Uncertainty analysis in the techno-economic assessment of CO_2 capture and storage technologies. Critical review and guidelines for use.

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Abstract. Uncertainty analysis is a key element of sound techno-economic analysis (TEA) of CO_2 Capture and Storage (CCS) technologies and systems, and in the communication of TEA results. Many CCS technologies are relatively novel, with only few large-scale projects constructed and in operation to date. Therefore, uncertainties in technology performance and costs are often substantial, making it imperative that they be characterized and reported. Although uncertainty analysis itself is not novel, with some methods already frequently used by the CCS TEA community, a document that provides a comprehensive overview of methods and approaches, as well as guidance on their selection and use, is still lacking. Given its importance, we seek to fill this gap by providing a critical review of uncertainty analysis methods along with guidance on the selection and use of these methods for CCS TEAs, highlighting good practice and examples from the CCS literature. The paper starts by identifying the different audiences for CCS TEAs, the different modelling approaches available for CCS technology performance and cost analysis, and the different roles that uncertainty analysis may play. It then continues to discuss established, as well as emerging, uncertainty analysis methods and addresses how and when each method is best used, as well as common pitfalls. We argue that the most commonly used method of one-parameter-at-a-time 'local' sensitivity analysis may often be a suboptimal choice, and that other approaches may be more suitable or lead to more insight, especially since uncertainty analysis software is becoming more widespread and easier to use. Finally, the paper discusses the benefits of advanced uses of uncertainty analysis in, for instance, the design of CCS experiments or in the design and planning of CCS infrastructure. Sound uncertainty analysis has an important role to play in TEAs of CCS technologies and systems, and there are many opportunities to bring the use of uncertainty analysis to a higher level than currently practiced. This review of and guidance on available methods is intended to help accelerate continued methods development and their application to more robust and meaningful CCS performance and costing studies.

1. Introduction

Sound uncertainty analysis is critical to the informed interpretation of carbon capture and storage (CCS) techno-economic analyses (TEA) [1], [2]. It can provide valuable insight into the impacts of assumptions and underlying model structure, and give an indication of model quality and robustness, as well as of how reliable the outputs of modelling studies are or can be. Without uncertainty analysis, the actual meaning and importance of CCS cost results from any techno-economic study are difficult to judge, especially for the target audience of such studies, who are often not involved in their production.

Over the years, many publications on uncertainty evaluation methods and approaches have found their way to the scientific domain (e.g., [3]–[5]), as have publications on the application of uncertainty analysis to TEA and CCS costing specifically (e.g., [6]–[8]). However, it is notable that often when uncertainty analysis methods are applied in TEAs, mostly simplified methods tend to be used (e.g., single parameter sensitivity analysis) whereas other (more complex) methods could provide additional valuable insight. Furthermore, new and promising uncertainty methods appear to remain unknown to (or unapplied by) the CCS TEA community. We believe this is partly due to unawareness of the full space of uncertainty analysis options, as well as a lack on guidance on when and how to use such options. Therefore, a critical review of the different options, complemented with guidelines on uncertainty evaluation can i) raise awareness to this issue, and ii) increase the effective and fit-for-purpose use of uncertainty analysis in CCS techno-economic studies, hopefully leading to improved understanding and communication of their results.

Building on a previous CCS costing guideline paper [9], this work sets out to provide a review of, and guidelines on, uncertainty analysis methods for use in CCS TEA. It combines knowledge and experience acquired in academia, research institutes and non-governmental organizations (NGOs). It is drafted in conjunction with two other guideline documents, one on techno-economic studies of CCS for industrial sources, and a second document looking into methods for carrying out costing of novel (low technology readiness level) processes (both forthcoming). The overarching goal of this manuscript is to advance the sound and fit-for-purpose use of uncertainty analysis in CCS TEA by providing practitioners and users with a reference document of relevant methods, tools and approaches, and a guideline of when and how to use them. These guidelines do not intend to provide an exhaustive account of every available method, rather to showcase different methods over a broad spectrum that can act as an illustration of the type of methods available. Naturally, these guidelines are equally applicable to TEAs of CO_2 utilisation and negative emission technologies.

