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ENvironmental Success under Uncertainty and Risk (ENSURe): A procedure for probability evaluation in ex-ante LCA

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A R T I C L E I N F O

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A B S T R A C T

In a context of ecological emergency, ex-ante Life Cycle Assessment (LCA) can be used to prioritize investments into technological concepts that are expected to make human activities less damaging to ecosystems and humans. Yet forecasts about the future environmental success of technological concepts come with high incertitude and require careful appraisal of the distinct levels of knowledge associated with the technology's indeterminacies. This study introduces the algorithmic procedure ENSURe (ENvironmental Success under Uncertainty and Risk) to apply ex-ante LCA when incertitude can be decomposed into risk, manageable with probability distributions, and uncertainty, a lack of knowledge so problematic that it prevents from defining probability distributions. The procedure applies a scenario discovery algorithm to identify combinations of requirements on the most uncertain factors to ensure a minimum conditional probability of success which stems exclusively from risk. The analysis of these requirements allows evaluating whether the total probability of success for the technological concept is above a decision-threshold. The procedure is demonstrated on the case of ex-ante LCA applied to the production of new microalgal compounds for health-management in fish farming. ENSURe can be extended to any type of model used to inform decisions under the co-existence of risk and uncertainty.

1. Introduction

In the wake of Collingridge's Social Control of Technology (Collingridge, 1980) and Beck's Risk Society (Beck, 1992) in the 1980–1990's, the field of Responsible Research and Innovation (RRI) (Owen et al., 2013) has problematized and advocated for a limitation of the undesired consequences of technological developments. Within this context, different types of models within industrial ecology and system analysis have provided decision support to various complex cases involving the interactions between the environment, people and industry to plan and anticipate. Among these approaches, ex-ante Life Cycle Assessment (LCA) (intended as "an LCA performed before the technology exists") stands out as a systemic and holistic ex-ante assessment of productive systems which leaves aside the retrospective scope of conventional LCA, allowing it to inform responsible innovation (Wender et al., 2014). Van der Giesen et al. (2020) describe the aim of ex-ante LCA as *"to guide R&D decisions to make a new technology environmentally competitive as compared to the incumbent technology mix"*. In this paradigm, ex-ante LCA does not forecast the future (Cucurachi et al., 2018) but explores scenarios to find the optimal technological choices to guide R&D accordingly through an iterative process. Using ex-ante LCA within such an iterative improvement paradigm constitutes the "responsive" dimension (Owen et al., 2013) of RRI in which technological development dynamically responds to societal needs and ex-ante LCA provides guidance. While ex-ante LCA here provides necessary guidance for existing innovation pathways (Genus and Stirling, 2018), it does not meet the need to make decisions about whether to invest time and resources into initiating the exploration of broad technological concepts. Indeed, in an undisputable context of ecological emergency (Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services, 2019; Ipcc, 2022), policy-driven planning of technological development should prioritize concepts that are likely to significantly improve the environmental performance of human activities.

Ex-ante LCA has been applied to specific, well-defined emerging technologies such as CO_2 reduction to formic acid production (Thonemann and Schulte, 2019), milk ultra-high-pressure homogenization (Valsasina et al., 2017) and front-side metallization of photovoltaic cells (Blanco et al., 2020). In this article however, we consider the use of ex-ante LCA in a context of an urgent need for decisions about which

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technological concepts should be further explored. Initiating research regarding a technological concept can eventually lead to different technological outcomes because these concepts are generally formulated as broad and open questions such as *"What about using microalgae in fish farms?"* or *"Should we look for seaweed to improve cattle production?"*. The exact modalities, such as function, location, design, and performance of the final technologies remain undefined. Ideally the decision makers of the innovation ecosystem (Carraresi and Bröring, 2022) in which such a technological concept emerges, from private entrepreneurs to politicians, should be informed early on about the probability of the concept to develop into a successful technology. Success here intended as improving environmental performance compared to a baseline situation. This exercise of projection of the uncertain consequences of a decision is already carried out by companies that forecast Return on Investment (ROI) (Magni, 2015) considering incomplete information and perform Real option-analysis (Block, 2007; Lee, 2011) for strategic decision-making where the value of specific performance indicators is compared to defined thresholds. At the policy level also, the European states' budgets are for instance disciplined based on arbitrary threshold deficit values together with additional assumptions on future financial balance evolutions (Priewe, 2020). Ex-ante LCA could be used in this same logic across the innovation ecosystem and as soon as concepts emerge, thus replacing financial indicators by environmental and social ones. Decision makers would invest time and resources in the exploration of a technological concept based on a threshold that they would set as a minimum probability of success. Instead of trying to correct emerging innovation trajectories, ex-ante LCA would assist in deciding whether a concept should even be explored, acknowledging the chaotic nature of technological development (Brian, 1989; Hung and Tu, 2011), especially in the environmental domain (Pizzol and Andersen, 2022), and the difficulty to control it along a responsive process (Owen et al., 2013).

In this context, ex-ante LCA aims at projecting the limited knowledge about the possible outcome of a technological concept into the space of environmental impacts. The result of this projection, practically simulated via propagation (Mendoza Beltran et al., 2018) of the model's inputs distributions, should be presented under the form of a "probability of success" to decision makers. The term "probability" here needs to be understood as "reasonable expectation" as proposed by R.T Cox (Cox, 1946). This interpretation also overlaps with a Bayesian perspective as it reflects the degree of belief, ideally supported by knowledge regarding the realization of an indeterminate event (Blanco, 2022).

In a typical ex-ante LCA model, the result (output) is determined by the combination of several factors (inputs, also commonly referred to as parameters) that are indeterminate in the sense that they are *"not measured, counted or clearly known"*(Cambridge University Press, n.d.). In such ex-ante LCA model, some indeterminate factors come associated with reasonable levels of knowledge that allow one to propose probability distributions regarding the future state of these factors. The propagation of these probability distributions, therefore, belongs to the computation of "risk" in Wynne's and Stirling's classifications of incertitude (Stirling, 2010; Wynne, 1992). Yet, the level of knowledge about the probabilities for other indeterminate factors is so problematic (Stirling, 2010) that its projection into the impact space can deceive decision-making. Wynne (1992) and Stirling (2010) define the factors for which probability distributions can hardly be proposed, for instance because factors dependencies are supposed but cannot be modeled, as "subject to uncertainty" (instead of "risk"). The authors highlight the importance of clearly distinguishing "risk factors" from "uncertain factors" for sound decision support (Scoones, 2019; Scoones and Stirling, 2020; Stirling, 2010; Wynne, 1992).

As LCA is inherently a quantitative assessment, practitioners could be tempted to apply wide uniform distributions to uncertain factors (Bergerson et al., 2020), propagate these distributions together with the risk factors, and present the results under the form of "probabilities". While this is in principle a conservative approach to uncertainty quantification in traditional stochastic models, it still conveys a misleading overestimation of confidence and knowledge (Thonemann et al., 2020; van der Giesen et al., 2020). A conscientious way of dealing with uncertain factors is to include them within *what-if* scenarios (Pesonen et al., 2000) while acknowledging that no probabilities can be assigned to their realizations. Stochastic propagation for factors with non-problematic levels of knowledge can be performed within these scenarios to generate probabilities of success which are conditional to the realizations of the scenarios. In complex cases where uncertainty is deep and defining relevant and likely scenarios cannot be done a priori, scenario discovery algorithms such as PRIM (Patient Rule Induction Method) (Bryant and Lempert, 2010) can be used as a computational algorithm to detect scenarios of interest, which are sets of intervals for indeterminate factors associated with a high proportion of cases of interest for the output. Scenario discovery was for instance used to identify different socio-economic pathways leading to the same CO_2 emissions outcomes (Guivarch et al., 2016) or discover which water management plans in Southern California would perform poorly (Groves et al., 2008). The advantage of scenario discovery is that it does not require prior knowledge of the distributions associated with uncertain factors as it allows reflecting exclusively on the probability of occurrence of the scenarios of interest. Thus, the complex decision-making process can be summarized into simpler questions provided that the scenarios of interest are based on easily interpretable factors (Bryant and Lempert, 2010).

Summing up, the joint presence of risk and uncertainty when attempting to decide on broad technological concepts means that ex-ante LCA is performed under a condition of "deep uncertainty" (Kwakkel and Jaxa-Rozen, 2016; van der Giesen et al., 2020) which means that the calculation of probabilities of impacts relies on problematic levels of knowledge. Deep uncertainty therefore prevents quantification and leaves decision makers and analysts with the sole options of "recognizing it", "managing it" (Funtowicz and Ravetz, 1993), abiding by a precautionary principle (Van Asselt and Vos, 2006) or postponing the decision until new knowledge has been acquired, thus transforming an uncertainty problem into a risk problem (Scoones and Stirling, 2020). In a complex context of environmental emergency, such a postponement is detrimental and decisions for technological planning still need to be made (Ipcc, 2022). We here address this need for informed decisions without using probability distributions to represent uncertainty while still being able to compare a probability of technological success with a decision threshold.

In this work, we present ENSURe (ENvironmental Success under Uncertainty and Risk), an algorithmic procedure to unveil if the total probability of success of a conceptual technology, in relation to environmental performance, exceeds a stipulated threshold. By combining the forms of incertitude from Stirling and Wynne, the prospective modeling approach, and the computational power of scenario discovery, ENSURe constitutes a novel approach which helps evaluating probabilities of success when both uncertainty and risk apply. We thus work towards more robust decision-making in the post-normal science age (Funtowicz and Ravetz, 1993), defined by high stakes and incertitude.

While the approach suits any model-based decision problem featuring factors subjected to risk and uncertainty, we demonstrate the ENSURe procedure with ex-ante LCA used to support a decision on whether time and resources should be spent on bioprospecting for new microalgal compounds (Jouannais and Pizzol, 2022) to enhance fish-health management. This case constitutes a deeply uncertain concept regarding the technological outcomes, is based on recent discoveries (Falaise et al., 2016; Krohn et al., 2022; Patel et al., 2021; Talero et al., 2015; Yaakob et al., 2014) showing interesting bioactivities of some microalgal compounds at laboratory scale and potential beneficial effects on fish health, resistance to diseases and growth performance (Lieke et al., 2020). This ex-ante LCA case study is well-suited to the demonstration of the methodology as it is based on a parameterized LCA models featuring dozens of factors subject to risk or uncertainty.

