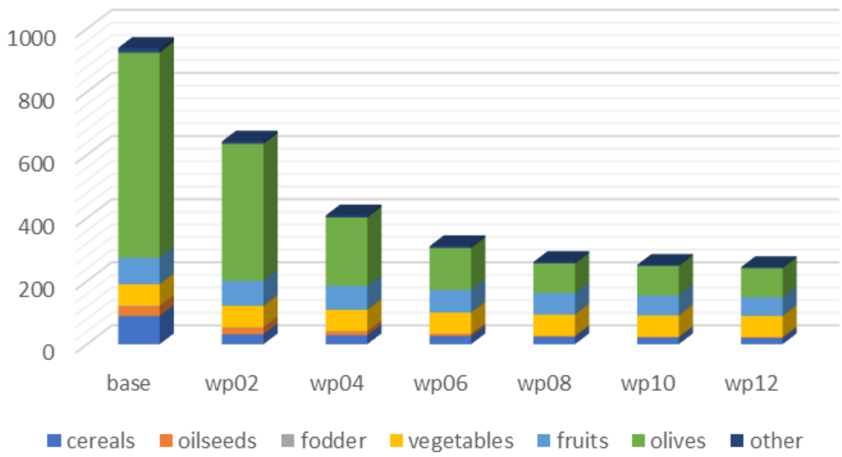

Figure 20: Sensitivity of irrigated area (in thousand hectares) to changes in water price. Source: own elaboration from CAPRI simulations for Andalusia in 2030.

The results of this sensitivity analysis highlight the importance of having adequate projections about future availability of water. In this sensitivity exercise, we have changed one parameter at a time and, therefore, the results should be interpreted accordingly. It is important to note that the sensitivity of model results to water prices differs from the effects of a water pricing policy. Water availability, water prices and irrigation technologies are interconnected and, therefore, defining a water pricing policy implies taking account of those interrelations.

4.3 Simulation model of technology uptake: E3ME-FTT

The E3ME-FTT-GENIE model is a simulation-based integrated assessment model, based on the descriptive modelling of dynamical human and natural behaviour, driven by empirically-determined relationships. At its core is the macroeconomic model E3ME, which represents aggregate human behaviour through a chosen set of econometric relationships that are regressed on the past 45 years of data and are projected 35 years into the future (until 2050). The macroeconomics in the model determine total demand for manufactured products, services and energy carriers in 61 world regions covering the globe.

Meanwhile, technology diffusion is simulated by bottom-up sub-models of technology uptake, the FTT family of technology modules. They determine changes in the environmental intensity of economic processes, including changes in amounts of energy required for transport, electricity generation and household heating. Since the development and diffusion of new technologies cannot be well modelled using time-series econometrics, cross-sectional datasets are used to parameterise choice models in FTT.

Finally, the combustion of fuels leads to greenhouse gas emissions, which impact the climate system. To determine these climate impacts, the global emissions as simulated by E3ME-FTT are fed to a carbon cycle-climate system model of intermediate complexity, the GENIE model.

Importantly, as a simulation-based model E3ME-FTT does not aim at optimising the decision-making of agents or future states of the system. There is thus no need to assume perfect knowledge and optimising behaviour. E3ME-FTT therefore allows for the possibility of fundamental uncertainty (see section 2.5), and assumes that agents make decisions based on imperfect knowledge.

A full description of the integrated model E3ME-FTT-GENIE is available in Mercure et al. (2018), while the E3ME manual is available in Cambridge Econometrics (2014). The FTT sub-modules for technology uptake in the power, transport and heating sectors are described in Mercure et al. (2012; 2018) and Knobloch et al. (2019). More details on the GENIE model are available in Holden et al. (2018).

4.3.1 Focus of the uncertainty analysis

E3ME-FTT-GENIE is effectively a combination of several models, each of which is immensely complex on its own. Here, we focus the uncertainty analysis on the future uptake of energy technologies, which is central to future greenhouse gas emissions, and modelled by the FTT (Future Technology Transformation) group of models. One model each is used to simulate the future uptake of technologies in the power sector (FTT:Power), transport sector (FTT:Transport) and heating sector (FTT:Heat). As all three models are based on the same theoretical framework, we focus the analysis on the model characteristics which all three of them have in common.

4.3.2 Identification of relevant uncertainties: Uncertainty matrix

As a first step, we identify relevant uncertainties within the FTT models by means of an uncertainty matrix (as described in section 3.1.1): What kind of uncertainties are located in which parts of the model? The resulting uncertainty matrix is shown in Table 15. The matrix can help to obtain an overview of uncertainties within the FTT models, by classifying them along the three dimensions of location, level, and nature (for more details on the different dimensions, see section 2.4).

Table 15: Uncertainty matrix for the location of key uncertainties within the E3ME-FTT models of technology uptake.

Nature / Location	Level					
	Statistical uncertainty		Scenario uncertainty		Recognised ignorance	
	Epistemic	*Variability*	*Epistemic*	*Variability*	*Epistemic*	*Variability*
Context			- Spatial resolution (59 world regions) - Temporal resolution (annually)		- Focus on uptake of energy technologies - Focus on cost and engineering data - No electricity grid modelling	
Structure			- No segmentation of the population within regions - Simplified age distributions		- Dynamic growth constraints - Basic principles of rational decision making - Myopic expectations of agents	
Input		- Technology costs - Technology lifetimes - Conversion efficiencies - Capacity factors - Technology stocks	- Future energy prices - Future carbon intensities of electricity - Energy service demand - Choice restriction matrix - Growth of infrastructure			
Parametric	- Non-pecuniary costs - Discount rates	- Heterogeneity of technologies and agents	- Replacement rates - Payback thresholds for early replacements	- Learning rates - Learning spill-overs between technologies		

The uncertainties in Table 15 were obtained based on the model descriptions and the underlying databases. While such a list can never be exhaustive, it covers the major uncertainties that the modellers are aware of. By definition, the matrix cannot include any uncertainties of which the modellers are not aware yet.

The exact location of individual uncertainties within the matrix is subjective, at least to a certain degree. For example, many of the uncertainties listed as ‘input uncertainties’ could also be classified as ‘parametric uncertainties’, and the other way around. The same holds for the distinction between statistical uncertainty, scenario uncertainty and recognised ignorance: These levels of uncertainty are not discrete classifications, but located on a continuous spectrum.

The following sub-sections describe the identified uncertainties within each location.

4.3.2.1 Context uncertainty

The spatial context of the FTT models is defined by the **spatial resolution** of the E3ME model, of which they are sub-components. This means that their spatial resolution is restricted to 61 world regions, which are either countries (e.g., Greece) or larger geographical units (e.g., 'Rest of Africa'). While these regions cover the entire globe, many of them are still quite large, with a potentially large heterogeneity within many world regions. Such a variance within regions is not explicitly represented by the FTT models, and thus a potential source of uncertainty – in particular when it comes to the analysis of technology uptake and resulting impacts on a sub-regional level, which may deviate from the regional average. Similarly, the FTT models are constrained to a quarter-annual **temporal resolution**, which means that any developments which occur within shorter time periods cannot be modelled and remain uncertain (such as the stability of the electricity grid, which would need to be modelled for every minute of every day).

The **lack of an explicit modelling of the electricity grid** with its dispatch of generators throughout any single day is also one of the deliberately chosen boundaries of the FTT models, which focus on longer time frames and larger geographical scales, compared to region-specific grid models. As a result, there is uncertainty as to whether the electricity grid in a region could actually accommodate increasing levels of renewable electricity generation, or increased levels of electricity demand from electric cars or heat pumps. Instead, the FTT models have a deliberate **focus on the uptake of energy technologies** (such as power generators, cars, heating systems) in different sectors. Furthermore, the modelling of technology uptake largely **focuses on cost and engineering data** (e.g. upfront investment cost, conversion efficiencies). While non-pecuniary costs are implicitly included by means of calibration of the model projections to historically observed time series (in FTT:Transport and FTT:Heat), factors of sociological, political or cultural nature are not explicitly represented in the modelling. Their potential impact on future technology uptake therefore remains uncertain (e.g., if a simulated policy would lead to political resistance and could therefore not successfully be implemented).

4.3.2.2 Structural uncertainty

The structure of all FTT models is characterised by their bottom-up representation of technology uptake, which is simulated based on the decision-making of heterogeneous groups of agents. The FTT models can therefore be classified as descriptive models of positive nature, aiming at a model representation of what might happen in reality, given a set of scenario inputs. This leads to several kinds of structural uncertainties, given that the modelling is based on representations of human behaviour, in particular of human decision-making.

The central structural assumptions therefore concern the dynamics of decision-making and how they are represented in the model. At its core, the decision between different technologies is conceptualised as a cost- and engineering-based comparison of all available technology options, for which the model estimates their respective levelised costs of providing an energy service (electricity, transport or heating). While the representation also includes intangible non-pecuniary cost elements (such as the preference for luxury cars or the discomfort of heating with coal), it is basically assumed that behaviour can be described according to the **basic principles of bounded rationality in decision-making**. However, it is known that people do not always decide rationally, and that human behaviour might be better described by alternative psychological frameworks, such as prospect theory (see section 2.3). Still, such theories have not (yet) been integrated into simulation models of energy technology uptake. The model representation of rational decision-making is therefore classified as a case of recognised ignorance: The modellers are aware of the underlying structural uncertainty, but due to the current limitations of the model structure, the uncertainty remains present. In section 4.3.4, we will try to change the model structure accordingly, in order to estimate the resulting impact of technology uptake.

A similar case of recognised ignorance in the model structure is the assumption about the expectations of agents, i.e. how decision-makers perceive the future (such as future changes in energy prices). In all FTT models, **myopic expectations of agents** are assumed. This means that in their decision-making, people act as if the future will look like the present, and do not anticipate any potential changes (such as increasing energy prices). This is a structural representation of bounded rationality, and therefore a conscious deviation from the basic principles of rational decision-making in the strict sense. However, it remains uncertain how people really form and take into account their expectations about future states of the world when it comes to deciding between alternative technology options, and different model structures are possible.