2. Scope and background

2.1. Audience for this paper

These guidelines target two types of audiences: techno-economic analysis *practitioners* and the *users* of techno-economic studies (Table 1). The first group is composed of people involved in the development, modelling, costing and analysis of (new) CCS technologies. They will be found mainly in research and development (R&D) agencies, academia, and in industrial organisations.

The second group are the users of TEA studies, as earlier described in Rubin et al., [2]. They are mostly technology (R&D) and policy decision makers. The purpose for this group is twofold: first to help them gain an understanding of the role of uncertainty and how it may affect assessments of technology performance, and second to provide an overview of available uncertainty analysis methods and their use, so that decision makers can request TEA practitioners to undertake the specific analysis that may fit their information needs best. A key example of the second group is funding agencies, who on a regular basis need to make informed decisions on funding technology proposals.

Table 1. Target audiences for this guideline document

Audience	Government	Industry	NGO's & universities
Practitioners: process developers/modellers, cost engineers and technology analysts in:	• R&D agencies	• Operators • Vendors • A&E firms • Venture capital • R&D organisations	• Academia
Users of CCS techno-economic studies in:	• Policymakers • Analysts • Regulators • R&D agencies • Funding agencies	• Operators • Vendors • A&E firms • Venture capital • R&D organisations	• Environmental • Media • Academia • Foundations

2.2. Types of techno-economic analyses and candidate parameter categories for uncertainty analysis

Before venturing into available uncertainty analysis methods, it is worthwhile to provide a rough description of the type of techno-economic models found in today's CCS literature, since different types of studies may require different types of uncertainty analysis. Table 2 presents a simplified overview of the types of techno-economic models and parameter categories that can be candidates for uncertainty evaluation (based on an earlier publication [10]). On the one end, there are simplified techno-economic models that, for instance, are used to get a first rough idea of technical and economic feasibility. These models may be based on simple first principles or more black box technology descriptions, and their economics are often derived from future projections of known equipment cost. On the other end of the spectrum are detailed techno-economic studies based on full physical (rigorous) technology models and detailed "bottom-up" cost models, such as the engineering-economic models often used in studies by e.g., the US Department of Energy's National Energy Technology Laboratory (DOE/NETL), the International Energy Agency Greenhouse Gas Programme (IEAGHG), and the Electric Power Research Institute (EPRI). In between, there are more or less detailed technical and economic modelling studies, here called intermediate complexity models, often using, e.g., shortcut models for technology description, and/or partial process design and equipment lists for costing. The choice for a certain model type may depend on the goal of the study, the availability of data and physico-chemical models, and the technology readiness level (TRL).

Table 2 is not meant as an exhaustive list of all parameters that need to be scrutinised, but rather provides an illustration of complexity levels. As the table clearly shows, the more detailed and complex the TEA, the more input parameters and models used, and therefore the more parameters that can, or should, be included in the uncertainty analysis. Also, especially for rigorous process models, it is good practice to investigate the effect of model structure. This, for example, could be reflected in the choice of models for mass transfer, as it may have a large effect on the technical process, and therefore its performance and cost (see e.g. [11], [12] for a discussion on how the choice of mass transfer models is relevant in solvent-based CO_2 capture systems, but it equally applies to other types of capture technology).

Table 2. Indicative technical and economic model types and candidate parameter (categories) for uncertainty scrutinization, based on [10]**.**

	Technical models		**Economic models**	
Model complexity level	**Description**	**Potential parameter categories to scrutinise**	**Description**	**Potential parameter categories to scrutinise**
Rigorous	Typically, full physical models based on first principles, including detailed flowsheets, mass and heat transfer, detailed kinetics, recycles, etcetera.	Below parameter categories as well as mass & heat transfer models, chemical kinetics models	Typically, detailed economic estimates, based on a detailed equipment list, using individual escalation and/or scaling factors and including all capital and operational costs	All of the below plus individual escalation and/or scaling factors, detailed capital and operational cost factors
Intermediate	E.g., short-cut models, excluding part of the physical description (often mass transfer, heat transfer, chemical kinetics)	Below parameter categories as well as, a.o., chemical equilibrium models and state parameters (P, T)	E.g., combinations of bottom up and top-down methods, using partial equipment lists and Lang/Hand type escalation factors	All of the below plus equipment sizes, purchased equipment costs, escalation factors
Simplified	Often mass and energy balance models based on literature or experimental results	Mass and energy input and output flows	Typically, top-down cost estimates, e.g., exponent models, using cost estimates from earlier studies	Financial parameters (lifetime, discount rate, etcetera); fuel & consumables cost; scaling exponents