2. Methods

This section first provides a definition of the terms used throughout the study (Sect. 2.1) and a formalization of the decision-making problem (Sect. 2.2). The ENSURe procedure is then explained in its generalized form (Sect. 2.3), i.e., for any model type, before the ex-ante LCA case application is detailed in Section 3.

2.1. Definitions of uncertainty, risk and indeterminacy

The definition of "uncertainty" is the subject of semantical debate. While Wynne (1992) defines different forms of "uncertainty" as risk, uncertainty, ignorance and indeterminacy, Stirling (2010) presents a typology of "incertitude" as risk, uncertainty, ambiguity, and ignorance. The common categories cover the same concepts, but Wynne's typology is ambiguous as it defines uncertainty as a type of uncertainty. In this work we pragmatically use "indeterminacy" as anything that prevents the modeler from using single deterministic values for factors in a model. We therefore interpret Stirling's typology of incertitude as "states of knowledges" regarding indeterminacy. Some factors in a model are therefore "indeterminate" from an ex-ante perspective, which means that one type of incertitude applies on them. "Uncertain factors" are specifically subject to uncertainty intended in Stirling's terms: they are associated with a problematic level of knowledge regarding their probability distributions. "Risk factors" are factors subjected to risk only.

2.2. Formalization of the decision-making problem

We define "a success", as a desired outcome regarding the phenomena that the model assesses. For example, in the case of ex-ante LCA, a success can be a technological concept eventually leading to a novel technology environmentally outperforming a baseline in specific impact categories. The baseline is case-specific and can be a fixed impact value, chosen for instance as a desirable minimum or maximum environmental impact, or a comparison with an alternative projected in the future in absence of the concept. In the case under analysis the decision to incentivize or invest into this technological concept is taken only if it can be shown that the total probability of success is higher than a decision threshold. We define "the total probability of success" as the overall probability of success for the technological concept. For a case where only risk would apply, the total probability of success would be approximated by the proportion of simulations leading to a success after the propagation of the input distributions. The adjective "total" is chosen to contrast with the "conditional" probabilities that are manipulated during the procedure. By definition, this total probability of success is inaccessible a priori as the decisions are taken under deeply uncertain conditions but ENSURe will allow comparing it to the decision threshold

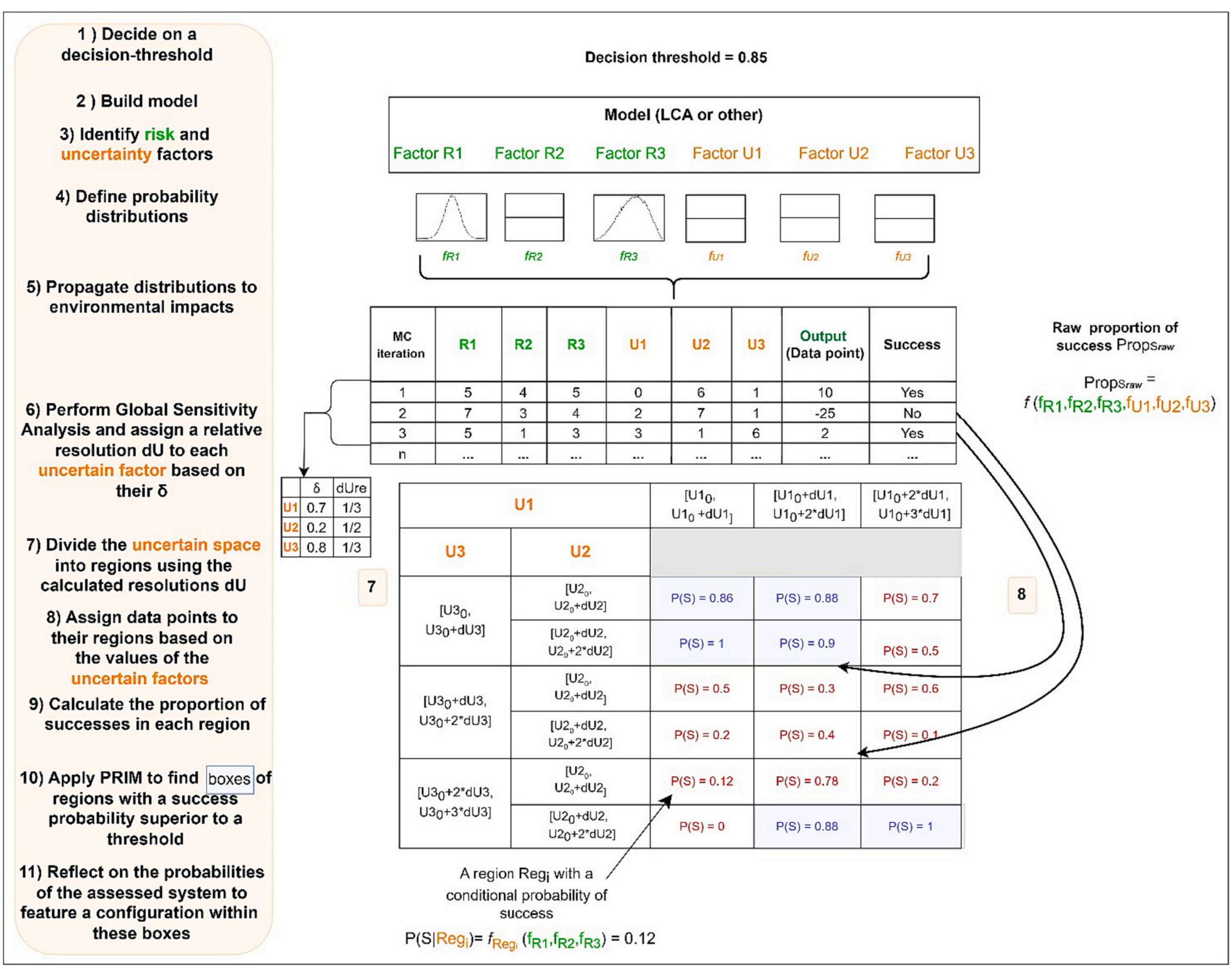

Fig. 1. Step-by-step representation of the ENSURe procedure. P(S): probability of a success, here represented as equal to the proportion of successes. Ux_0 is the minimal value in the range for Ux. The presented mathematical notations are further developed in SI A.1.

of the decision-makers.

2.3. ENSURe procedure

The objective of ENSURe is to discover sets of value ranges for the uncertain factors that are associated with outcomes for which the probability of success is superior to the decision threshold. The space of technology configurations contained within such a set of value ranges is called a "box", following the original terminology by Friedman and Fisher (1999) who developed the algorithm to identify such boxes (cf. 2.3.3).

This procedure allows reflecting only on the probability of the final technology having such a configuration instead of trying to define a priori reasonable probability distributions for all uncertain factors. Fig. 1 illustrates the step-by-step algorithmic procedure of ENSURe which is further explained in the following paragraphs. A mathematical formulation of the procedure and underlying theory is available in SI A.1.

The procedure starts by defining a decision-threshold for the decision-making problem (cf. 1 in Fig. 1) and building the associated model (cf. 2 in Fig. 1).

2.3.1. Uncertainty and risk propagation

All indeterminate factors, whether they are subject to risk or uncertainty (cf. 3 in Fig. 1), are first propagated jointly via a Monte Carlo sampling scheme according to their distributions (cf. 4 and 5 in Fig. 1). The establishment of probability distributions for the risk factors can be performed using approaches such as expert elicitation (Huijbregts, 1998; O'Hagan, 2019), statistical analysis regarding phenomena which are similar to the modeled ones (Jouannais and Pizzol, 2022; Tu et al., 2018) and pedigree matrices (Ciroth et al., 2016). The uncertain factors are instead sampled using uniform distributions defined within arbitrarily large boundaries while abiding by physical and logical constraints (cf. example in 3.3). Uniform distributions are chosen due to the lack of knowledge that could justify another distribution and because they are the easiest option to populate the uncertain space with an even number of points in all regions, which is suitable for the following steps of the procedure. Each output of the model constitutes a data point, and the successes are identified among the points.

2.3.2. Regionalization of the uncertain input space for conditional probabilities of success

The proportion of successes among the data points resulting from the joint propagation of all factors ($Prop_{S_{raw}}$,cf. 5 in Fig. 1) cannot be interpreted as a total probability of success as this would boil down to treating uncertainty as risk, i.e. considering that the uniform distributions assigned to the uncertain parameters were chosen based on an acceptable level of knowledge. The only probabilities that should be assessed are those exclusively stemming from the propagation of risk. Thus, only probabilities which are conditional to specific, fixed combinations of values for the uncertain factors should be assessed.

We cannot assess all combinations of uncertain factors to calculate conditional probabilities of success as this would lead to an infinite number of assessments. Therefore, the regionalization aims at assessing these conditional probabilities of success into small regions of the uncertain space, instead of for specific combinations of uncertain factors' values. To do so, each uncertain factor's range is divided into intervals of equal factor-specific length. For instance, a range from 0 to 100 m for a factor *Ua* is divided into 10 intervals of length 10 m. This length is the resolution *dUa* for this uncertain factor. The resolution divided by the total range is called the relative resolution dUa_{re}, which is also the inverse of the number of intervals (e.g., factor *Ua* has a relative resolution of 1/10). This segmentation of all uncertain factor's ranges divides the entire uncertain space defined by the ranges of the uncertain factors into small y-dimensional regions *Reg* of dimensions $\{dU1, dU2, \ldots, dUy\}$ where y is the total number of uncertain factors (cf. 7 in Fig. 1). Each region contains the data points for which the uncertain factors' values are between the limits of the region (cf. 8 in Fig. 1). The smaller the regions are, the closer the proportions of successes within the region gets to conditional probabilities of success stemming exclusively from the propagation of risk factors. Indeed, the propagation of the chosen distribution for an uncertain factor *Ua* in such region is limited to the factor's variation over a small interval *dUa*.