Apart from the decision-making core itself, a fundamental characteristic of the FTT model structure is the implementation of **dynamic growth constraints**, which endogenously determine how quickly new technologies can grow within the market. Without any growth constraints, it would implicitly be assumed that any new technology could dominate the market within very short time periods, something that contradicts the historical evidence (C. Wilson et al. 2013). Instead, the diffusion of technologies is characterised by s-shaped logistic diffusion profiles, in which initial phases of slow growth are followed by a faster diffusion into the mass market (C. Wilson and Grubler 2011). This is both related to the transmission of information between potential technology adopters, and the fact that the production capacities in industry cannot be transformed instantaneously (Rogers 2010; J.-F. Mercure 2018). Therefore, in the FTT models, the potential growth rate of any technology in any time period is endogenously constrained by the technology's market share in the previous time period. While the resulting patterns of technological change are consistent with historically observed technology transitions, the exact dynamics remain uncertain, and different structural representations in the model would lead to different projections of technology uptake.

Furthermore, the model structure is based on some simplifying assumptions regarding the representation of technology stocks and the population of decision-makers within each region. First, the **same age distribution** is assumed for all technologies, which implies that all technologies are assumed to be replaced with the same rate (e.g., if the average technological lifetime is 20 years, 5% of the technology would need to be replaced within each year). In reality, the age distribution might look differently for different technologies. Due to the limited data availability on age distributions, however, such differences are not represented in the model structure. The same applies to the representation of decision-makers. In reality, the population in each region is characterised by many different characteristics, some of them may have an impact on technology uptake (such as the limited availability of finance). Due to the related data requirements and additional complexities, however, the FTT models do **not include such segmentations of the population within regions**. While such a splitting of the population is currently under development for a separate project, it is not yet included into the model structure.

4.3.2.3 Input uncertainty

Input uncertainties refer to the uncertainty arising from the input data which is needed for the FTT models, which either (i) describe the characteristics of the system to be modelled, or (ii) the external drivers of this system. Most of this data is either subject to statistical or scenario uncertainty.

Input uncertainty at the level of statistical uncertainty is present for all data which can, in principle, be measured. In the FTT models, these are foremost all variables that describe the technological and economic characteristics of different technologies – such as **technology costs** (e.g., upfront investment costs and maintenance costs of a car or heating system), **technological life times** (i.e., how many years is a technology going to be used?), **energy conversion efficiencies** (i.e., the energy input required for generating a certain energy service), **capacity factors** (i.e., to which extent will a technology be used throughout its lifetime) and **technology stocks** (i.e., how many units of a technology type are currently being used in different world regions). All of this data is measurable and mostly available, but still subject to statistical uncertainty – for example, because the available measurements are not completely reliable (e.g., the conversion efficiency under real-world conditions might deviate from engineering estimates), or are not fully known (e.g., the true capacity factor of cars or heating systems is usually only known to the person using it, while the model estimate is based on statistic approximations). Hence, the uncertainties are not epistemic (they could be eliminated in principle), but due to the variability which is inherent to the real-world systems.

Input uncertainty at the level of scenario uncertainty is present for all data that describes future realisations of FTT model variables, as well as drivers which are external to the FTT models as such. Per definition, future input data (until 2050 in the current model configuration) cannot be measured, but is subject to scenario assumptions. Therefore, the uncertainties are of epistemic nature: They cannot be eliminated by means of performing more accurate measurements. This includes **future energy prices**, the **future carbon intensities of electricity** and the **energy service demand** (i.e., the demand for electricity, road transport or heating). Furthermore, scenario assumptions have to be made concerning the **future growth and availability of related infrastructure** – such as of storage potential in the electricity grid, or the future expansion of district heating networks. Last but not least, the possibility of switching between different technologies can be constrained by means of a **choice restriction matrix**, where each value within the matrix can be used to regulate the flow from one technology to another technology. For example, it is usually assumed that people who currently heat their homes with gas or central heating would not choose a coal heating systems instead, even if it should be considerably cheaper. While such assumptions are based in empirical observations and feasibility considerations, they still remain uncertain, and can be modified if needed.

4.3.2.4 Parametric uncertainty

Closely related to (and not always clearly distinguishable from) input and structural uncertainties are parametric uncertainties, which originate from uncertainty regarding the choice and calibration of model parameters.

In the FTT models, an important parametric uncertainty at the level of statistical uncertainty is the calibration of **non-pecuniary cost parameters**. These are not taken from engineering or literature estimates, but found by means of calibration. For each technology in each region, the parameter is specified in such a way that the rate of change of the trajectory of technology diffusion is continuous at the start of the model simulation. The parameter is meant to represent all factors that have an impact on technology uptake, but which are not explicitly specified within the model (e.g., subjective preferences or policy support schemes which are not explicitly incorporated into the baseline). However, these values remain uncertain, in particular in case of new technologies with only small market shares (in which case the non-pecuniary cost parameter may be determined based on the preferences of only a small sub-set of the whole population), and are potentially subject to change in the future. Further uncertainties in this category are the **heterogeneity of technology characteristics** (i.e., the standard deviations of the main cost parameters) and the **discount rates** (i.e., how much decision-makers value future costs relative to upfront costs).

At the level of scenario uncertainty, the most important uncertainties in the FTT models are related to the assumed **replacement rates of technologies** (i.e., which share of the technology stock gets replaced each year, either due to technical failures or due to economic considerations) and the assumed **learning rates** (i.e., the projected relative reduction in upfront investment costs that is associated with every doubling of the cumulative installed capacity of a certain technology). Furthermore, the model structure for endogenous cost reductions allows to define **learning spill-overs between technologies** that are specified as separate technology categories in the model, but are still closely related to each other (e.g., different types of electric cars or heat pumps). Such spill-over values are defined in a matrix, based on plausibility considerations, but remain uncertain.

4.3.3 Analysing modelling assumptions: Pedigree analysis

As a next step, the plausibility of identified uncertain assumptions in the FTT models is analysed. This is done by performing a qualitative pedigree analysis (see section 3.1.2), that assigns subjective pedigree scores to each individual assumption. Ideally, this is done by a group of stakeholders. However, as no resources are available for such a stakeholder workshop, a simplified approach is taken in this case, in which the pedigree scores are assigned by the analyst.

We focus the analysis on structural uncertainties that are related to the modelling of human decision-making. Specifically, the following three structural model assumptions were selected for a pedigree analysis (all of which are described in more detail in section 4.3.2.2):

- Dynamic growth constraints
- Basic principles of rational decision making
- Myopic expectations of agents

Table 16: List of evaluation criteria which are used in the pedigree analysis of behavioural assumptions in the E3M3-FTT model (adapted from Pye et al. 2018).

Uncertainty dimension	Criteria	Description
Methodological	Proxy	The extent to which the assumptions that we use in the model are proxies for the reality that we seek to represent, given the purpose of the model. Examples include over simplifications, first order approximations, incompleteness.
	Empirical basis	The degree to which observations, measurements and statistics are used to estimate a parameter or assumption.
	Rigour	Refers to the norms for methodological rigour in this process applied by peers. Well-established and respected methods for measuring and processing the data would score high on this metric, while untested or unreliable methods would tend to score lower.
	Validation	The extent to which assumptions have been cross-checked and validated against other observations and measurements.
Epistemological	Theoretical understanding	The extent to which our theoretical understanding of the real world processes provides a reliable basis for estimates.
Societal/ Value-laden	Choice space	The degree to which alternative choices of assumptions could be made i.e. the degree to which other acceptable/ plausible assumptions are available.
	Justification	The degree to which the approximation made in the model can be justified as a reasonable, plausible or acceptable assumption, given one's understanding of the reality. Can these assumptions be defended?
	Agreement amongst peers	The degree to which the assumption made in the model (by the analyst) is likely to coincide with other experts in the field.

These assumptions were selected because they are of potentially large importance for the model projections of technology uptake and resulting energy use and emissions, as well as for the potential effect of different policy instruments. These structural assumptions on the behavioural characteristics of the system are of qualitative nature, and can therefore not easily be analysed by means of quantitative methods (such as sensitivity or scenario analysis, which can easily be applied to most input and parametric uncertainties).

The set of criteria for performing the pedigree analysis are based on Pye et al. (2018), who have performed a similar analysis for a model of the British electricity system. Scores between 0 to 4 can be given to each model assumption, where 0 denotes a weak pedigree and 4 a strong pedigree. The overall pedigree score of an assumption is then calculated as the (unweighted) average of all individual pedigree criteria. The assigned pedigree scores for all individual dimensions, as well as the overall pedigree score for each assumption, are presented in Table 17, Table 18 and Table 19.

The pedigree analysis resulted in different overall pedigree scores for all analysed model assumptions, ranging from 1,5/4 to 2,9/4.

Table 17: Pedigree score card for structural assumption of dynamic growth constraints in E3ME-FTT (adapted from Pye et al. 2018).

Model assumption: Dynamic growth constraints for energy technology diffusion							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	*Exact*			X			*Poor*
Empirical basis	*Observation*		X				*Speculative*
Methodological rigour	*Best available*			X			*None*
Validation	*Many sources*		X				*None*
Theoretical understanding	*Agreed*			X			*Speculative*
Choice space	*Wide*		X				*None*
Justification	*Full*	X					*Speculative*
Agreement amongst peers	*Complete*				X		*None*
Overall pedigree score		2,5					

Table 18: Pedigree score card for structural assumption of rational decision-making in E3ME-FTT (adapted from Pye et al. 2018).

Model assumption: Basic principles of (bounded) rationality in decision-making							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	*Exact*			X			*Poor*
Empirical basis	*Observation*				X		*Speculative*
Methodological rigour	*Best available*		X				*None*
Validation	*Many sources*				X		*None*
Theoretical understanding	*Agreed*			X			*Speculative*
Choice space	*Wide*				X		*None*
Justification	*Full*				X		*Speculative*
Agreement amongst peers	*Complete*				X		*None*
Overall pedigree score		1,5					

Table 19: Pedigree score card for structural assumption of myopic expectations of agents in E3ME-FTT (adapted from Pye et al. 2018).