2.3. What do the existing TEA guidelines say about uncertainty assessment?

As discussed in the introduction, a comprehensive set of guidelines for uncertainty analysis of techno-economic studies of CCS technologies is currently lacking. Two widely used guideline documents for CCS TEA in general, The DOE/NETL Quality Guidelines for Energy System Studies (QGESS [13]) and the European Best Practice Guidelines for Assessment of CO_2 Capture Technologies [14], provide a note on uncertainty analysis. Both recommend the use of sensitivity analysis to help generate an understanding of uncertainty in input data, financial assumptions, and state of technology development. They, however, limit themselves to the most simple of sensitivity analyses (one-at-a-time sensitivity analysis, see 3.3.1), without discussing alternative methods and without providing guidance on how to undertake uncertainty analysis in a methodologically sound way.

The techno-economic studies by organisations such as the IEAGHG or the Zero Emissions Platform (ZEP), are also often used as guidelines for good TEA practice. The IEAGHG studies use the standardised IEAGHG techno-economic and financial parameters for their studies (e.g., [15]). The IEAGHG studies generally include sensitivity analyses, aiming to offer a picture of how changes to the standard IEAGHG assumptions could impact CCS costs. The key parameters generally investigated are fuel prices,

discount rate, discount rate after plant closure, plant life time and CO_2 transport and storage costs, subject to the objective of the study [16]–[18]. Recent studies [19] also included assessments of potential techno-economic scenarios, where the authors a) explored technical parameters that can have a significant impact on the CO_2 capture costs; b) provided overviews of the TRLs of the CO_2 capture technologies and their impact on costs, and c) highlighted technical differences in the literature which make cost-reviews more challenging. The TEA studies by ZEP only investigate sensitivity to plant efficiency and capital costs [20] for CO_2 capture plants and extends that with operational costs, distance, and utilisation level for CO_2 transport [21]. Only in their CO_2 storage costing study, ZEP also included sensitivities on high level technical parameters like field and well capacity [22].

The abovementioned guideline documents and techno-economic studies use, what are often called, local sensitivity analysis methods for uncertainty analysis, especially the one-at-a-time, and one-way type of sensitivity analysis (see section 3.3.1). Another observation is that these studies mostly focus their sensitivity analyses on economic input parameters (although there are exceptions). When addressing technical parameters, they do so mostly at high level, aggregated, parameters such as power plant efficiency, rather than the underlying technical *input* parameters that might exist in a first-principle process model.

3. Uncertainty analysis

3.1. Definitions of uncertainty analysis

In the CCS TEA literature, Rubin et al. [2], make a distinction between uncertainty, variability and bias. Therein, the author defined uncertainty to reflect "a lack of knowledge about the precise value of one or more parameters affecting CCS costs" ([2]:187). In this definition, uncertainty exists solely in the value of parameters. Variability was defined to refer "to the different value a given parameter may take on (for example, across a collection of facilities, or at different points in time at a given facility). In this case the values of the parameter are assumed to be known (or knowable), and thus subject to quantitative data analysis" ([2]:187). This means that the variability of a given parameter can be measured and can thus be quantified by, e.g., a probability density function (PDF). This would be much more difficult (or arbitrary) in the case of uncertainty, where the lack of knowledge (true uncertainty) would hamper defining a precise PDF[1]. Furthermore, the author defined bias to refer "to assumptions that skew an analysis in a particular direction while ignoring other valid alternatives, factors or data" ([2]:188), meaning that the outcomes of a study may change when favouring one input parameter value over another.