To limit the number of regions to assess, we assign the number of intervals, i.e. 1/dUre, for each uncertain factor based on its sensitivity (cf. 6,7 in Fig. 1). The latter is measured with the Borgonovo's delta index δ (Borgonovo and Iooss, 2016) regarding the difference of impact between the technological concept and the alternative. Borgonovo's approach (Borgonovo and Iooss, 2016) is a density-based global sensitivity analysis (GSA) and δ is based on the area difference between the output density and the conditional output density for a fixed value of the factor, averaged over all its values. δ is therefore a moment-independent measure, as it considers the whole output distribution instead of a specific moment for variance-based sensitivity analysis. Alternatively, variance-based sensitivity measures could be chosen, such as the Sobol index (Saltelli, 2002). The analyst decides on a minimum and maximum relative resolution, i.e., a maximum and minimum number of intervals, to assign respectively to the most and least sensitive uncertain factors. The number of intervals for all the other uncertain factors is calculated between these two extremes as inversely proportional to their delta index δ via the equation presented in SI A.2. Thus, the more sensitive an uncertain factor is, the less it is permitted to vary in the regions in which the conditional probabilities of success are assessed. A value of 1 for the maximum relative resolution, implies that the probability distribution associated with the least sensitive factor is fully treated as risk (with a uniform distribution) and its influence on the probability assessment is considered neglectable. We can therefore approach true conditional probabilities of success, exclusively dependent on the propagation of risk factors, by decreasing the minimum and maximum relative resolutions.

Overall, the regionalization step is necessary to approach conditional probabilities of success across the entire uncertain space without resorting to a computation of these for each combination of uncertain factors.

2.3.3. Scenario discovery (PRIM) to reveal uncertain boxes of success

Once the regions *Reg* have been defined, the empty regions that happened not to contain any data point are discarded and the proportions of successes, i.e., conditional probabilities of success, are assessed in the remaining ones (cf. 7,8 in Fig. 1). Then, the PRIM (Patient Rule Induction Method) algorithm (Friedman and Fisher, 1999) is applied to discover boxes of regions, i.e., groups of regions, that are associated with a probability of success superior to the decision threshold (cf. 10 in Fig. 1). Note that this means that PRIM is applied over the regions and not over the data points resulting from the stochastic propagation of the distributions through the model (cf. Fig. 1). The PRIM algorithm is designed to iteratively select "boxes" with a high predictive potential for an output of interest within a multidimensional input set. By applying a "hill climbing optimization procedure" (Friedman and Fisher, 1999), PRIM iteratively "peels-off" sub-boxes, i.e. discards sub-boxes of the input variables while maximizing an objective function to increase the predictive potential of the resulting box regarding the output of interest. The exact objective function and the settings ruling PRIM are chosen by the analyst depending on its goal (cf. 2.3.4). In this study we used the PRIM python implementation proposed by Kwakkel and Jaxa-Rozen (2016). For each iteration of PRIM, the box with the highest density is kept and the selected data points are then removed from the sample before the next iteration is performed on the remaining points. The iterations stop when no remaining box can be found with a chosen minimum density, mass, and coverage (cf. 3.5).

The total probability of success is evaluated by the analysis of the boxes identified by PRIM. While reasonable probability distributions cannot be proposed for the uncertain factors a priori, the focus can be placed on the identified boxes only, which correspond to spaces defined by some uncertain factors only, thus drastically reducing the complexity of the problem. If the decision-makers are now sure (Probability =1) that the assessed phenomena (in our case study, a future technology development) will feature a configuration within the identified boxes, this means that the total probability of success is superior or equal to their decision threshold. This is a direct conclusion from the law of total probability with conditional probabilities detailed in SI A.1. Otherwise, it cannot be strictly concluded that the probability of success is either superior or inferior to the threshold (cf. SI A.1), uncertainty remains and the ENSURe procedure can be repeated with different settings or decision threshold (cf. 3.5 and 5.1). However, if the procedure made the decision-making problem simpler so that it can now be stated that there is a probability P(β) of the technology eventually featuring a configuration in the boxes, the total probability of success is superior to P(β) multiplied by the decision threshold (cf. SI A.1).

2.3.4. Choices and trade-offs within the ENSURe procedure

The three main phases of ENSURe, namely the Monte Carlo sampling and model simulations, the regionalization of the uncertain space into regions of conditional probabilities, and the use of PRIM, can be configurated to optimize the procedure according to the objectives. The number of data points and regions quickly get constrained by available computational resources. Dividing the uncertain factors' ranges into more interval by decreasing the minimum and maximum relative resolutions allows a more precise distinction of risk and uncertainty (cf. SI A.1) but also creates a larger number of regions with few or no data points (cf. 4.1).

The objective function for the PRIM algorithm was chosen to be the "lenient" one proposed by Kwakkel and Jaxa-Rozen (2016), which is fit for different types of variables and considers the gain of density together with the loss of observations at each peeling step. Bryant and Lempert (2010) highlight how PRIM can be used as a "scenario discovery" tool to assist policy-making under deep uncertainty by selecting boxes with the desired trade-off between *density, mass, coverage, and interpretability*. The *density* is the proportion of observations (in our case the proportion of regions) of interest in the box, *mass* is the proportion of total observation contained in the box, and *coverage* is the proportion of total observations of interest. *Interpretability* refers to the fact that having too many factors constraining the boxes makes it difficult to interpret the results for stakeholders and policy makers (Bryant and Lempert, 2010). PRIM can be parameterized with the minimal density, mass, and coverage that a box can feature.

3. Case study description and LCA application

The technological concept under study is the bioprospecting of new microalgal compounds to enhance fish health in European fish farms. This technological concept is not a unique emerging technology, as initiating bioprospecting, i.e., searching compounds of interest within biodiversity, can eventually lead to substantially different technological configurations depending on what is found and how the market integrates it (Jouannais and Pizzol, 2022). The diversity of microalgal compounds (Falaise et al., 2016) together with the diversity of fish health issues (Assefa and Abunna, 2018; Bang-Jensen et al., 2019) leave the technological outcome of this technological concept uncertain. Initiating research on this concept could for example generate a German production of powerful microalgal antibiotics tackling a particular fish pathogen at very low doses, or the production in Southern Europe of nutraceuticals which are closer to feed supplements than medicines. The diversity of outcomes associated with the development of this concept presents potential suboptimal configurations and the case thus constitutes a good example of technological concept that needs to be assessed before its development is initiated. Thus, since the future application of microalgae for health management in fish farming is characterised by deep uncertainty, this case study is very suitable for testing the method hereby proposed.

The microalgal compound production part of the LCA model and the associated indeterminacies have been modeled and studied in previous works (Jouannais et al., 2022; Jouannais and Pizzol, 2022). The LCA model used in the present study is a combination of this model with a new parameterized model of a Danish trout farm (Jouannais et al., 2023). We refer the reader to this work (Jouannais et al., 2022, 2023; Jouannais and Pizzol, 2022) for an exhaustive description. The alternative technology is the production of trout without the microalgal compound.

The next sub-sections explain the main aspects of the LCA model (cf. 2 in Fig. 1), show how the distinction between risk and uncertain parameters was made (cf. 3 in Fig. 1) and detail the choice of ENSURe's settings for the step 6 to 10 in Fig. 1.

3.1. Parameterized product system

The functional unit of the consequential LCA is 1 kg live weight of sea-reared trout before slaughtering. The trout farm corresponds to a combination of primary data from Denmark and Italy reconstituting a detailed life cycle inventory with divisions between the different growth stages from inland hatchery to sea-reared trout of 2.4 kg live weight (Jouannais et al., 2023). The microalgal compound production, which can be an input to all trout growth stages, takes place in an indeterminate production mix stochastically sampled across 10 European countries previously identified for their high potential for microalgal biomass production (Jouannais and Pizzol, 2022; Skarka, 2012). The size of a mix (number of plants) and the producing locations are therefore indeterminate. Each location of a mix produces the microalgal strain and compound in a vertical tubular reactor whose techno-operational setup is indeterminate. The life cycle inventory for the microalgal compound is obtained via a parameterized dynamic and location-specific simulation of the microalgae cultivation.

The simplified product system is shown in Fig. 2 together with three groups of indeterminate factors affecting different parts of the system. The first group covers the indeterminacy of the production and nature of the production of an indeterminate microalgal strain and compound in Europe. The second group reflects the indeterminacy of the trout farm's potential for improvement, which covers the level of losses (mortality) and the suboptimal feed conversion ratio experienced by the farm before using the compound, together with the unknown impact associated with the production of the chemotherapeutants used in the farms. This group also reflects the microalgal compound's improvement performance, i.e., the beneficial effect of the compound on the fish farm. The third group describes the indeterminacy in the background system.

3.2. Effects of factors on the compound's improvement performance and fish farm's potential for improvement

In the model, the use of microalgal compound can have a double effect to improve the biological performance in each fish growth stage. It can reduce the losses and can decrease the biological feed conversion ratio (FCR) based on two distinct factors. These effects on a growth stage are achieved with an indeterminate input amount of microalgal compound and reflect a vast range of bioactivities for the compound.

Furthermore, each growth stage division is parameterized so that it can be modeled as undergoing higher levels of losses than the current ones. This allows projecting the fish farms (with or without the compound) under different future regimes of health issues that the compound will tackle, thus modulating the farms' potential for improvement. The model does not involve explicit temporal aspects, and the factors' values simply describe the configuration of the system at time of application.

We refer the reader to Jouannais et al. (2023) for an exhaustive description of the fish farm model.