Model assumption: Myopic expectations of agents							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	*Exact*		X				*Poor*
Empirical basis	*Observation*	X					*Speculative*
Methodological rigour	*Best available*		X				*None*
Validation	*Many sources*			X			*None*
Theoretical understanding	*Agreed*		X				*Speculative*
Choice space	*Wide*		X				*None*
Justification	*Full*		X				*Speculative*
Agreement amongst peers	*Complete*			X			*None*
Overall pedigree score		2,9					

The lowest overall pedigree got assigned to the assumption of rational decision-making when it comes to choosing between different technology options: Plenty of empirical evidence suggests that humans do not make such decisions fully rationally, only based on cost and engineering considerations (Grubb, Hourcade, and Neuhoff 2014; Gillingham and Joskow 2016; Gerarden, Newell, and Stavins 2017). While alternative model representations are possible (Wilson and Dowlatabadi 2007; Knobloch and Mercure 2016), it is a still ongoing debate which type of representation would be both a better representation of real-world behaviour and also feasible to implement in large-scale energy models (Mercure et al. 2016). The assumption is therefore further analysed in section 4.3.4, where an alternative specification of decision-making is implemented into the model structure of one of the FTT models, in order to analyse the potential impact on model projections.

4.3.4 Analysing the uncertainty of policy effectiveness with E3ME-FTT

In section 2, we have argued that the uncertainty regarding human behaviour and decision-making is of primary relevance for modelling the Nexus, for example when it comes to technology uptake or the potential effectiveness of policy instruments. In section 4.3.3, we have described that the E3ME-FTT models of technology uptake are based on the basic principles of (bounded) rationality in decision-making, and that this structural assumption constitutes a major uncertainty in these models. However, the analysis was only on a qualitative level, and it remained unclear what the impacts of such behavioural uncertainties in the model structure would be in quantitative terms. What would be the difference in model projections that would result from changing the assumptions on technology choice behaviour?

In the original specification of the FTT models, there is no parameter for "rationality in decision-making" that could be changed. An analysis of behavioural uncertainty[4] is therefore not possible by means of a sensitivity analysis. Instead, it requires a modification of the model structure itself, as described in section 3.2.3. For this purpose, we have replaced the decision-making core of one of the FTT models by a more general version. Depending on the parameter setting, the new model formulation either yields the original formulation of bounded rationality, or can be replaced by an

[4] Note that 'behavioural uncertainty' refers to uncertainty from the perspective of the modeller, regarding what is the most appropriate model representation of decision-making by agents. This is different from uncertainty as perceived from the perspective of these agents (see section 2.3).

alternative structural assumption on decision-making. As a case study, we exemplarily perform this structural uncertainty analysis for the FTT model of technology uptake in the residential heating sector, FTT:Heat.

As an alternative description of decision-making we use prospect theory (Kahneman and Tversky 1979; Tversky and Kahneman 1991; Amos Tversky and Kahneman 1992). It aims at a realistic description of observed behaviour in decision-making situations, based on a wide range of experiments. The theory is considered to offer the best available representation of observed decisions (Barberis 2013). Centrally, in prospect theory, decision-making is subject to loss aversion. According to empirical research, losses have a stronger impact on choices than gains, and it depends on a person's individual reference point what is seen as losses and gains (Kahneman, Knetsch, and Thaler 1991). It therefore makes a difference if someone owns an apple and compares it to an orange, or owns an orange and compares it to an apple. Samuelson and Zeckhauser (1988) show that loss aversion impacts observed choices of jobs and cars, amongst others. They find that models which ignore the implications of loss aversion will overestimate how peoples' choices respond to changing economic characteristics (such as prices), and underestimate the stability of the status quo in the real world.

Prospect theory has successfully been used in empirical research on energy technology uptake (Frederiks, Stenner, and Hobman 2015; Greene 2011; Häckel, Pfosser, and Tränkler 2017). However, despite its large relevance for energy policy (Gillingham et al. 2009), the theory is rarely applied to energy modelling (for an example, see Safarzyńska and van den Bergh 2018), and not considered in any major energy or integrated assessment model.

In the following sub-sections, we introduce loss aversion into a modified version of E3ME-FTT:Heat. At the example of the residential heating sector, we demonstrate to which extent it impacts model projections of technological change, and the effectiveness of different policy instruments. This serves as a demonstration of the importance of behavioural uncertainty in modelling, and how it can be analysed.

4.3.4.1 Theoretical background on loss aversion

Although prospect theory was originally developed for analysing risky choices (such as lotteries or gambles), it is equally useful for choices in which risk is only of secondary importance – such as when choosing between consumption goods, which differ in their individual attributes (Thaler 1980; Tversky and Kahneman 1991). Due to loss aversion, people perceive deviations from their current situation as less attractive than what rational choice theory would imply, and therefore show an irrationally strong preference for the status quo and their current entitlements (Thaler 1980; Samuelson and Zeckhauser 1988).

In a classic experiment by Knetsch (1989), each participant is randomly given either a mug or a candy bar. They then get the option to exchange their present for the alternative object. Resulting choices reveal a striking asymmetry in preferences, depending on the reference point: Around 90% of the participants who were given a mug chose to keep it, but only 10% of participants who were assigned a candy bar chose to trade it for the mug. Rational choice theory predicts that average preferences should be the same in both sub-groups. In reality, the loss of giving up the assigned object is felt more strongly than the gain of receiving an alternative object, making the exchange less attractive. In a related experiment by Kahneman, Knetsch and Thaler (1990), participants are either given a mug or nothing. Everyone is then asked for which price they are either willing to sell their mug (if they were given one), or willing to buy a mug (if they were not given one). On average, the sellers' willingness to accept (to sell the mug) is more than twice the buyers' willingness to pay (for the mug). Giving up the mug seems to be evaluated as a loss, which looms larger than the resulting monetary gain.

Tversky and Kahneman (1991) distil the evidence from various experiments into a reference-dependent model of loss aversion in riskless choice, which is the starting point of our analysis. Conceptually, the model considers a choice between two options (x and y) that differ on two valued dimensions (d1 and d2). Depending on the reference point, any difference on a dimension, Δd_i, is evaluated as a loss or gain (i.e., as a relative disadvantage or advantage). For each loss or gain, the subjectively perceived decision value, $v(\Delta d_i)$, is determined by the following value function:

$$v(\Delta d_i) = \begin{cases} \Delta d_i \ if \ \Delta d_i \geq 0 \\ \Delta d_i * \lambda \ if \ \Delta d_i < 0, \end{cases}$$

λ is the coefficient of loss aversion, which described the relative impact of losses on the decision-making, compared to gains of the same magnitude. The overall evaluation of a choice option equals the sum of $v(\Delta d_i)$ over both dimensions.

If λ=1, the value function yields the rational choice model. If λ > 1, however, due to loss aversion, losses have a greater impact on choices than gains, and it depends on the reference point what is perceived as losses by an individual decision-maker.

4.3.4.2 A conceptual model of loss aversion in technology choice

Reference-dependent technology choice for a single decision-maker

We apply Tversky and Kahneman's (1991) reference-dependent model of loss aversion in riskless choice to the adoption of energy end-use technologies, such as the choice between alternative car models or heating systems. Although such decisions also include risk (e.g., uncertain future energy price), we argue that peoples' preferences foremost depend on the valued dimensions of different technologies - such as their purchase price, or estimated energy costs during a technology's lifetime. We start with the simplified case of one individual decision-maker, before extending the analysis to a heterogeneous population.

Suppose that a person needs to replace an energy technology which is coming to the end of its lifetime, and can choose between two technology options (*x* and *y*), both of which provide the same energy service (e.g., transport or heat). For simplicity, suppose that preferences for this choice are determined by two dimensions (d_1 and d_2): upfront capital cost (i.e., the purchase price and eventual installation costs), and the (discounted) total energy cost during a technology's lifetime.

Table 20: Cost attributes of two alternative energy end-use technologies (*x* and *y*), under different assumptions on their cost characteristics (cases a-d).

Case	Technology x (d_1) Capital cost (Euro)	(d_2) Energy cost (Euro)	*Total cost (Euro)*	Technology y (d_1) Capital cost (Euro)	(d_2) Energy cost (Euro)	*Total cost (Euro)*
a	200	200	*400*	300	200	*500*
b	200	200	*400*	200	200	*400*
c	100	300	*400*	300	100	*400*
d	200	200	*400*	200	100	*300*

Table 20 shows the respective cost dimensions for four hypothetical cases, labelled (a)-(d). In case (a), technology *y* has higher overall costs. In case (b), both technologies are identical in overall costs and both dimensions. In case (c), both technologies still have the same overall cost, but differ in their dimensions: Technology *x* has low capital and high energy costs, while technology *y* has high capital and low energy costs. In case (d), technology *y* has lower overall costs.

Table 21: Gains and losses from switching between two alternative technologies (x and y), evaluated with and without loss aversion, for different hypothetical technology characteristics (a-d). Gains (in green) and losses (in red) stem from differences in upfront capital costs (ΔC) and total energy cost over a technology's lifetime (E). Switching technologies is considered an attractive choice when the sum of evaluated losses and gains is positive (indicated in green).

		Switching from technology x to y			Switching from technology y to x		
		$v(\Delta C)$	$v(\Delta E)$	Sum	$v(\Delta C)$	$v(\Delta E)$	Sum
a	Rational	-100	0	**-100**	100	0	**100**
	Loss aversion	-225	0	**-225**	100	0	**100**
b	Rational	0	0	**0**	0	0	**0**
	Loss aversion	0	0	**0**	0	0	**0**
c	Rational	-200	200	**0**	200	-200	**0**
	Loss aversion	-450	200	**-250**	200	-450	**-250**
d	Rational	0	100	**100**	0	-100	**-100**
	Loss aversion	0	100	**100**	0	-225	**-225**

Table 21 shows the resulting choice evaluations from the perspectives of rational choice theory and prospect theory, respectively. From a rational choice perspective, choices are straightforward: Technology *x* should be preferred in case (a), and technology *y* in case (d). In cases (b) and (c), as total costs are identical, any objective decision-maker should be indifferent between both options. Preferences should not depend on the technology which is being replaced.