Other scholars use a wider definition of uncertainty by focusing on all kinds of knowledge or information, rather than only on parameters. For instance, "incomplete information about a particular subject" ([23]:387), "lack of confidence in knowledge related to a specific question" ([24]: 504) and "any deviation from the unachievable ideal of completely deterministic knowledge of the relevant system" ([25]:5). These three definitions all focus on the lack of knowable knowledge, values, or information, and in that way, they are closest to Rubin's definition of uncertainty.

[1] This differentiation between uncertainty and variability relates closely to what is called *epistemic* and *aleatoric* uncertainty in the uncertainty quantification (UQ) literature [73]. The UQ community thus refers to both as uncertainty, but of a different nature. Epistemic uncertainty is also called *reducible uncertainty*, *ignorance uncertainty* or *subjective uncertainty* [74]. Aleatoric uncertainty, on the other hand, refers to *inherent variability* of a quantity of interest or *unpredictability due to stochasticity* [73], indeed equivalent to Rubin's definition of variability [2].

We here adopt a wide definition of uncertainty, that includes both parameter [1], [2], [26] and non-parameter uncertainty (i.e., knowledge uncertainty [27] and uncertainty in the model structure and boundaries: methodological, model structure, and contextual uncertainty [1], [26]). At the same time, we embrace the difference between uncertainty and variability (or epistemic and aleatoric uncertainty), because they play an important role in the selection of uncertainty analysis methods, as we will discuss later.

3.2. Purposes of uncertainty analysis

Before outlining different uncertainty analysis methods that are commonly used in CCS techno-economic analysis, we first discuss the different purposes uncertainty analysis may have. The first, straightforward, purpose is to provide insight into potentially different outputs as a result of different input assumptions. This is a way to answer "what if", or, diagnostic, type of questions [28], [29]. A more sophisticated purpose can be to provide an estimate of a certain output happening. This relates more to "what will", or prognostic questions [28], [29], because the model specifies a certain outcome of happening with a certain probability. Related to this, uncertainty analysis can help understand which input parameters influence the model outputs most and should therefore be scrutinised and/or parametrised most thoroughly (for instance, through Factor Priorisation, FP, [28]). This can help answer the question of "where to put most effort" when quantifying model input values. Conversely, uncertainty analysis may provide insight into the parts of the model(s) that have less influence on the outputs, thereby answering "which parts of the model can we simplify" and providing a basis for model reduction (Factor Fixing, FF [28]). An advanced use of uncertainty analysis is model testing, i.e., testing how a model behaves when fed with extreme parameter values or scenarios. If the model behaves as expected (i.e., provides the expected outputs), it increases confidence that the model structure is correct. If unexpected outputs occur, this may indicate that model equations are incorrect, or incorrectly implemented. Finally, uncertainty analysis can also generate insight into the strength of models and/or the input data fed to them (further discussed in 3.4.1), which is of great importance when models are used for policy and decision making.

3.3. Established uncertainty analysis methods

This section describes established uncertainty analysis methods, i.e., methods that have well established principles and that have been commonly used in techno-economic analysis for decades. We start out with a general description of sensitivity analysis and local sensitivity analysis methods and then continue with a description of global (e.g., Monte Carlo based) uncertainty analysis. This section ends with describing pitfalls and good practices for the established methods.

To allow explanation of the different methods, a very simple and generic mathematical representation of uncertainty analysis is introduced in the main text:

$$\mathbf{y} = g(\mathbf{x}) \qquad 1$$

Where, g is a techno-economic model (i.e., a mathematical function). Despite the simple representation here, g can be a very complex system of equations solved analytically or numerically. $\mathbf{x}$ is an array of n model inputs $\{\mathrm{x}_1, \mathrm{x}_2, \dots, \mathrm{x}_\mathrm{n}\}$ and $\mathbf{y}$ is an array of m model outputs $\{\mathrm{y}_1, \mathrm{y}_2, \dots, \mathrm{y}_\mathrm{n}\}$. We call k the number of parameters out of the set n $(k \leq n)$ that is actually varied in a sensitivity analysis. This will suffice the explanation of the methods below. Slightly more comprehensive mathematical representations can be found in Appendix A.