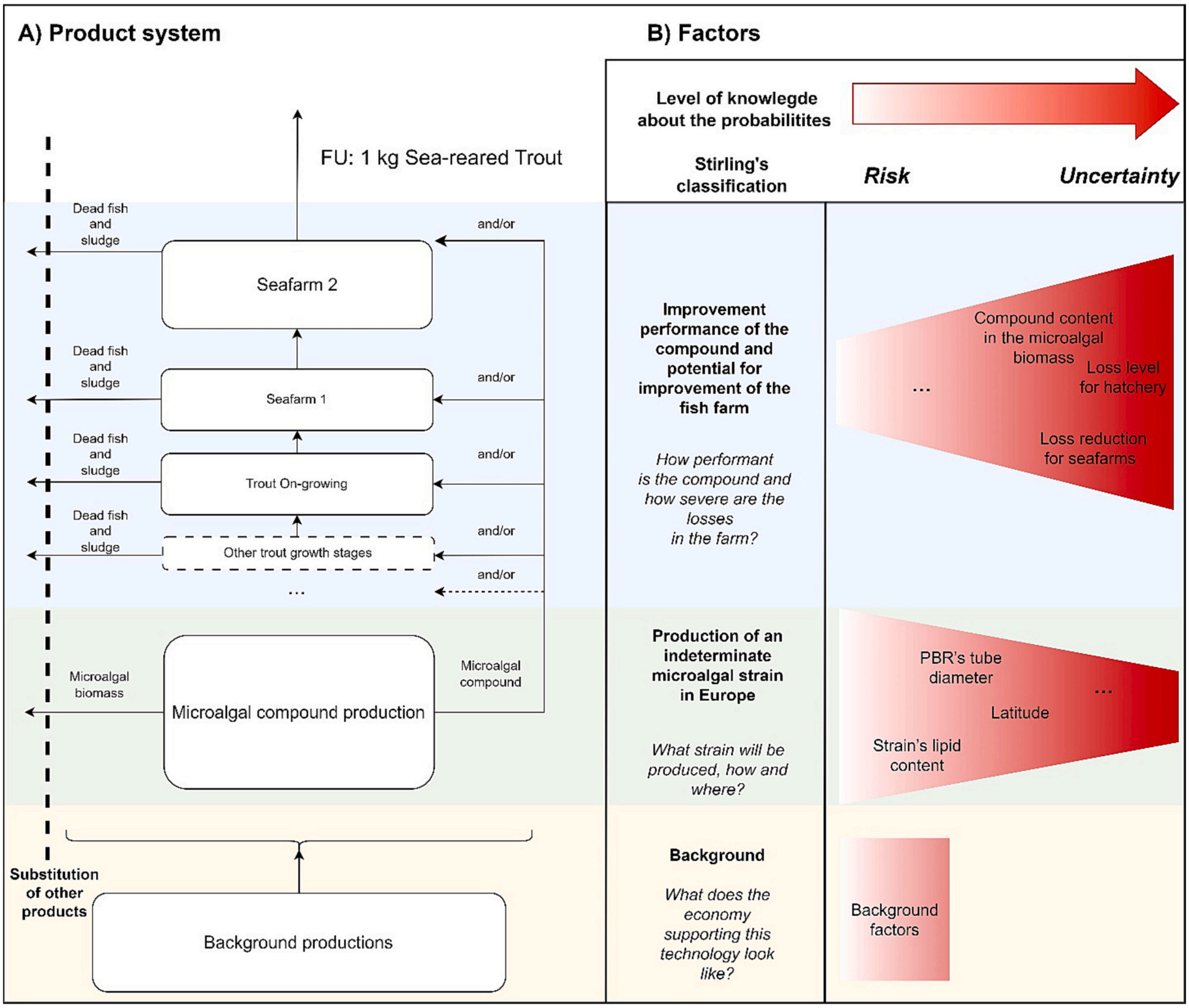

Fig. 2. A) Simplified product system for case study. B) Groups of factors affecting the system and associated level of knowledge. The groups of factors are located on the same level (same colored band) as the processes they affect in the product system. The trapeze's width illustrates the proportion of factors corresponding to the level of knowledge. No actual proportion is measured and only the trend is illustrated.

3.3. Risk and uncertain factors

While the distinction between risk and uncertainty can be obvious for some factors, the decision to categorize a factor in one category or the other is eventually subjective. This is illustrated by the intentionally fuzzy delimitation chosen by Stirling who differentiates "problematic" and "unproblematic" levels of knowledge. As show in Fig. 2, there happens to be an overlap between the three groups of factors in the product system and the associated levels of knowledge about probabilities. We used this case-specific overlap to draw a clearer distinction between risk and uncertainty factors.

Probability distributions can reasonably be proposed for the factors defining the production of an indeterminate microalgal strain in Europe which therefore classify as "risk factors". Indeed, data on microalgal biodiversity (lipid content, thermal requirements etc.) and techno-operational design of photobioreactors (tube diameter, flow rate etc.) can ground the definition of probability distributions as documented in previous works (Jouannais et al., 2022; Jouannais and Pizzol, 2022).

The background factors also classify as risk factors and the probability associated with these factors directly stem from the "uncertainties" (though not in Stirling's terms) defined within ecoinvent, which is the background LCA database. These probability functions are generated using a qualitative pedigree matrix in which the level of knowledge about the amounts reported is graded on a scale from 1 to 5 regarding the reliability, the completeness, the temporal, geographical and technological correlations, and the sample size (Ciroth et al., 2016; Muller et al., 2016). The use of the pedigree matrix is a canonical example of treating incertitude as risk because a qualitative description of the level of knowledge is mathematically converted into a probability distribution.

The factors defining the improvement performance of the compound and the potential for improvement for the farm are considered uncertain. The knowledge associated with these parameters is scarce compared to other factors and no grounded guesses can be made about their distributions. The level of knowledge for these "uncertain factors" is so problematic that the propagation of arbitrarily large uniform distributions for the factors' values allows a mere exploration of the input factor space. For instance, the uniform distributions chosen for the factors defining the loss reduction in the different growth stages range from 0 to 100 % and are therefore only constrained by logic, as losses cannot be reduced by >100 %.

All the model's factors are presented and classified in SI B.

3.4. Aggregated factors for a compound's improvement performance and a farm's potential for improvement

The LCA models used in this study are high-dimensional and allow simulation of many different configurations for the microalgae and fish farms. However, such a level of detail adds difficulty to the decision-making exercise. Indeed, it may require decision makers to form beliefs about many low-level factors that they may not be familiar with. For instance, assigning probabilities to certain regions for the FCR reduction in a specific fish growth stage (e.g., from 80 g to 1 kg) is more difficult than reflecting on the overall FCR reduction for the whole production. Overall FCR values can indeed be compared to national statistics because they constitute widely used performance indicators at the farm level.

Furthermore, applying regionalization (cf. 2.3.2) on many uncertain factors may lead to too many regions with very few data points depending on the computing resources and the total number of simulations that can be generated.

For these two reasons, namely interpretability and computability, we propose five aggregated factors that can be used to regionalize the uncertain space. These aggregated factors are calculated within the model and depend on the values of different uncertain factors to reduce the dimensionality of the problem and ease the decision-making exercise (cf. 3.5).

Four aggregated factors are used to summarize the improvement performance of the microalgal compound. First, we quantify the total dose of microalgal compound per functional unit ($g.kg^{-1}$). Second, we calculate the overall economic FCR as the ratio of feed input over the live, ready-to-sell fish output and calculate the overall economic FCR reduction induced using the compound, in % of economic FCR in the alternative production. We also calculate the overall biological FCR (feed/(dead + live fish)) reduction, in % of biological FCR and the compound content in the microalgal biomass ($g.\ g_{dried\ biomass}^{-1}$). The potential for improvement in the farm is summarized in one aggregated factor, namely the increase in loss level, i.e., the ratio of the loss level in the projected alternative over the current loss level.

These aggregated factors depend only on uncertain factors and therefore reflect exclusively uncertainty and not risk. Their mathematical definitions are available in SI A.3.

3.5. Specific ENSURe settings for the case study

For this case study, 500,000 technology configurations were stochastically generated via random sampling, where, in each configuration each model factor is assigned a different value. Each simulation output, i.e., each data point, is associated with its specific technology configuration.

The conceptual technology is defined as successful if the impact of trout production using the microalgal compound is lower than the impact without using it. The life cycle impacts for the technological concept and for the alternative are calculated in pairs for each Monte Carlo iteration (cf. 5 in Fig. 1). The LCA considers four impact categories from ReCipe Midpoint (H): Freshwater ecotoxicity (FETinf), Global warming (GW), Terrestrial Ecotoxicity (TETinf), Freshwater Eutrophication (FE). In addition, the eutrophication impact category from TRACI was used to encompass nitrogen and phosphorus emissions both in seawater and freshwater. No normalization or weighting was considered and addressing the possible burden shifting between impact categories in the decision is outside the scope of this work.

The regionalization step was first performed at what we defined as a "high dimensionality level", using 24 uncertain factors and one aggregated factor which constitute 25 dimensions. Using so many factors results in the definitions of a large number of regions, and the number of data points per region was expected to be too low in each region. Difficult interpretation of the boxes was also anticipated (cf. 2.4.4). Therefore, we also applied the procedure with a regionalization step at a "low dimensionality level" using only one factor and four aggregated factors. The influence of the 24 factors on the output of the model is still captured in the second case, because the aggregated factors are calculated based on these factors.

The decision threshold was set at 0.85. The minimal density, coverage, and mass for a box to be discovered by PRIM were fixed at 0.9, 0.01 and 0.01 respectively. The minimum and maximum relative resolutions were respectively set at ¼ and 1 to divide the uncertain space at the high dimensionality level, and 1/8 and 1 for the space at low dimensionality level.

After the choice of the settings for ENSURe, the algorithm performs the steps 6 to 10 in Fig. 1, based on the results of the propagation of the distributions through the model (step 5 in Fig. 1).

4. Results

4.1. Discovering boxes at the high dimensionality level

When applying the regionalization at the high dimensionality level, the PRIM algorithm could identify at least one success box for each impact category.