From a prospect theory perspective, the technology options are evaluated based on the two-step value function (see pervious section), where the coefficient of loss aversion is set to 2,25 (based on Amos Tversky and Kahneman 1992). The resulting attractiveness of choice options depends on the decision-maker's subjective reference point, which is taken to be his currently owned technology. Switching from the status quo to the alternative technology can lead to changes in one or more dimension, and each change is perceived either as a loss or gain, relative to the reference point. Due to loss aversion, relative disadvantages of an option (losses) now loom larger than relative advantages (gains).

Loss aversion has no impact on preferences or choices in case (b), where all dimensions are identical. In case of (a) and (d), where one technology has a clear advantage over the other, switching to the overall more expensive technology is now perceived as even less attractive, compared to rational preferences. However, the resulting choices remain unaffected. This is different for the trade-off in case (c), where overall costs are identical, but the underlying dimensions are reversed: The disadvantage (loss) in one dimension is felt more strongly than the simultaneous advantage (gain) in the other dimension, which suggests a strong preference for the status quo technology.

Defence-dependent technology choice for a heterogeneous population

Technology adoption within a larger population is not determined by a single representative agent, but depends on the distributed decisions of heterogeneous people, with different preferences. Also, there is variation within different sub-groups of technology groups (such as gas heating systems), as different technology models are produced by different manufacturers, which need to be installed in a diverse range of houses.

For representing such diversity, we extend the analysis to the case of a heterogeneous population. A Gaussian normal distribution is specified around each of the cost dimension values in Table 20, assuming a relative standard distribution of 20% around the respective mean values.

Figure 21 presents the probability distributions of net gains/losses of switching between two technologies *x* and *y*, resulting from a Monte Carlo simulation with 50,000 runs. The location on the x-axis equals the (perceived) net values of technology switching, which is seen as attractive in case of positive net values (right of the dashed line). Solid lines show the distributions of net values from a rational choice perspective, while filled shapes correspond to the distributions as perceived under loss aversion. Average choices are defined by the distributions' means, which are identical to the case of a single decision-maker. Different than before, however, choices are distributed: An option may be seen as unattractive by one part of the population, while it is considered attractive by the other part.

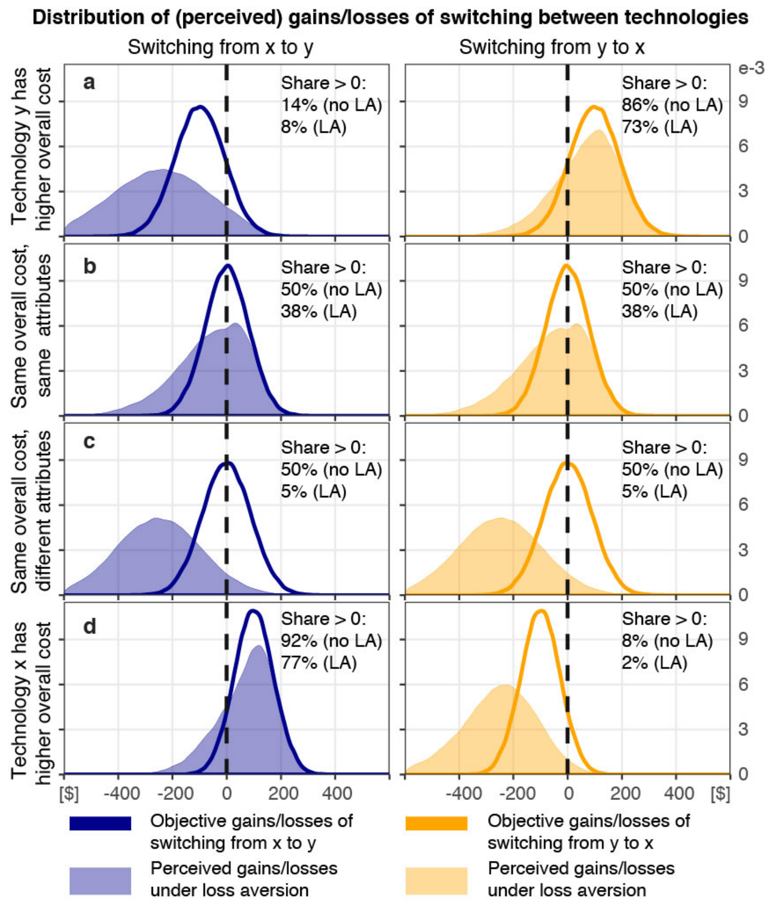

Figure 21: Probability distributions of the monetary gains/losses associated with switching between two alternative technologies (x and y). Distributions of objective cost differences are shown as solid lines, distributions of gains/losses as perceived under loss aversion (LA) are shown as filled shapes.

In all cases, the inclusion of reference-dependent loss aversion into the model reduces the share of the population which is predicted to switch between technologies, by a ratio of 15-90%. The effect is most striking for a trade-off between dimensions, as it is assumed in case (c). Because both technology options have the same overall cost, objective preferences should be equally distributed, so that 50% of the population would find it favourable to switch technologies. Under reference-dependent preferences, however, loss aversion implies that the disadvantages in one dimension have more impact on choices than the advantages in the other dimension. As a result, only 5% of the hypothetical population finds it attractive to switch technologies, while 95% prefer the status quo. This strong expression of the status quo bias manifests itself in both directions: People either stick to technology *x* or *y*, whichever is their reference point.

4.3.4.3 Simulating reference-dependent technological change over time

Up until here, we have analysed technology choice in a static setting, without considering the dynamic impact of loss aversion on technology stocks and market shares over time. As a next step, we simulate technology diffusion over 50 years. We assume an average lifetime of 10 years for both technologies. This implies that within each year of the simulation, 10% of the population are faced with the choice from section 0. Initial market shares are set to 99% for technology *x*, and 1% for technology *y*.

Within each simulation period *t*, the model first calculates the choice preferences, which are defined as the fraction of the population which would choose to switch from technology *i* to technology *j*. This fraction is denoted as $F_{i\rightarrow j,t}$, and equals

$$F_{i\rightarrow j,t} = S_{i,t-1} * P\left(\sum v(\Delta d_{i\rightarrow j}) > 0\right).$$

$S_{i,t-1}$ is the market share of technology *i* in the previous period, which determines the share of the population for which the reference point is technology *i*. $P\left(\sum v\left(\Delta d_{i\rightarrow j}\right) > 0\right)$ denotes the probability that switching from technology *i* to *j* is perceived as beneficial, which requires that the sum of evaluated gains and losses on both dimensions *d*, $v(\Delta d_{i\rightarrow j})$, is larger than zero. As costs are static, this probability remains constant throughout time. Based on the choice preference $F_{i\rightarrow j,t}$ and market share $S_{i,t-1}$, flows in market shares from technology i to j can then be calculated as

$$S_{i\rightarrow j,t} = F_{i\rightarrow j,t} * {S_{i,t-1}}/{L_i},$$

where L_i is the average life expectancy of technology *i*. The new market share of *i* is then simply its market share in the previous period, minus the flow in market shares from *i* to *j,* plus the flow of market shares from *j* to *i*:

$$S_{i,t} = S_{i,t-1} - S_{i\rightarrow j,t} + S_{j\rightarrow i,t}$$

Figure 22 compares the simulated development of market shares (solid lines) and choice preferences (dashed lines) over time, with and without loss aversion. In all cases, market shares converge to the distribution of preferences within the population. When comparing the simulation results with and without loss aversion, there are three striking differences.

First, loss aversion leads to different distributions of choice preferences, compared to rational decision-making (as already discussed for the static case, see section 0). Second, reference-dependence implies that the distribution of preferences changes throughout time, due to continuous shifts in the distribution of reference points. This is unlike rational decision-making, for which choice preferences are static as long as objective technology characteristics do not change. Third, and perhaps most importantly, different choice preferences throughout time imply different trajectories of technological change.

The extent to which loss aversion affects technological change is roughly proportional to the extent to which it alters the underlying distributions of choice preferences, as shown in Figure 21. Due to the asymmetric nature of loss aversion, the largest difference can be seen for a trade-off between two dimensions (while total costs are the same), as it is assumed for case (c). Under rational decision-making, each technology option should be preferred by 50% of the population, and their market shares converge to 50% within the simulation period. Under loss aversion, only 5% of the population would prefer technology *y* in the first year, and 25% after 50 years. Such strong and persistent preferences for the status quo drastically reduce the extent of technological change: Even after 50 years, the market would remain dominated by the current incumbent.

It is important to note that the assumed trade-off between capital and energy costs in case (c) is a commonly encountered cost profile in low-carbon transitions. For example, let *x* be an energy-inefficient technology with low capital and high energy costs, while technology *y* is a much more energy-efficient alternative (with very high capital and low energy costs). Option *y* is still new and rather expensive, and therefore objectively unattractive. Policy-makers therefore introduce a purchase subsidy, which reduces technology *y*'s overall costs to the level of technology *x*. Under rational decision-making, such a policy would be predicted as being sufficient. When considering loss aversion, however, cost-competitiveness is no guarantee for success: As long as both technologies largely differ in important characteristics, switching remains unattractive, and technology *y*'s market uptake therefore much slower than anticipated.