3.3.1. Sensitivity analysis

Sensitivity analysis (SA) studies how uncertainty in the output of a model is apportioned to different sources of uncertainty in the input of a model [30], [31]. Its main purpose is thereby to identify which inputs most significantly impact the model, helping to prioritise the effort of a modeller on further

quantifying the model inputs, while making the model more robust. The model inputs to which the output is most sensitive deserve the most rigorous quantification; the inputs to which the model is least, or not sensitive, can be allowed less stringent quantification, or can be set to fixed (sometimes even random) value. Below we describe commonly used sensitivity analysis methods used in CCS costing, distinguishing between local sensitivity analysis and global sensitivity analysis. The descriptions are made around three main aspects: definition (what), method (how) and their applicability (when).

Local sensitivity analysis

By far the most commonly used sensitivity analysis methods are local, meaning that one or more variables are varied around selected base, or nominal, values. This also implies that local methods do not include the uncertainties in the whole solutions space (set of potential outputs) of the model) [28]. The reason for the wide use of local methods is their ease of use and of interpretation of their results

What: Local sensitivity analysis can roughly be divided in three types: one-at-a-time sensitivity analysis, one-way sensitivity analysis and n-ways sensitivity analysis (scenario analysis, sometimes called N-at-the-time -NAT- sensitivity analysis was excluded from below description, because a very special class of uncertainty analysis). The simplest local method is one-at-a-time (OAT) sensitivity analysis [3], [4], where the model output is only evaluated against a minimum and a maximum value of a given input parameter. This is most commonly known as the plus/minus 10% way of varying an input parameter (example in Figure 1). An extension to OAT sensitivity is *one-way sensitivity analysis* [4]. Here, one parameter at a time is varied but over its entire predetermined range, sampling multiple points. The added value is that a response to an input becomes visible between its extremes, allowing to also identify potential non-linearities between input and output (see, e.g., the IEA figure [32] in Figure 2). One-way sensitivity analysis can be further extended to multiple ways sensitivity analysis (or n-ways sensitivity analysis) [4]. This method varies multiple parameters at a time, and uses for each parameter, a set of different values from its entire range. It has the ability to investigate the model output space as function of many parameters with less runs than would be required when only using one-way-sensitivity. In addition, it is able to show interdependencies between input parameters (Example provided in Figure 3).

How: The main methodological step in sensitivity analyses is to choose the perturbations to the nominal value of the parameters under investigation. This is only trivial when input-output relations are linear and there is no interaction between input parameters. For OAT analysis for instance, it is common practice to vary each input parameter with a fixed percentage, e.g. +/- 10%, or +/- 50%. Note however, that in case of non-linear relations a variation of 10%, 50%, or other, may lead to a different ranking of sensitivity to inputs. Alternatively, each parameter can be given a different minimum and maximum, for instance based on expert knowledge of the minimum and maximum values a parameter can have. From a purist perspective, the former approach (using the same plus and minus) is more appropriate, since the local nature of OAT analysis strictly does not allow a statement of the total variance of output $\mathbf{y}$ as a function of input $\mathbf{x}$. Rather, OAT analysis merely produces a ranking of sensitivity to input parameters when varied close to their nominal value. However, from a pragmatic perspective, it seems illogical to vary all parameters with the same percentage around their nominal value if it is known that their real ranges differ substantially, and the practitioner would like to get a first impression of the maximum range of the output parameters. The methodologically correct use of strict OAT analysis is limited, and there may be good reason to choose another method.

One-way sensitivity analysis in this perspective is more versatile than OAT sensitivity analysis, because it allows to sample multiple perturbations from the input parameter's nominal value. Here, it is advised to choose the minimum and maximum values more widely, and preferably according to known, or

realistic, limits. The main choice here is rather how many points to include, and where to sample them. For (or when suspecting) non-linear relations, it is advisable to add more points in those sections of the curve that are likely to show the highest non-linearities. For inputs with a linear relation to output, it would suffice to only use one minimum and maximum values without sampling points in between. These considerations also apply to n-way sensitivity analysis.