This means that we could identify one space of uncertain factors' values that would be robustly associated with a total probability of success superior to 85 %. For the global warming impact (GW), only one box was found (cf. Fig. 3 A). This success box is defined by three factors and one aggregated factor, out of the 25 uncertain factors used for the regionalization, and out of the 13 that were assigned a relative resolution lower than 1 (cf. Fig. 3 B). The box's limits are a dose of microalgal compound lower than 3.1 $g.kg^{-1}$ output live fish in the first part of the last growing stage at sea (*SFDK1_micro_dose*), and lower than 1.5 $g.kg^{-1}$ in the second part of the sea stage (*SFDK2_micro_dose*). In addition to these limits, the biological FCR of this stage must be affected so that it becomes lower than the middle value between its current and minimum theoretical values (*SFDK2_FCR_red_ratio_frac* > *0.5*). Finally, the compound content in the microalgal biomass must be higher than 35 % (*bioact_molec_dbio* > *0.35*). As the discovered box displays only four limits, no other requirement applies on the other uncertain factors that can vary freely within their wide ranges while ensuring a probability of success superior to 85 %. This means for instance that no predicting is required on the future increase in losses experienced by the farm, or on the compound dose delivered to any growth stage but the last one.

Fig. 4 shows the two boxes that were found for Eutrophication, corresponding to two different ways of ensuring an 85 % chance that the technology will outperform the alternative. The first box is obtained by limiting only four factors: the microalgal compound doses in the two divisions of the sea stage are both limited to 2.2 g. kg live fish $^{-1}$ (*SFDK1_micro_dose* and *SFDK2_micro_dose* < *0.022*), the biological FCR in the last part of the sea stage must be modified to at least 50 % closer to its minimum value (*SFDK2_FCR_red_ratio_frac* > 0.50) and the compound content in the microalgal biomass must be at least 42 % (*bioact_molec_dbio* > 0.42). The second box informs us that it is also possible to reach a 85 % probability of success by tightening the constraint on the biological FCR reduction in the last growth stage (*SFDK2_FCR_red_ratio_frac* > 0.75 instead of 0.5), removing the limits on the compound doses, and limiting the new level of losses in the first part of the sea stage to being at least five percentage points higher than it currently is (*SFDK1_loss_lev* > 0.05). However, PRIM returned for this box limit a quasi *p*-value of 0.09 (cf. SI A.7). This limit could thus be considered non-significant compared to the other limits for which the quasi *p*-values are several orders of magnitude below (cf. SI A.7).

The boxes obtained for the other impact categories are presented in SI A.5.

While boxes can be identified at the high dimensionality level, their interpretation is difficult and their use for decision-making requires careful consideration. With 25 factors/aggregated factors and 500,000 data points, the minimum relative resolution could only be set to 1/4

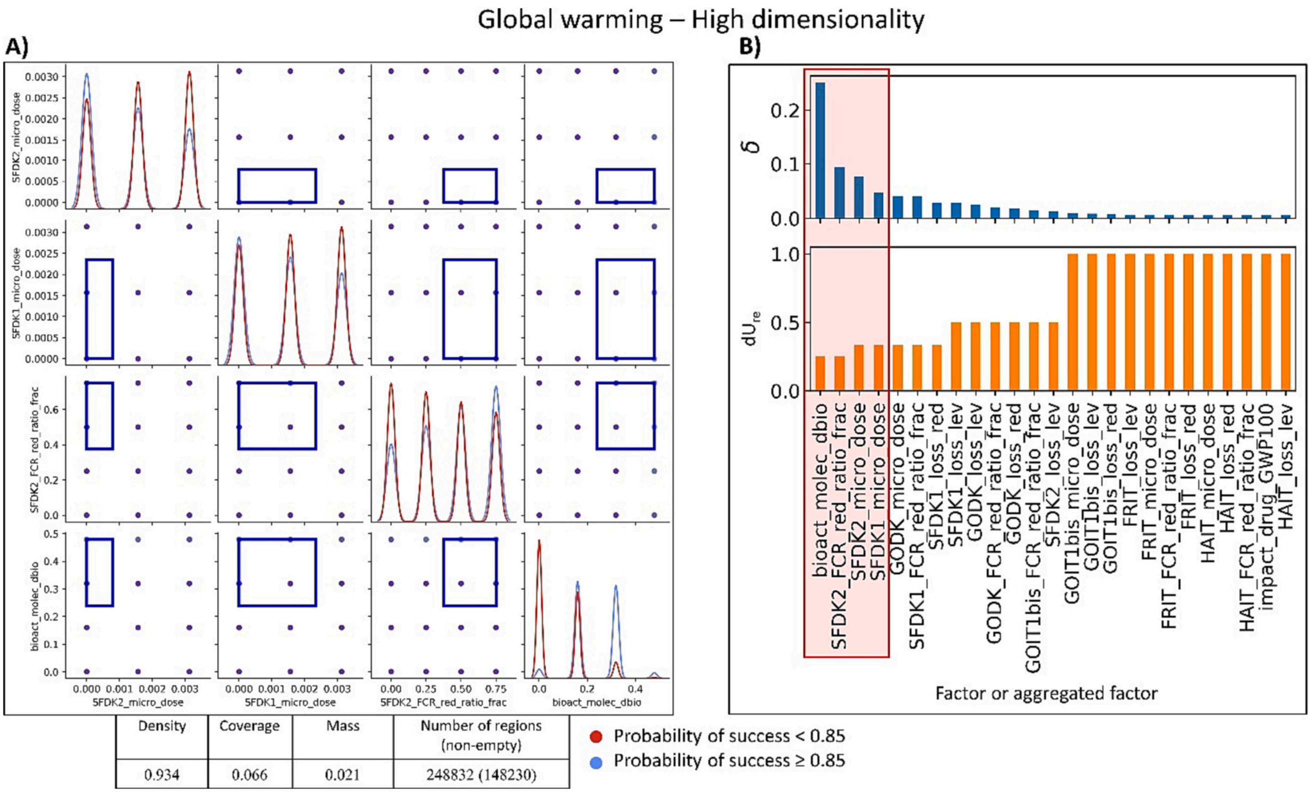

Fig. 3. A) Box discovered by PRIM at the end of ENSURe, at the high dimensionality level, for the Global Warming impact. The original graphic representation for PRIM proposed and programmed by Kwakkel and Jaxa-Roxen (Kwakkel and Jaxa-Rozen, 2016) was adapted to the present use. The dots were made transparent and then appear purple to see the stacking of the regions due to the one-dimensional projection. The blue rectangle corresponds to the limits of the box. A dot represents the lower boundary of a region which expands until the next dot (cf. 2.3.2). An assistance for box visual interpretation is presented in SI A.4. B) Borgonovo's δ for each factor/aggregated factor describing the uncertain space and the corresponding assigned relative resolution dU_{re}. The red rectangle contains the four factors/ aggregated factors that were constrained by PRIM as visible in A). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

and the average number of points per region fell between 28 and 3 depending on the impact category. These numbers are too low to assess meaningful probabilities in each region (cf. 4.1).

4.2. Discovering boxes at the low dimensionality level

The low dimensionality level is only described by five aggregated factors and one factor, which allowed us to set the minimum relative resolution to 1/8 with an average number of points per region varying from 100 (GW) to 290 (TETinf).

For global warming impacts (GW), four boxes were found, and therefore four configurations under which the total probability of success would be superior to 85 %. Two of the four boxes are shown in Fig. 5 and the last two can be found in SI A.5. The first box covers 10 % of the success regions with a density of 1. The limits of the box indicate a reduction of the economic FCR higher than 22 % combined with a reduction of the biological FCR higher than 15 %. The quasi p-value for the latter is however equal to 0.10 which is several orders of magnitude higher than for the other limits, cf. SI A.7). These two constraints would need to be met with a dose of microalgal compound <2.5 g.kg live fish^{-1} during the whole life cycle and this compound should constitute at least 20 % of the dried microalgal biomass. The second box features a limit on the compound dose which is less demanding than in the first one (< 3.5 g.kg $^{-1}$). Unlike the first box, it does not have any limit on the biological FCR but requires a higher compound content in the biomass (30 %).

While ENSURe applied at the high dimensionality level on FE only allowed to find consistent boxes with a decision threshold at 65 %, applying the procedure at the low dimensionality level generated 5 boxes at 85 % (cf. SI A.5).

4.3. Example of conclusion for the technological concept

At the low dimensionality level and for the five impact categories, PRIM did not identify any box where the value of the factor "compound content in the microalgal biomass" is lower than 18 %. This means that it is impossible to consider a probability of success superior or equal to 85 % for the conceptual technology without predicting that the compound will at least reach this concentration in the biomass. The fact that this aggregated factor was limited for all boxes is due to its high sensitivity, as measured by Borgonovo's delta. The compound content in the microalgal biomass was the most sensitive aggregated factor for FETinf and GW. When considering these impact categories as outputs, the range for the compound content was divided into 8 intervals (relative resolution of 1/8, cf. Figs. 5,6), while the GSA processing only assigned it a relative resolution of ¼ when considering Eutrophication. This impact category was more sensitive to the economic and biological FCR reductions (cf. SI A.5).

Achieving a compound content of at least 18 % can already be considered as a very demanding requirement but does not fully disqualify the conceptual technology from being explored, having set a total probability of success superior to 85 % as threshold. Indeed, a compound content over 18 % indicates that the compound should likely be a primary metabolite which is accumulated by the microalgae and associated with normal growth and development. While secondary metabolites are often bioactive because involved in meditating the interactions with other organisms, microalgal primary metabolites such as Beta 1–3 glucans and Poly-unsaturated fatty acids (PUFA) have also shown bioactivities and can accumulate up to >18 % of the biomass (Barsanti et al., 2001; Guedes et al., 2011).