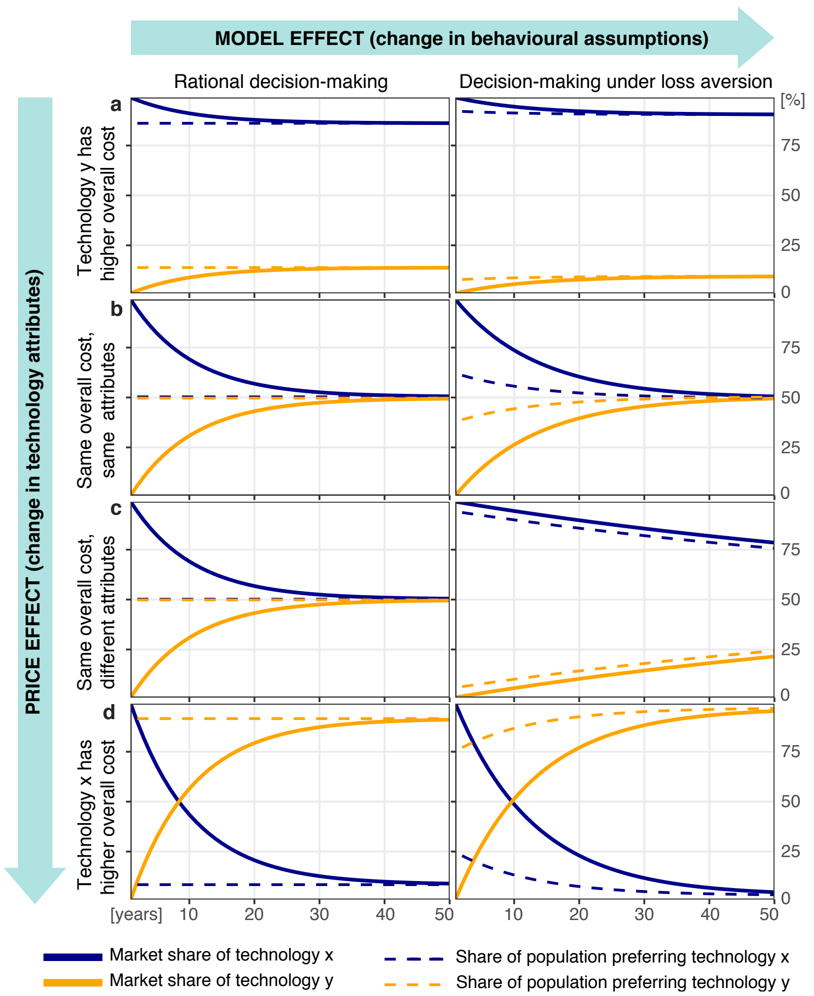

Figure 22: Simulated changes in technology market shares (solid lines) and technology preferences (dashed lines) over time (50 year simulation period), within a heterogeneous population of decision-makers, for cases (a)-(d). Panels on the left show the simulation results under the assumption of rational decision-making, panels on the right show the simulation results for decision-making which is subject to loss-aversion. Initial market shares of technologies *x* and *y* are 99% and 1%, respectively.

4.3.4.4 Implementation of loss aversion into FTT:Heat

As a next step, we implement the model of loss aversion into FTT:Heat (for a model description and further details, see Knobloch et al. 2019, 2017), which is part of E3ME-FTT (J.-F. Mercure, Pollitt, Edwards, et al. 2018; J.-F. Mercure, Pollitt, Viñuales, et al. 2018). The model simulates the uptake and replacement of 13 different heating technologies in all E3ME world regions, up until 2050.

In each year up to 2050, a fraction of households decides between available heating systems, and this annual fraction depends on replacement needs. The model simulates decisions from a bottom-up perspective: under given behavioural assumptions, which technologies would households prefer, and how fast can new technologies grow within the market? In each year, technology choices are determined by a pairwise comparison of all available options, based on distributed costs and preferences. Costs are normalised to the generation of one unit of useful heat, and are derived from three main components: Upfront investment costs, maintenance-repair costs, and energy costs. All cost values are distributed around their mean values, and future costs are discounted. Additionally, an empirically calibrated 'intangible' cost component is added. It represents technology characteristics which are valued by households (such as convenience or co-benefits), but not captured by the engineering-based cost data. Upfront investment costs can endogenously decrease over time, as a function of each technology's cumulatively installed capacity ('learning by doing'), which makes the model highly path-dependent.

The current choice modelling in FTT:Heat is based on bounded rationality: Households are specified to have myopic expectations (i.e., they act without foresight, only based on cost data in each respective period), and only have limited information on available technologies (i.e., if a technology has a small market share, it is only considered by a proportionally small share of the population). However, apart from these restrictions, the comparison of considered options remains tied to the assumptions of rationality.

For the inclusion of prospect theory into FTT:Heat, we have replaced its original decision-making core with the reference-dependent model from section 4.3.4.3, extending it to 13 choice options and three dimensions. In each period, the model estimates the distributions of potential losses and gains from technology switching for any possible pair of heating technologies, by means of a Monte Carlo simulation. Losses and gains can result from each cost component and the 'intangible' cost component. The distribution of reference points is taken to be the market shares of technologies in the previous period, in each respective region. If the coefficient of loss-aversion is set to 1, the new decision-making core yields its original version, which allows an easy comparison of model results under alternative assumptions on decision-making.

For demonstrating the modified version of FTT:Heat, we exemplarily simulate four scenarios, based on previous work (Knobloch et al. 2019):

- Scenario a projects current trends of technology diffusion into the future. It implicitly considers existing policies (via the 'intangibles'), but does not introduce new policies.
- Scenario b simulates a residential *carbon tax*, which is added to the household price of fossil fuels. The tax starts at 50€/tCO_2 in 2020, and increases by 5€/tCO_2 per year.
- Scenario c simulates a *technology subsidy,* which is paid on the upfront investment costs of heat pumps, solar thermal and modern biomass systems. The subsidy rate is set to -50% of the investment costs between 2020-2030, and then linearly phased out until 2050.
- Scenario d simulates the combined effect of the carbon tax and the technology subsidy.

Model results with and without loss-aversion

The impact of loss aversion on the model projections of global heat generation by technology type and CO_2 emissions can be seen in Figure 23, for scenarios (a)-(d). Table 22 presents the underlying market shares of renewable and highly energy-efficient heating technologies (referred to as renewables from hereon), at the start (in 2015) and end of the simulation (in 2050).

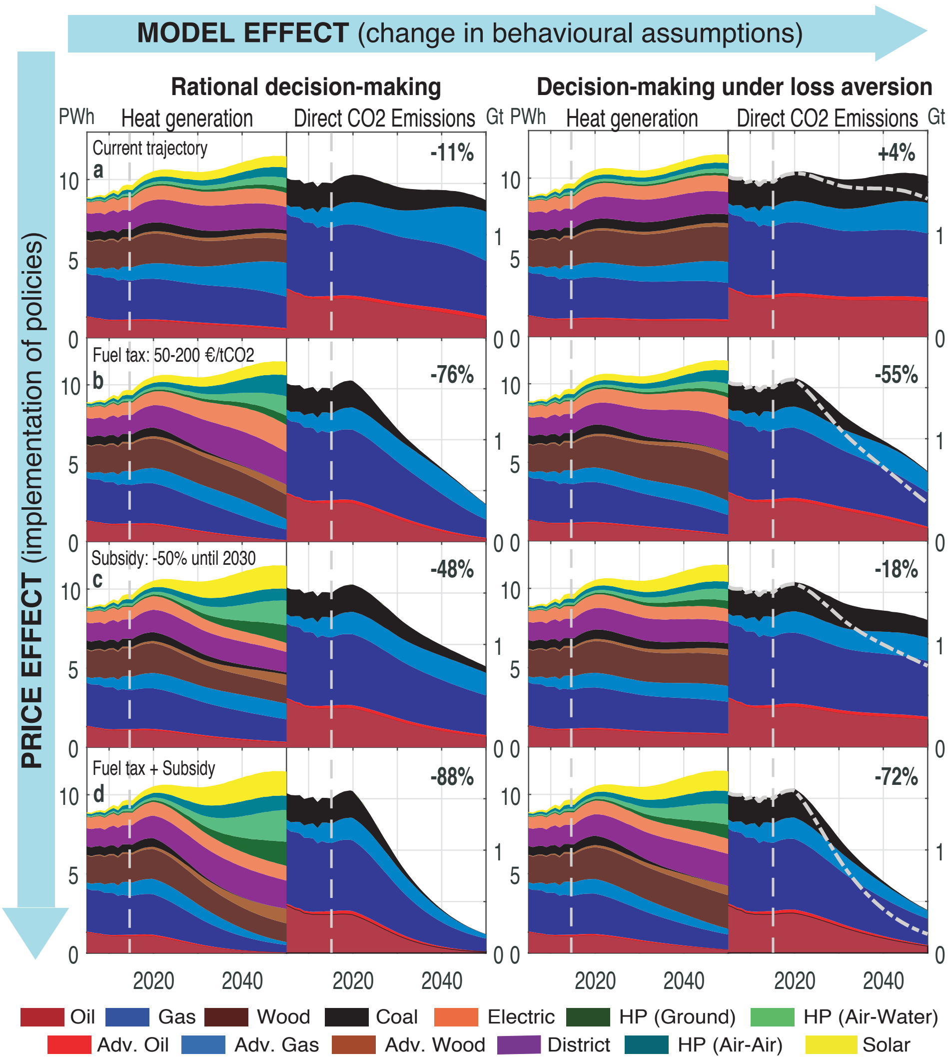

Figure 23: Global heat generation by technology and resulting direct CO_2 emissions from 2005-2050, under the current technological trajectory (a) and in three policy scenarios (b-d), as simulated by FTT:Heat. Panels on the left show the simulation results under the assumption of rational decision-making, panels on the right for decision-making which is subject to loss-aversion. Vertical lines indicate the start of the model simulation in 2015. Bold numbers refer to the change in direct CO_2 emissions in 2050, relative to their level in 2015. In the right panels, dashed lines indicate the level of CO_2 emissions as simulated under rational decision-making.

It can be seen that in all of the simulated scenarios, the future uptake of renewable heating technologies is much slower under decision-making with loss aversion, relative to the model formulation without loss aversion. In 2015, the global market share of renewables was 9%. Until 2050, under current trends this share is projected to increase to 24% without loss aversion, compared to only 14% with loss aversion. This means that the change in behavioural assumptions reduces the projected uptake of renewable by 40%. Similar dynamics can be observed for the simulated impacts of policy instruments in scenarios b-d. The carbon tax and the subsidy are projected to increase the uptake of renewables in both model versions, relative to current trends. However, the consideration of loss aversion in the model reduces the impact of policies significantly.

Table 22: Projected global market share of renewable and highly energy-efficient heating technologies (modern biomass, solar thermal and electric heat pumps) in 2050, as simulated by FTT:Heat, under the current technological trajectory (a) and for three policy scenarios (b-d).

Year	2015	2050		2050
Scenario	---	**(i) Bounded rational decision-making**	**(ii) Decision-making with loss aversion**	***Relative difference (ii) to (i)***
a	9%	24%	14%	*-40%*
b	9%	41%	24%	*-40%*
c	9%	48%	27%	*-43%*
d	9%	60%	42%	*-29%*

The reason for the lower uptake of renewables under loss aversion is the relatively larger impact of losses on the underlying decision-making. Typically, fossil fuel-based and renewable heating technologies have reversed cost characteristics. The former have relatively low upfront investment costs, but relatively high energy expenses over time. In comparison, renewable heating technologies are characterised by relatively high upfront costs, but low energy costs (or almost zero in case of solar thermal). Without any policy support, renewables are mostly still more expensive in terms of overall costs, and objectively only attractive in relatively few cases. In such a situation, the potential impact of loss aversion is thus limited, similar to case (a) in section 4.3.4.3.

The carbon tax increases the energy costs of fossil fuel-based technologies, and thereby increases the competitiveness of renewables Depending on local energy prices, renewables and fossil technologies might then have similar overall costs. However, parity in total costs does not change the fact that both technology groups have reversed cost dimensions. Without the additional introduction of subsidies, renewables still have higher capital costs. Due to loss aversion, this relative disadvantage (loss) has a relatively stronger impact on decisions than the advantage in energy costs (gain), when evaluated from the reference point of fossil-fuel technologies.

The projected differences in technology uptake have obvious consequences for the amount of direct CO_2 emissions which are emitted by residential heating systems. Under current trends, annual emissions are projected to decrease by 11% until 2050 when assuming bounded rational decision-making. When considering loss aversion, however, emissions are projected to increase by 4%. The change in behavioural assumption leads to a 17% higher estimate of emission levels in 2050. Differences in emission levels due to different behavioural assumptions are even larger in case of the policy scenarios: Projected annual emissions in 2050 are 85% higher in the carbon tax scenario, 57% higher in the subsidy scenario, and 127% higher for a combination of both policies, compared to decision-making without loss aversion. Cumulative emissions over the entire simulation period (2015-2050) are 6% (3GtCO_2) larger in scenario a, and around 20% (6-7GtCO_2) larger in the policy scenarios b-d.

Interpretation of results

For analysing the potential impact of prospect theory on technology choices and policy-induced low-carbon transitions, we implemented a simple model of reference-dependent energy technology choice into FTT:Heat, which is part of the E3ME model.

In prospect theory, loss aversion implies stronger preferences for technologies which are perceived as the subjective reference points of decision-makers. Because losses loom larger than gains, relative disadvantages on one dimension are valued more strongly than relative advantages on another dimension. It depends on the situation if such asymmetries also influence technology choices. If one technology has a clear advantage on one dimension, while other dimensions are similar to the alternative options, loss aversion leads to more pronounced preferences without necessarily changing the resulting choices. Reversely, this means that impacts on choices are strongest if there is a trade-off between dimensions: Even if both cancel out from an objective perspective, subjectively more weight is given to relative disadvantages. In such situations, loss aversion can easily change the overall evaluation of options, and therefore lead to different predicted technology uptake than when assuming rational decision-making. This case is of primary relevance for low-carbon transitions, which require that energy-intensive fossil-fuel based technologies are replaced with capital-intensive renewable and energy-efficient technologies – a direct trade-off between dimensions.

From the perspective of modelling, it is particularly important that reference dependence is based on an asymmetric decision-making process. For example, switching from a petrol-powered car to an electric car is evaluated differently than switching from an electric car to a petrol-powered car. Both situations imply different perspectives on what is perceived as gains and losses, and hence different evaluations of technology switching. Such asymmetries cannot be represented by an adjustment of cost attributes. Instead, they require a different model representation of decision-making itself. As illustrated for the case of residential heating, the inclusion of prospect theory into a global simulation model of technology uptake leads to significantly different results. The projected diffusion of renewable technologies is around 30-40% lower than what would be projected without loss aversion, resulting in higher levels of direct CO_2 emissions by the residential sector.

From a policy perspective, loss aversion therefore has two important implications. First, it requires a different design of policy instruments, such as taxes and subsidies. Typically, such incentives are meant to make low-carbon technologies sufficiently attractive, so that they can financially compete with fossil-fuel technologies. However, loss aversion implies that while a similar level in overall costs is a necessary precondition, it is not always sufficient for incentivising a switch between technologies. Even when total costs are on par, remaining differences in the underlying dimensions can make it unattractive for people to take up the alternative technology. Second, loss aversion should be included in the ex-ante evaluation of policies and their potential effects. Not considering loss aversion likely overestimates policy impacts and the resulting extent of technological change in the future, while it underestimates the persistence of the status quo.

5 Conclusions

In this deliverable, it was shown that uncertainty is relevant for any kind of modelling, and in particular in the context of modelling complex interacting systems, as they are analysed in the Sim4Nexus project. A whole range of multi-faceted uncertainties exists in models, which can be classified according to their location within the model, the level of uncertainty, and its epistemological nature. Different established methodologies exist for the identification, analysis, and communication of uncertainties in models. Quantitative methodologies, such as sensitivity and scenario analysis, are a powerful tool for analysing the uncertainties which stem from model parameters and inputs, as well as their interactions with each other. Qualitative methodologies, such as uncertainty mapping and pedigree analysis, can be particularly useful for the analysis of structural uncertainties and modelling assumptions, which go beyond the variation of model parameters. A particular case of structural uncertainty is the uncertainty regarding the behaviour of people, for example when it comes to the choice of technologies. As the real-world effectiveness of any type of policy instrument finally depends on its impact on human decisions, behavioural uncertainty is of primary importance when it comes to the model simulation of policy effectiveness.

The application of different methodologies for the analysis of different types of uncertainties has been demonstrated at the example of three models which are used within the Sim4Nexus project. The newly developed 'pragmatic approach for uncertainty analysis in large and complex models' can be easily applied to all other kind of models. Together with the guidelines for uncertainty communication, the methodologies presented in this deliverable can therefore help to facilitate the analysis and communication of uncertainties as part of the development of other system dynamics models for the different case studies, as well as the analysis of uncertainties within the 'serious game'.

Appendix

Detailed analysis of model assumptions in the Greek SDM

Table 23. Mapping of model assumption 1 (of the Greek SDM).

Model assumption 1: The Nexus components that are considered in order to assess the sustainability of resource use in a case study are Water, Land Use, Energy, Food, and Climate	
Location: *context uncertainty*, uncertainty within the system boundaries	**Level:** *recognized ignorance*, Other Nexus approaches that extend to include more components than WEF are ongoing and maybe prove that other Nexus components, such as soil, waste, and ecosystems are important to include.
Nature of uncertainty: *epistemic, undefined relations*	

Strength of model assumption 1							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact		x				Poor
Empirical basis	Observation		x				Speculative
Methodological rigor	Best Available				x		None
Validation	Many Sources				x		None
Theoretical understanding	Agreed		x				Speculative
Choice space	Wide				x		None
Justification	Full		x				Speculative
Agreement amongst peers	complete			x			None
Overall pedigree score		2.125					

Influence on results of model assumption 1			
Greatly determines model results	2	x	2
Greatly determines results of modelling step	1		
Only local influence	0		

Table 24. Mapping of model assumption 3 (of the Greek SDM).

Model assumption 3: The urban land use proportioning is not modelled	
Location: *context uncertainty*, uncertainty within the system boundaries	**Location:** *context uncertainty*, uncertainty within the system boundaries
Nature of uncertainty: *variability*	**Nature of uncertainty:** *variability*

Strength of model assumption 3							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact		x				Poor
Empirical basis	Observation		x				Speculative
Methodological rigor	Best Available			x			None
Validation	Many Sources			x			None
Theoretical understanding	Agreed		x				Speculative
Choice space	Wide					x	None
Justification	Full		x				Speculative
Agreement amongst peers	complete	x					None
Overall pedigree score		**2.5**					

Influence on results of model assumption 3			
Greatly determines model results	2		**1**
Greatly determines results of modelling step	1	x	
Only local influence	0		

Table 25. Mapping of model assumption 4 (of the Greek SDM).

Model assumption 4: The GHG emissions model is simplified to be incorporated in the SDM, with yields that are calibrated to give out the forecasted GHG emissions.	
Location: *structure uncertainty*, simplified equations	**Location:** *structure uncertainty*, simplified equations
Nature of uncertainty: *epistemic, uncertain relations*	**Nature of uncertainty:** *epistemic, uncertain relations*

Strength of model assumption 4							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact			x			Poor
Empirical basis	Observation	x					Speculative
Methodological rigor	Best Available			x			None
Validation	Many Sources		x				None
Theoretical understanding	Agreed			x			Speculative
Choice space	Wide			x			None
Justification	Full		x				Speculative
Agreement amongst peers	complete		x				None
Overall pedigree score		**2.625**					

Influence on results of model assumption 4			
Greatly determines model results	2		**0**
Greatly determines results of modelling step	1		
Only local influence	0	x	

Table 26. Mapping of model assumption 5 (of the Greek SDM).

Model assumption 5: The uniform distribution of water demand, water sources, energy demand, energy production and food production throughout space.	
Location: *structure uncertainty*, simplified distribution	**Location:** *structure uncertainty*, simplified distribution
Nature of uncertainty: *variability*	**Nature of uncertainty:** *variability*

Strength of model assumption 5							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact				x		Poor
Empirical basis	Observation			x			Speculative
Methodological rigor	Best Available				x		None
Validation	Many Sources			x			None
Theoretical understanding	Agreed			x			Speculative
Choice space	Wide				x		None
Justification	Full				x		Speculative
Agreement amongst peers	complete				x		None
Overall pedigree score		1.375					

Influence on results of model assumption 5			
Greatly determines model results	2	x	2
Greatly determines results of modelling step	1		
Only local influence	0		

Table 27. Mapping of model assumption 6 (of the Greek SDM).