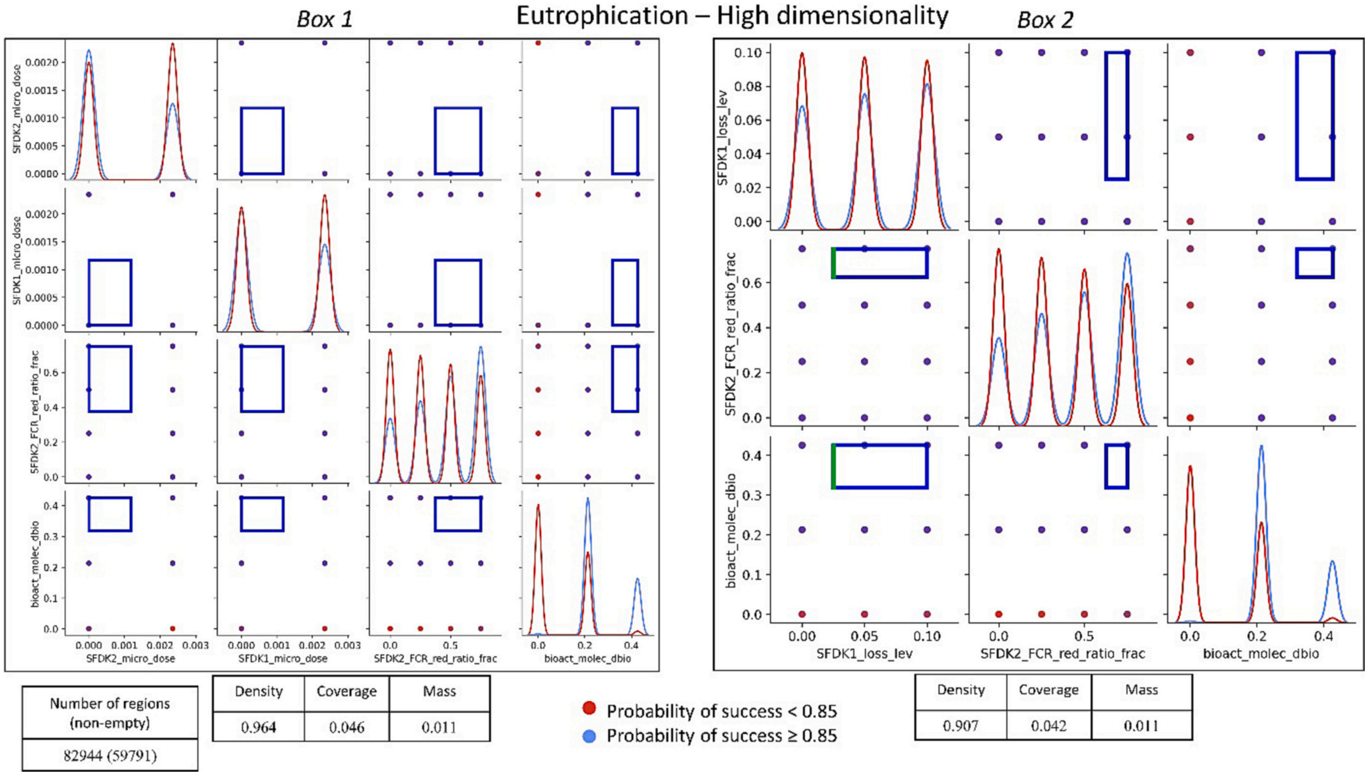

Fig. 4. Boxes discovered by PRIM at the end of ENSURe, at the high dimensionality level, for the Eutrophication impact. The Borgonovo's δ for each factor/aggregated factor and the assigned dU_{re} are presented in SI A.5. A green border on a box means that the PRIM output indicated a quasi *p*-value that was substantially higher than for the other borders (qp >0.02) (cf. SI A.7). An assistance for box visual interpretation is presented in SI A.4. The "peeling trajectory" illustrating PRIM functioning is presented in SI A.6. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

In addition to stringent requirements about the compound content, the majority of boxes are defined by an ambitious reduction of the economic FCR by at least 20 % (e.g., boxes 1,2, for GW in Figs. 5 and 3,4 for GW, 2,3,4,5 for Eutrophication in SI A.5), regardless of the increase in the level of losses (e.g., box 1, 2 for GW in Fig. 5) or by setting limits on them (e.g., box 2 for FE in SI A.5). The combination of these demanding requirements to ensure a total probability of success superior to 85 % appears unlikely.

It is impossible to state that there is a 100 % probability for the conceptual technology to eventually meet them simultaneously by featuring a technological configuration in these boxes. Therefore, it cannot be concluded that the total probability of success for the conceptual technology is superior to the decision threshold of 85 %. Note that it cannot be mathematically concluded that the total probability of success is strictly below 85 %. Uncertainty therefore remains (cf. SI A.1). We further discuss this conclusion in 4.2.

These results indicate that given the substantial incertitude represented by the probability distributions of many factors, decision-makers would need to be very confident in the performance of the discovered compound before supporting the bioprospecting of these in a context where 85 % success probability was required. Technology developers could also use the results to orient their bioprospecting towards compounds that are highly concentrated in their respective microalgal strains as it is a strong requirement to ensure a high probability of success once the market-scale technology is deployed. The other uncertain factors that constitute the discovered boxes cannot directly orient bioprospecting as they mainly characterize the performance of the compound on the fish and the status of the fish farm, which will only be revealed late in the development process. However, the bioprospecting could try to focus on compounds that target diseases which mainly affect the fish in its late growing stages as only factors related to the reduction of the FCR in the late stages were shown constrained in the boxes at high dimensionality (cf. Fig. 3 and 4).

5. Discussion

5.1. ENSURe's robustness and trade-offs

Applying the regionalization step on many factors at the high dimensionality level caused problems for the computability and therefore interpretability of the results. The model of the technological concept here used relies among other things on a dynamic simulation of microalgal cultivation in different European production mixes, which is computationally intensive. Simulating millions of data points requires large computing resources and time, and we could only reasonably compute 500,000 data points because each point required several simulations to generate production mixes for the microalgal compound (Jouannais et al., 2022). Overall, the case study required approximately 325,000,000 LCAs and simulations of microalgal productions operated in parallel over multiple servers and cores over approximately ten days. The case study is thus particularly computationally demanding due to the long process simulation, but these computational limits can be partly generalized. Since ENSURe is limited by computing resources, trade-offs arise in terms of its performance. We propose three main criteria to evaluate the performance of the procedure. The first criterion is *reliability,* defined as the capacity of ENSURe to find boxes which do not contain false positive regions. In other words, reliability is high when the identified boxes only contain regions for which the conditional probability of success would asymptotically tend to being superior to the threshold with more data points. The second criterion is *purity* and represents the degree of distinction between risk and uncertainty achieved by the regionalization step. Purity is minimal when the uncertain space is not regionalized, which is equivalent to setting all relative resolutions to 1, and increases with lower relative resolutions, thus

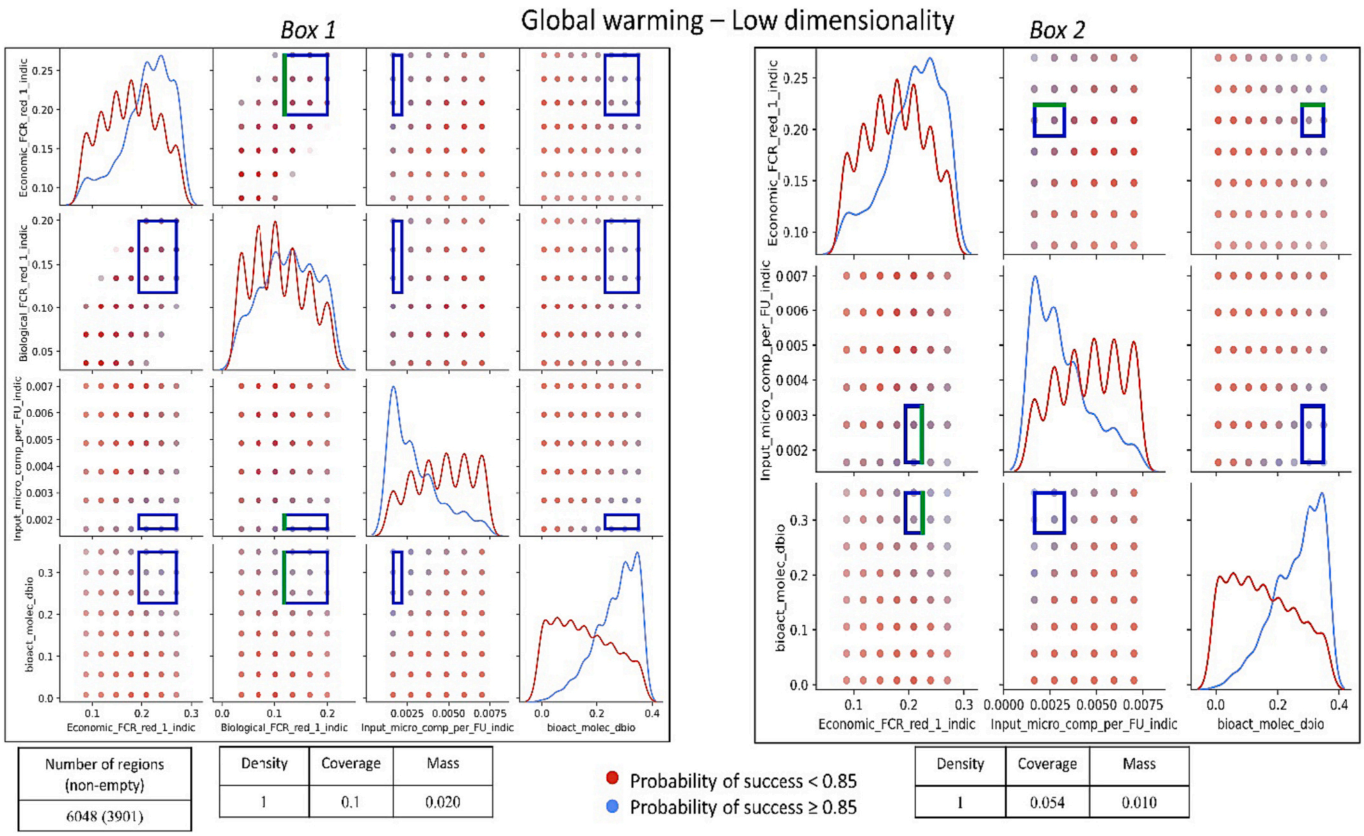

Fig. 5. Boxes discovered by PRIM at the end of the ENSURe, at the low dimensionality level, for the Global Warming impact. The Borgonovo's δ for each factor and aggregated factor and the assigned dU_{re} are presented in Fig. 6. A green border on a box means that the PRIM output indicated a quasi p-value that was substantially higher than for the other borders (qp >0.02) (cf. SI A.7). The "peeling trajectory" illustrating PRIM functioning is presented in SI A.6. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

approaching "pure" conditional probabilities in each region (cf. 2.3.2 and mathematical formulation in SI A.1) The third criterion *comprehensiveness* is maximized when all boxes, even the smallest ones, have been found. The trade-offs between criteria depend on the case study and its computing requirements and can be managed by modulating ENSURe's settings as illustrated below.