Model assumption 6: The temporally uniform distribution of water demand, water sources, energy demand, energy production and food production on a yearly basis.	
Location: structure	**Location:** structure
Nature of uncertainty: variability	**Nature of uncertainty:** variability

Strength of model assumption 6							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact				x		Poor
Empirical basis	Observation				x		Speculative
Methodological rigour	Best Available				x		None
Validation	Many Sources			x			None
Theoretical understanding	Agreed	x					Speculative
Choice space	Wide				x		None
Justification	Full				x		Speculative
Agreement amongst peers	complete				x		None
Overall pedigree score				**1.5**			

Influence on results of model assumption 6			
Greatly determines model results	2	x	**2**
Greatly determines results of modelling step	1		
Only local influence	0		

Table 28. Mapping of model assumption 7 (of the Greek SDM).

Model assumption 7: Freshwater resources modelled as a whole, without the distinction between surface water and groundwater.	
Location: context	**Location:** context
Nature of uncertainty: variability	**Nature of uncertainty:** variability

Strength of model assumption 7							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact				x		Poor
Empirical basis	Observation				x		Speculative
Methodological rigour	Best Available				x		None
Validation	Many Sources			x			None
Theoretical understanding	Agreed	x					Speculative
Choice space	Wide			x			None
Justification	Full			x			Speculative
Agreement amongst peers	complete					x	None
Overall pedigree score		1.625					

Influence on results of model assumption 7			
Greatly determines model results	2	x	2
Greatly determines results of modelling step	1		
Only local influence	0		

Table 29. Mapping of model assumption 8 (of the Greek SDM).

Model assumption 8: Classification of crops in 14 distinct crop categories.	
Location: structure	**Location:** structure
Nature of uncertainty: variability	**Nature of uncertainty:** variability

Strength of model assumption 8							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact		x				Poor
Empirical basis	Observation			x			Speculative
Methodological rigour	Best Available			x			None
Validation	Many Sources	x					None
Theoretical understanding	Agreed	x					Speculative
Choice space	Wide			x			None
Justification	Full						Speculative
Agreement amongst peers	complete	x					None
Overall pedigree score		**2.625**					

Influence on results of model assumption 8			
Greatly determines model results	2	x	**2**
Greatly determines results of modelling step	1		
Only local influence	0		

Table 30. Mapping of model assumption 9 (of the Greek SDM).

Model assumption 9: Different yield coefficients of each crop type in each RBD were used as provided by the Hellenic Statistical Authority (ELSTAT) for base year 2010. Yield coefficients remain constant in time.	
Location: *input uncertainty*, the uncertainty concerns the input variable "agricultural production yield coefficient"	**Location:** *input uncertainty*, the uncertainty concerns the input variable "agricultural production yield coefficient"
Nature of uncertainty: *epistemic*	**Nature of uncertainty:** *epistemic*

Strength of model assumption 9							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact	x					Poor
Empirical basis	Observation				x		Speculative
Methodological rigor	Best Available			x			None
Validation	Many Sources			x			None
Theoretical understanding	Agreed		x				Speculative
Choice space	Wide				x		None
Justification	Full		x				Speculative
Agreement amongst peers	complete		x				None
Overall pedigree score		**2.4**					

Influence on results of model assumption 9			
Greatly determines model results	2		**0**
Greatly determines results of modelling step	1		
Only local influence	0	x	

Table 31. Mapping of model assumption 10 (of the Greek SDM).

Model assumption 10: Different meat, milk, eggs, and honey yield coefficients per type of animal per head in each RBD were used as provided by the Hellenic Statistical Authority (ELSTAT) for base year 2010. Animal production yield coefficients remain constant in time.	
Location: *input uncertainty*, the uncertainty concerns the input variable "livestock production yield coefficient"	**Location:** *input uncertainty*, the uncertainty concerns the input variable "livestock production yield coefficient"
Nature of uncertainty: *epistemic*	**Nature of uncertainty:** *epistemic*

Strength of model assumption 10							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact	x					Poor
Empirical basis	Observation			x			Speculative
Methodological rigor	Best Available		x				None
Validation	Many Sources		x				None
Theoretical understanding	Agreed			x			Speculative
Choice space	None			x			Wide
Justification	Full			x			Speculative
Agreement amongst peers	complete		x				None
Overall pedigree score		**2.4**					

Influence on results of model assumption 10			
Greatly determines model results	2		**0**
Greatly determines results of modelling step	1	x	
Only local influence	0	x	

Table 32. Mapping of model assumption 11 (of the Greek SDM).

Model assumption 11: Agricultural value of crop and livestock products is determined per unit of produced goods according to ELSTAT values for the base year 2010. The values per unit of agricultural products (crop, livestock) are kept constant through time.	
Location: *input uncertainty*, the uncertainty concerns the input variable "agricultural value per crop/livestock unit"	**Location:** *input uncertainty*, the uncertainty concerns the input variable "agricultural value per crop/livestock unit"
Nature of uncertainty: *variability*	**Nature of uncertainty:** *variability*

Strength of model assumption 11							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact	x					Poor
Empirical basis	Observation				x		Speculative
Methodological rigour	Best Available			x			None
Validation	Many Sources			x			None
Theoretical understanding	Agreed	x					Speculative
Choice space	None			x			Wide
Justification	Full			x			Speculative
Agreement amongst peers	complete			x			None
Overall pedigree score		**2.4**					

Influence on results of model assumption 11			
Greatly determines model results	2		**1**
Greatly determines results of modelling step	1	x	
Only local influence	0		

Table 33. Mapping of model assumption 12 (of the Greek SDM).

Model assumption 12: The values of water losses coefficients for different irrigation technologies were set according to the suggested literature value ranges and calibrated to fit Greek reported agricultural water demand data.	
Location: *parameter*	**Location:** *parameter*
Nature of uncertainty: *variability*	**Nature of uncertainty:** *variability*

Strength of model assumption 12							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact				x		Poor
Empirical basis	Observation	x					Speculative
Methodological rigour	Best Available				x		None
Validation	Many Sources	x					None
Theoretical understanding	Agreed				x		Speculative
Choice space	None					x	Wide
Justification	Full			x			Speculative
Agreement amongst peers	complete				x		None
Overall pedigree score		1.75					

Influence on results of model assumption 12			
Greatly determines model results	2		**1**
Greatly determines results of modelling step	1	x	
Only local influence	0		

Table 34. Mapping of model assumption 13 (of the Greek SDM).

Model assumption 13: The values of per capita residential and touristic water consumption were set according to suggested literature ranges and calibrated to fit reported urban water demands.	
Location: *parameter*	**Location:** *parameter*
Nature of uncertainty: *variability*	**Nature of uncertainty:** *variability*

Strength of model assumption 13							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact					x	Poor
Empirical basis	Observation	x					Speculative
Methodological rigour	Best Available						None
Validation	Many Sources	x					None
Theoretical understanding	Agreed				x		Speculative
Choice space	None					x	Wide
Justification	Full				x		Speculative
Agreement amongst peers	complete				x		None
Overall pedigree score		1.375					

Influence on results of model assumption 13			
Greatly determines model results	2		**1**
Greatly determines results of modelling step	1	x	
Only local influence	0		

Table 35. Mapping of model assumption 14 (of the Greek SDM).

Model assumption 14: The definition of a base line scenario holds the assumption that decarbonisation policy cannot be taken for granted. Instead a business as usual scenario is defined as the base line scenario.	
Location: structure	**Location:** structure
Nature of uncertainty: variability	**Nature of uncertainty:** variability

Strength of model assumption 14							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact		x				Poor
Empirical basis	Observation		x				Speculative
Methodological rigour	Best Available			x			None
Validation	Many Sources			x			None
Theoretical understanding	Agreed			x			Speculative
Choice space	None			x			Wide
Justification	Full			x			Speculative
Agreement amongst peers	complete	x					None
Overall pedigree score		**2.5**					

Influence on results of model assumption 14			
Greatly determines model results	2		**2**
Greatly determines results of modelling step	1		
Only local influence	0		

Table 36. Mapping of model assumption 15 (of the Greek SDM).

Model assumption 15: The values of National Factors Power Plant were taken from the E3ME model and are the same values for the whole of Greece. These factors were categorized in 8 groups (Coal, Oil, Gas, Solar, Wind, Hydro and Biomass) and these values were used to estimate the electricity generated in GWh of each RBD of Greece by multiplying each factor with the corresponding value of each group.	
Location: parameter	**Location:** parameter
Nature of uncertainty: variability	**Nature of uncertainty:** variability

Strength of model assumption 15							
		Pedigree score					
Criteria	**Highest score**	4	3	2	1	0	**Lowest score**
Proxy	Exact				x		Poor
Empirical basis	Observation		x				Speculative
Methodological rigor	Best Available			x			None
Validation	Many Sources		x				None
Theoretical understanding	Agreed			x			Speculative
Choice space	None				x		Wide
Justification	Full			x			Speculative
Agreement amongst peers	complete				x		None
Overall pedigree score		**1.875**					

Influence on results of model assumption 15			
Greatly determines model results	2		**1**
Greatly determines results of modelling step	1	x	
Only local influence	0		

Table 37. Mapping of model assumption 16 (of the Greek SDM).

Model assumption 16: The initial values of areas of land uses were taken by ELSTAT which was assumed to be the most trustworthy data source. The land uses were categorized into the following groups according to crop or cattle species: fruits, rice, fodder permanent, fodder temporary, tobacco, cotton, sugar beet, pulses, potatoes, vegetables, olives, other cereals, citrus, maize and beehives, cattle heads, sheep heads, buffaloes heads, goats heads, swine heads, horses/donkeys heads, rabbits heads, poultry heads respectively.	
Location: Input	Location: Input
Nature of uncertainty: Variability	Nature of uncertainty: Variability

Strength of model assumption 16							
		Pedigree score					
Criteria	Highest score	4	3	2	1	0	Lowest score
Proxy	Exact				x		Poor
Empirical basis	Observation			x			Speculative
Methodological rigor	Best Available		x				None
Validation	Many Sources			x			None
Theoretical understanding	Agreed			x			Speculative
Choice space	None					x	Wide
Justification	Full			x			Speculative
Agreement amongst peers	complete		x				None
Overall pedigree score		**1.875**					

Influence on results of model assumption 16			
Greatly determines model results	2	x	**2**
Greatly determines results of modelling step	1		
Only local influence	0		

Table 38. Mapping of model assumption 17 (of the Greek SDM).

Model assumption 17: The monthly water demand for each crop was set according the literature based on data for Cyprus with the assumption that the water crops needs are the same in all the RBDs. The data were calibrated to fit the Greek water irrigation demand recorded by ELSTAT.	
Location: input	Location: input
Nature of uncertainty: variability	Nature of uncertainty: variability

Strength of model assumption 17							
		Pedigree score					
Criteria	Highest score	4	3	2	1	0	Lowest score
Proxy	Exact			x			Poor
Empirical basis	Observation		x				Speculative
Methodological rigor	Best Available			x			None
Validation	Many Sources			x			None
Theoretical understanding	Agreed		x				Speculative
Choice space	None				x		Wide
Justification	Full		x				Speculative
Agreement amongst peers	complete		x				None
Overall pedigree score		2.37					

Influence on results of model assumption 17			
Greatly determines model results	2	x	2
Greatly determines results of modelling step	1		
Only local influence	0		

Table 39. Mapping of model assumption 18 (of the Greek SDM).

Model assumption 18: The values of Emission Factors were taken from E3ME model and are the same values for the whole Greece. The Emission Factors were categorized in 6 groups and each group was divided in more subgroups: Coal Emission Factors (Power Generation, ETS Industry), Gas Emission Factors (ETS Industry, non-ETS Industry, non-ETS Transportation, Household, Other), Oil Emission Factors (Power Generation, ETS Industry, non-ETS Industry, Other, Construction, Agricultural, Household, ETS Transportation, non-ETS Transportation), Biomass Emission Factors (Power Generation), Agricultural Factors (Cattle, Sheep/Goats, Swine, Horses/Donkeys, Manure, Rice, Managed Agricultural Soil, Field Burning, Urea) and LULUCF Factors (Cropland, Grassland, Forest, Wetlands).	
Location: parameter	Location: parameter
Nature of uncertainty: variability	Nature of uncertainty: variability

Strength of model assumption 18							
		Pedigree score					
Criteria	Highest score	4	3	2	1	0	Lowest score
Proxy	Exact				x		Poor
Empirical basis	Observation		x				Speculative
Methodological rigor	Best Available			x			None
Validation	Many Sources		x				None
Theoretical understanding	Agreed			x			Speculative
Choice space	None				x		Wide
Justification	Full			x			Speculative
Agreement amongst peers	complete				x		None
Overall pedigree score		**1.875**					

Influence on results of model assumption 18			
Greatly determines model results	2		**1**
Greatly determines results of modelling step	1	x	
Only local influence	0		

Table 40: Sensitivity Index of crops (Greek SDM).

Crops	Sensitivity index
COTTON	0.065
FODDER PERMANENT	0.048
OLIVES	0.025
MAIZE	0.024
RICE	0.023
FRUITS	0.019
OTHER CEREALS	0.017
CITRUS	0.013
VEGETABLES	0.007
FODDER TEMPORARY	0.006
TOBACCO	0.003
POTATOES	0.002
PULSES	0.002
SUGAR BEET	0.002

Table 41: Sensitivity Index of livestock (Greek SDM).

Cattle species	Sensitivity index
SHEEP HEADS	0.327
SWINE HEADS	0.262
CATTLE HEADS	0.260
GOAT HEADS	0.128
HORSES/DONKEYS HEADS	0.009
RABBITS HEADS	0.006
POULTRY HEADS	0.006
BEEHIVES	0.000
BUFFALOES HEADS	0.000

Table 42: Sensitivity Index of Emission Factors (Greek SDM).

Emission factors	Sensitivity index
WETLANDS (LULUCF)	0.000
RICE(AGRI)	0.000
UREA (AGRI)	0.000
NON-ETS TRANSPORTATION (GAS)	0.000
SWINE (AGRI)	0.001
HORSES/DONKEYS (AGRI)	0.002
POWER GEN (GAS)	0.003
OTHER (GAS)	0.005
POWER GEN (OIL)	0.005
NON-ETS INDUSTRY (GAS)	0.007
CONSTRUCTION (OIL)	0.008
HOUSEHOLD (GAS)	0.009
MANURE (AGRI)	0.009
CROPLAND (LULUCF)	-0.009
OTHER (OIL)	0.011
GRASSLAND (LULUCF)	-0.011
NON-ETS INDUSTRY (OIL)	0.018
ETS INDUSTRY(GAS)	0.018
ETS-TRANSPORTATION (OIL)	0.019
ETS INDUSTRY(COAL)	0.022
FOREST (LULUCF)	-0.034
SHEEP/GOATS (AGRI)	0.051
CATTLE (AGRI)	0.056
AGRI (OIL)	0.077
HOUSEHOLD (OIL)	0.086
ETS-INDUSTRY (OIL)	0.094
MANAGED AGRI SOIL (AGRI)	0.150
NON-ETS TRANSPORTATION (OIL))	0.387

Review comments

ADDRESSING REVIEWERS' COMMENTS	
Comment	**Response**
1. Many thanks for sending over this excellent report. It includes the main aspects that I would expect to see and I therefore do not recommend major additions or revisions to structure. Some general thoughts:	A large effort was made to take into account all reviewer comments, in order to overcome the weaknesses identified by the reviewer. These changes are described below.
2. In a recent conference paper I was considering the link between uncertainty and optimisation. I realised there is a classic contra-positive relationship: empirical modelling rejects perfect knowledge and therefore cannot optimise. But optimisation models assume optimisation (rational behaviour) and therefore are forced to assume perfect knowledge (i.e. it is not a leading, or maybe even intentional, decision). As in Sim4Nexus there is a variety of simulation and optimisation models, maybe this can be brought in somewhere?	We have extended the conceptual comparison of optimisation and simulation models in section 2.5 ('uncertainty in different types of models') accordingly. As suggested, the section now also explicitly compares the implications of fundamental uncertainty for the feasibility of optimisation and simulation approaches. The respective assumptions regarding perfect/imperfect knowledge have also been added to table 3.
3. A more theoretical point about Bayesian statistics – maybe this could be mentioned somewhere. I raise it because you talk about complexity and the complexity scientists stress this point. But from my (very basic) understanding, the existence of fundamental uncertainty means that the standard calculations don't work and we end up with the situation described above.	We have added a paragraph on the limits of statistical methods in the context of fundamental uncertainty, in which not all relevant possible outcomes are known (at the end of section 2.2, 'risk versus uncertainty'). These limits apply both to frequentist and Bayesian statistics.
4. I wonder about whether it would be possible to say a bit more on how uncertainty is treated in different models. E.g. the climate models have a treatment of risk as standard, but this is because of the limited number of inputs/outputs (as you say and the section on CAPRI also discusses). Are there any good examples of uncertainty analysis (i.e. beyond basic sensitivity analysis) in the other modelling approaches?	We have included a new paragraph which includes various references to useful examples for the analysis and communication of uncertainties in different contexts and fields of science (at the beginning of section 3), including a range of quantitative and qualitative methodologies.
5. It could be good to mention somewhere delphi analysis, as initially developed by the RAND corp. This is a very good example of where models could be used to inform uncertainty, but in a setting where scenarios are developed in a much more qualitative manner through expert interaction.	We have added a paragraph on Delphi Method analysis (at the end of section 3.2.3), in which we discuss the potential usefulness of quantitative models to inform such forms of analysis.

6. In Section 4, there seems to be a missing discussion on how the agents in the model view uncertainty. For the SDM this may not be relevant as system dynamics is an accounting rather than behavioural framework. But CAPRI mentions equilibrium and comparative statics, so I guess has an assumption about perfect knowledge? It seems an important omission given some of the earlier discussion. Similarly, gaps in knowledge is a key assumption in E3ME/FTT, which is discussed but only as a specific assumption.	For CAPRI, we have added a new paragraph that explicitly discusses this model's assumptions regarding perfect knowledge and agent behaviour (beginning of section 4.2). For E3ME-FTT, we have now also clarified at the beginning of the respective sub-section (4.3) that the model does not assume perfect knowledge or optimising behaviour. For the SDM, we have added a paragraph which explains that the model is based on an accounting framework, and behavioural assumptions are thus of secondary importance in this context (section 4.1.2).
7. Section 4.3.4 is very interesting, and may be publishable in its own right. To me, the assumption being questioned is rational behaviour, rather than uncertainty. This comes back to the point above about how the two are linked – with perfect knowledge loss aversion wouldn't really make sense. Having said that, I appreciate that this section is on model uncertainty rather than agent uncertainty.	We have clarified in the beginning of section 4.3.4 that the focus in this section is indeed on analysing the uncertainty regarding human behaviour from the perspective of the modeller. We have also included a new reference to section 2.3, in which this important distinction is discussed in more detail.
8. I would be hesitant to describe the models in Sim4Nexus as 'complex'. This is stretching the definition a bit and could be challenged by ABM operators.	We have clarified in the introduction (footnote 1) that 'complex' is meant in the sense that the models in Sim4Nexus deal with dynamic systems (such as agriculture or the economy), which are represented within the respective models by means of a large number of interacting variables.
9. On the SDM (and lesser extent E3ME-FTT), the assumptions feel more like approaches internal to the modelling effort. E.g. Assumption 1 states that some issues are 'not modelled'. If I have interpreted correctly, the assumption used instead is either that they don't change (i.e. not impacted by the other areas) or that they do change but it doesn't matter (i.e. don't have feedback effects). NB this section is very long, would it be better to put the discussion of the individual assumptions into an appendix and just a summary in the main text?	We have added a paragraph (within section 4.1.2) which clarifies that the model assumptions 1-3 of the SDM are essentially similar to assuming that the modelled variables do not change. As any changes would be unlikely to have strong impacts on the model end results, they can safely be ignored. As suggested by the reviewer, we have considerably shortened the section on the SDM, by moving all pedigree tables into a new appendix section.
10. The current version of E3ME-FTT has 61 regions – I believe this is the version being used in Sim4Nexus.	The number of regions which are modelled by E3ME-FTT has been corrected to 61.
11. The first sub-heading in 4.3.4.2 should be 'reference dependent'.	The spelling error in the sub-heading has been corrected.

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