The number of regions within the uncertain space grows exponentially with the number of uncertain factors and intervals. Increasing the number of intervals decreases the average number of data points on which a probability of success is estimated in each region. At the high dimensionality level, dividing each of the 25 uncertain factor and aggregated factors' ranges into only four intervals would lead to 4^{25} regions with an average number of points per region being infinitesimal. Thanks to the use of Borgonovo's δ to assign distinct relative resolutions to factors, the average number of points per region was maintained at 28 for TETinf but due to different Borgonovo's δ, this number fell to three points per region for FETinf. This hinders *reliability* as it causes false negative and false positive regions assessed as "Success" based on very few data points, while more simulations could show a probability of success lower than 0.85 in these same regions. While increasing the minimum relative resolution from 1/4 to 1/3, thus dividing the range of the most sensitive parameter into 3 intervals instead of 4, would drastically increase the number of points per region, it would also allow a larger variation of the uncertain factors within these regions and reduce the *purity* of the procedure. If *reliability* is low, a lower minimal density can be set so that the algorithm can find boxes with a density <1, such as the boxes found for Eutrophication (cf. Fig. 4). These settings can allow finding boxes that are meaningful despite the noise due to false positives and negatives. The discarding of regions that happened to be empty is also an aspect of these performance trade-offs. Unless the model features very local non monotonic behaviors, the empty regions which are spread equiprobably across the uncertain space should not prevent PRIM from finding relevant boxes that may contain empty regions mainly surrounded by regions of interest.

The PRIM algorithm was here parameterized to find all boxes with a mass superior to 0.01, meaning that the minimum number of regions in a box is 0.01 multiplied by the number of not empty regions. As pointed out by Friedman and Fisher (Friedman and Fisher, 1999) who set the basis for PRIM, the lower the mass of a box is, the higher is the risk of a box delimitation being affected by noise ("over-fitting" problem). When PRIM is applied within ENSURe, noise is due to false positives and negatives among regions in the space. Thus, fixing the minimal mass value as small as possible would potentially lead to PRIM identifying all false positives as small boxes and hinder *reliability*. On the other hand, looking exclusively for success boxes above a large mass affects the *comprehensiveness* of ENSURe by potentially overlooking boxes. For example, when applying regionalization at the high dimensionality level, setting a minimum mass at 0.01 made PRIM leave 90 % of the success regions outside of the discovered boxes for all impact categories. This is probably because the success regions are sparsely distributed in the uncertain space due to the false negatives and positives. Therefore, PRIM cannot identify a unified and consistent box with a sufficient mass containing these regions.

In fact, for FE and at the high dimensionality level, no box at all could be found with a decision threshold at 0.85 but only at 0.65. The straightforward conclusion could be that the total probability of success for this impact category is not higher than 0.65, but the limitations addressed above prompt to remain cautious with this interpretation.

Fig. 7 summarizes the trade-offs between *purity*, *reliability*, and *comprehensiveness* that are influenced by ENSURe's settings and the case

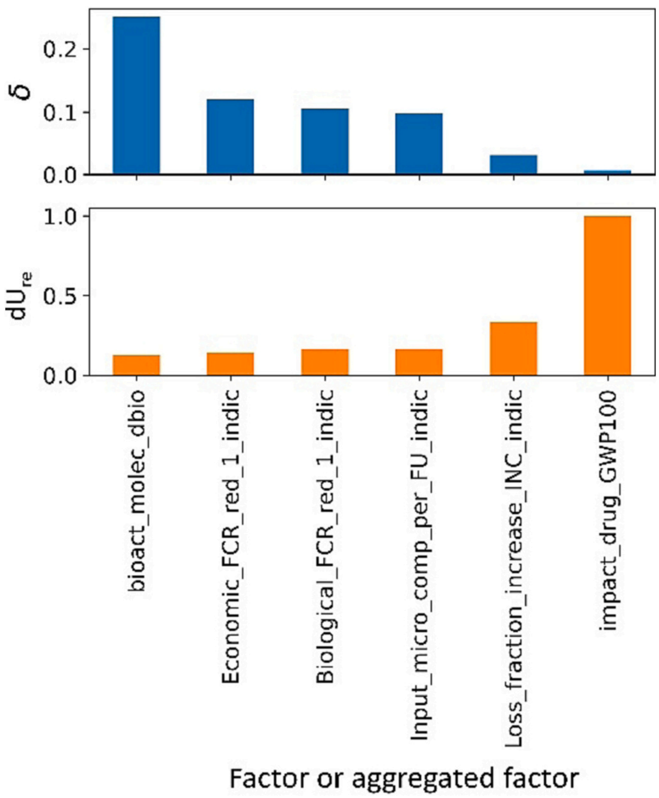

Fig. 6. Borgonovo's δ for Global warming impact at the low dimensionality level and corresponding relative resolutions dUre.

study.

In addition to finding the right trade-offs regarding ENSURe's settings, insightful results can also be obtained by carefully reducing the ranges considered for the uncertain factors. This reduction can be done by first allowing PRIM to find large boxes and then using the boxes limits to define new ranges for the concerned factors in a new iteration of the procedure. This iterative approach allows discovering boxes with a lower resolution.

Decreasing the dimensionality of the problem by combining factors into aggregated factors is the solution we used to manage trade-offs in performance and provide results that have sufficient *reliability, comprehensiveness, and purity* for decision-making. It must be noted that reducing the dimensionality by using aggregated factors implies losing information at the most detailed level of the modeling. The same aggregated factor value can be obtained from different combinations of factors values. This means that the probabilities assessed with ENSURe are given considering that for one aggregated factor value, all potential combinations are equiprobable. Thus, the incertitude associated to these multiple combinations for one aggregated factor value is therefore treated as risk while the factors on which the aggregated factors are based were first identified as "uncertain". This particularity constitutes a limit to consider when using aggregated factors.

5.2. *Refining the evaluation*

For this case study in which the procedure could not prove that the total probability of success was over the threshold, decision-makers have multiple options. Firstly, they can settle for this result and dismiss the technological concept because ENSURe did not allow us to state that the total probability of success was over the decision threshold. The modelers can also change the settings of the procedure to refine the evaluation. The first option is to decrease the decision threshold in the procedure until they can find a box associated with a probability of 1. This will inform about the minimum total probability of success and allow decision-makers to assess whether this probability is too far from the initial decision threshold. Another option is to lower the minimum density chosen for PRIM to see if boxes with a slightly lower density can be associated with a probability of 1. This would mean that the total probability of success is not far from the decision threshold. The last option is to lower the minimum *mass* of discoverable boxes in PRIM which will allow the algorithm to find additional boxes on which decision-makers can reflect. However, these boxes will necessarily be associated to smaller shares of the uncertain space which implies more demanding limits on the ranges of the uncertain factors. These scenarios will probably be too specific to be likely. In addition, one must remain aware of the caveats that stem from low-mass boxes regarding *reliability* of the results (cf. 4.1). Additionally, ENSURe could be run using the approach to multiple boxes proposed by Guivarch et al. (2016), in which the points of interest (in our case, regions) located in a discovered box are not deleted but their status in instead changed to "of no interest" for the next iterations of PRIM. As described by the authors, this approach may improve the diversity of discovered boxes.

Finally, the decision could be better informed if it was shown with certitude that the total probability of success is below the decision threshold. This can be done using the simple relationship *P(success) = 1-P(failure)*. Thus, ENSURe can be applied to find boxes associated with a decision-threshold regarding the probability of a failure (e.g., 15 %), which is equal to one minus the decision threshold for a success (1–15 % = 85 %). This will allow showing whether the probability of failure is superior to a threshold (15 %), and therefore proving whether the probability of success is less than one minus this threshold (85 %).

5.3. *Setting the context to talk about probabilities*

While differentiating risk and uncertainty allows one to better approach the notion of probability regarding the outcome of technological development, additional considerations are needed to approximate "*real-world probabilities*"(Thompson and Smith, 2019). As Wynne (1992) states, *"Science can define a risk, or uncertainties, only by artificially 'freezing' a surrounding context which may or may not be this way in real-life situations. The resultant knowledge is therefore conditional knowledge."* In this context, sound decision-making for policy-planning requires explicit hypotheses on the main drivers of technological development. Hence, the probabilities that we assessed via ENSURe can only be considered as such if we assume, among other aspects detailed in previous works (Jouannais et al., 2022; Jouannais and Pizzol, 2022), that microalgal producers will always seek to optimize the areal productivity of their plants and that bioengineers can find any strain-specific techno-operational setup to cultivate a microalgal strain at 30 % of its maximum productivity (Jouannais et al., 2022). Once this context is established, the evolution of the conceptual technological can more accurately be pictured as a random process whose first step will be the discovery of a specific microalgal strain and compound.

5.4. *Interpretation in a perspective of technological planning and guidance*

The present work uses ENSURe in the theoretical context of risk and uncertainty, but the approach can also be used in perspective of technological governance and planning. Let's examine our choice of considering the unknown locations of the compound's producing mix as belonging to risk, with markets developing equiprobably around random regions in Europe (cf. 3.1 and 3.3). It could be argued that nothing separates the nature of the incertitude applying to the unknown set of factors (size of the mix, latitudes, and longitudes) describing the production mix (category 1) from the one applying to factors associated with the compound's effect on the farm (category 2). They could both be considered as equally uncertain, and the production mix incertitude could be included in the uncertain space within the procedure. Treating this incertitude as risk as we did means that the discovered boxes are

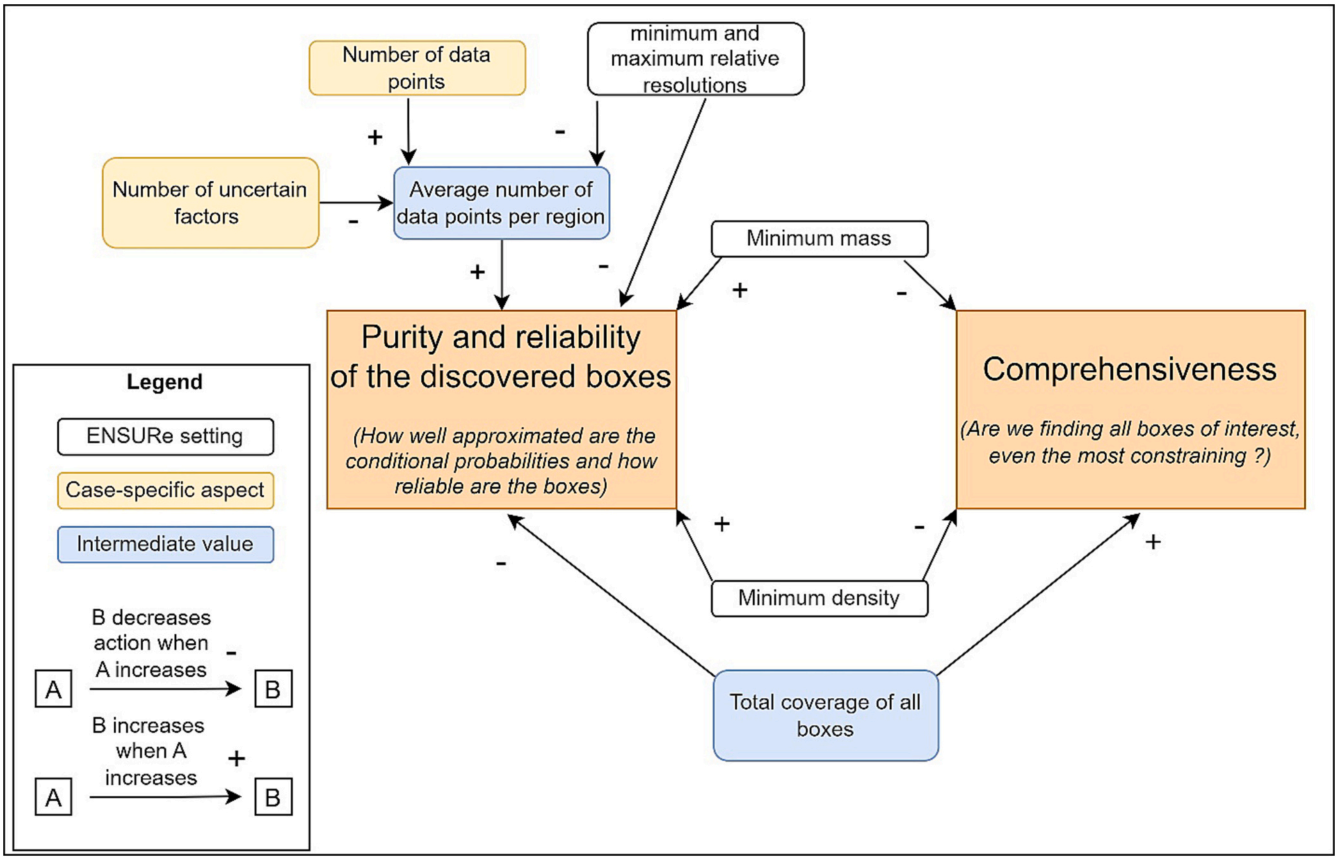

Fig. 7. Effects of the case study and ENSURe's settings on the trade-offs between purity, reliability and comprehensiveness. An intermediate value stems from the combination of the case-specific aspects and the choice of the procedure settings. dU_{remin} and dU_{remax} respectively are the minimum and maximum relative resolutions.

associated with a total probability of success superior to 85 % if the geographical development can occur across Europe equiprobably. In other words, ENSURe here discovers boxes of uncertain factors that would allow making a safe-enough decision about the conceptual technology in a context where the geographical development is not constrained by regulations. This position constitutes a cautious stand, within which the evolution of the market associated with the technology is considered chaotic and uncontrollable (unresponsive) (Genus and Stirling, 2018) under the current economic system. We thus account for potential environmentally suboptimal configurations such as very valuable microalgal compounds being produced in countries requiring high fossil energy inputs per kg of compound because of low solar irradiance, low temperature and/or carbon intensive electricity mixes etc.

On the contrary, treating the geographical development of the production mix as uncertainty within ENSURe could allow finding boxes which are constrained on the production mix factors. This would for instance enable discovering minimal and maximal latitudes under which the technology should be confined to ensure a targeted probability of success.

In general, while we here presented a use of ENSURe to assist decision-making about initiating research on a technological concept in presence of uncertainty, with the previous example we argue that the procedure can also be employed for the guidance and planning of technological development. In this case, the factors being treated as risk constitute what decision-makers and regulators cannot, or do not intend to regulate. The factors treated as uncertainty represent political and technological freedom of maneuver for decision-makers and societal regulation of technological concepts.

5.5. Deciding whether to prioritize an unexplored conceptual technology

We have demonstrated the use of ENSURe on a technological concept on which a substantial incertitude applies. In this context, deciding to invest resources in the technological concept only if the total probability is shown higher than 85 % constitutes a very conservative and cautious stand. Daily individual or political actions are taken with a lower level of subjective certitude and ENSURe can be applied with lower decision thresholds. Furthermore, sound decision-making and technological planning could require more insightful decision criteria that do not consider only the probability of success but analyze the "risks" (in risk assessment terminology, i.e., "hazards") of further developing an initial technological concept. Thus, ENSURe could be parameterized to not only consider the probability but also the magnitude of this success and the severity of a failure, i.e., how better or worse the final technology would be compared to the alternatives. This is particularly relevant when considering technological concepts associated with lock-in possibilities (Brian, 1989; Carraresi and Bröring, 2022; Hung and Tu, 2011) and possible suboptimal configurations regarding environmental impacts. A probabilistic view on innovation calling for cautious consideration of risks before exploring technological concepts is also provided in Nick Bostrom's Vulnerable World Hypothesis (Bostrom, 2019), which depicts technological development as a random draw in an urn containing two types of balls. One type represents technological concepts that inevitably lead to the self-annihilation of humanity. The author exemplifies these concepts with theoretical "easy-nukes" but also global warming worsening directions. While microalgae-based solutions for fish farming could unlikely constitute a paramount threat to Humankind, it could be argued that all investment of time and resources in concepts with low chance of improving the status quo an constitute an irrational bet in times of ecological and social emergency. The use of ex-ante LCA within ENSURe enables an insight into Bostrom's urn to cautiously preselect the balls we draw.

6. Conclusion

This study presented ENSURe, a new modeling procedure to deal with deep uncertainty in the prospective assessment of future systems. The application of ENSURe on an ex-ante LCA case study demonstrated its purpose by identifying sets of conditions that allow reaching a high success probability decision-threshold of 85 % without treating uncertainty as risk. The case study was particularly demanding regarding computing resources that prevented further iterations of the procedure to refine the evaluation of the total probability of success. This probability could not be shown superior to the decision-threshold. The challenging computing needs allowed exploring the different performance trade-offs for the procedure which can be piloted according to the case-study, the objectives and expectations of the analysts and decision-makers.

While Stirling's risk propagation acts as a projection of stakeholders' belief and knowledge into the output space via the model, ENSURe acknowledges that only partial projection is possible in the presence of risk and uncertainty. Thus, ENSURe assists in evaluating the total probability of success, but not the full probability distributions for the outputs. We therefore keep uncertainty and risk differentiated without forcing a probabilistic approach to uncertainty and make modeling approaches such as ex.ante LCA comply with these key concepts in post-normal science.

By separating risk and uncertainty, ENSURe prevents modeling from falling further down into "model-land" (Thompson and Smith, 2019), in which assigning tentative probabilities to events, or mathematical relationships between factors sometimes constitutes an additional abstraction and a deceptive impression of quantifying all incertitude. Instead, the approach takes advantage of the fact that stakeholders often fail to simultaneously assign probability distributions to multiple factors that may be interdependent, but this does not prevent them from informing about the probability of reaching a certain scenario defined by several factors.

Our approach joins GSA to assist modeling approaches such as ex-ante LCA in providing insightful results for decision-making. While GSA supports practitioners and decision makers in prioritizing their data collection efforts to reduce uncertainty in the output of their models, ENSURe informs them about which conditions should be met to ensure a certain probability of success and decide on further exploring a concept.

With ENSURe, ex-ante LCA and other modeling approaches can move forward into assessing broad technological concepts or any emerging technology for which incertitude is not limited to risk. While the other forms of incertitude, namely ambiguity or even ignorance (Stirling, 2010) still resist quantitative assessments, we tackle the need for early-stage decision making for a better planning of technological development under ecological emergency.

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CRediT authorship contribution statement

Pierre Jouannais: Conceptualization, Methodology, Formal analysis, Investigation, Visualization, Writing – original draft, Writing – review & editing. **Carlos Felipe Blanco:** Conceptualization, Methodology, Resources, Validation, Writing – review & editing. **Massimo Pizzol:** Conceptualization, Project administration, Validation, Supervision, Writing – review & editing, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The code allowing reproduction of the results is available at https://github.com/PJGilmw/LCA_deep_uncertainty_fish_micro.

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