An important consideration for the choice of method is its computational cost (i.e., the amount of time that it takes to run an analysis). It also depends on the computing hardware available: the computational cost of running an analysis is much higher for any model on a two-core laptop than on a supercomputing cluster where multiple dozens of cores work in parallel. For OAT, the computational cost can be estimated as $C = 2k + 1$ [4], where k is the number of inputs that is varied. The computational cost of one-way sensitivity analysis is obviously higher than OAT sensitivity analysis: $C = (2 + a)k + 1$, where a is the amount of sampled points in addition to its extremes and the base case. Because n-ways sensitivity analysis varies input parameters simultaneously, its computational cost is typically lower than that of one-way sensitivity analysis. As for one-way sensitivity analysis, C depends on the number of sampled values of each input x_i. In addition, it is more difficult (and thus requires more computational effort) to determine the influence of *individual* parameters when using n-ways analysis. For example, $C = 2k$ to calculate all order sensitivities for generalised min/max full factorial designs, i.e., when only two values (a minimum and a maximum) for each input x_i are sampled; $C = 2k + 2$ to calculate first order (individual), interaction and total order sensitivity indices for min/max full factorial designs [4], [28]. Similarly, when a range of values for each x_i is sampled, the computational costs increases to $C = (2 + a)k$, with a being the amount of sample points in addition to its extremes.

When: Local sensitivity analysis is best used to answer diagnostic, or "what if" type of questions, where it has less use to prognostic studies due to its local nature. It can be used very well for a first and quick screening of influential variables, both in process modelling and economic analysis. In this case it is less relevant if the nature of the input parameter variance is pure uncertainty or rather variability (see above), because we are more interested in a ranking of parameters, than in the actual predicted output of the model. Though being simple, local sensitivity analysis shows some relevant disadvantages. Its main drawback is arguably the inability to estimate the influence of variable interactions (OAT and one-way sensitivity analysis) and non-linearities (OAT sensitivity analysis) [28]. Especially in complex and highly non-linear mathematical models this can lead to a false ranking of importance [3], or to the discarding of inputs as relevant based on their single variable sensitivity, while they may actually be relevant in combination with other parameters. This means that local sensitivity analysis is more suited to simple models (like simple factorial cost estimates) than to complex models (like full physical process models). Also, local sensitivity analysis can be inefficient if k is large and only some input parameters are influential. This is, again, especially the case for computationally intensive models.

In addition to diagnostic questions, local sensitivity analysis can also be very useful to test the model structure, by running extreme cases. If for instance, in an economic model, the discount rate is set to a very high value, the levelised cost of product should also become very high. If this is not the case, the modeller knows there may be a mistake in the model formulation.

Common pitfalls in (local) sensitivity analysis

The following list provides some common pitfalls, to prevent mistakes in the use of sensitivity analysis for CCS techno-economic analysis and elsewhere:

- Local sensitivity methods are perceived as sufficient, where in reality they may not fulfil the purpose of the study. This, in turn, leads to spending time applying methods that may not

generate the answers that are needed, or that are less suitable given a certain scope of the problem/question.

- Showing the sensitivity of (too) many model outputs to the model inputs, thereby confusing the audience of the study [28]. Often only a few output parameters are really interesting and is better practice to show only those, while being transparent on the full number of parameters studied.
- Performing piecewise sensitivity analysis where it is not justified. Piecewise sensitivity analysis examines the model in parts or compartments. Often, uncertainty is propagated through the model compartments in non-linear and interactive ways, and piecewise analysis could therefore provide false insights. Examples could include the piecewise examination of uncertainty in a process model and a cost model, where it might be more justified to investigate the uncertainty of the integrated techno-economic model.
- Using the wrong representation of results for a chosen method. For instance, representing the results of a OAT sensitivity analysis in a spider plot. This may happen if modellers are not familiar with the full range of possible approaches and good practices of graphic representation.

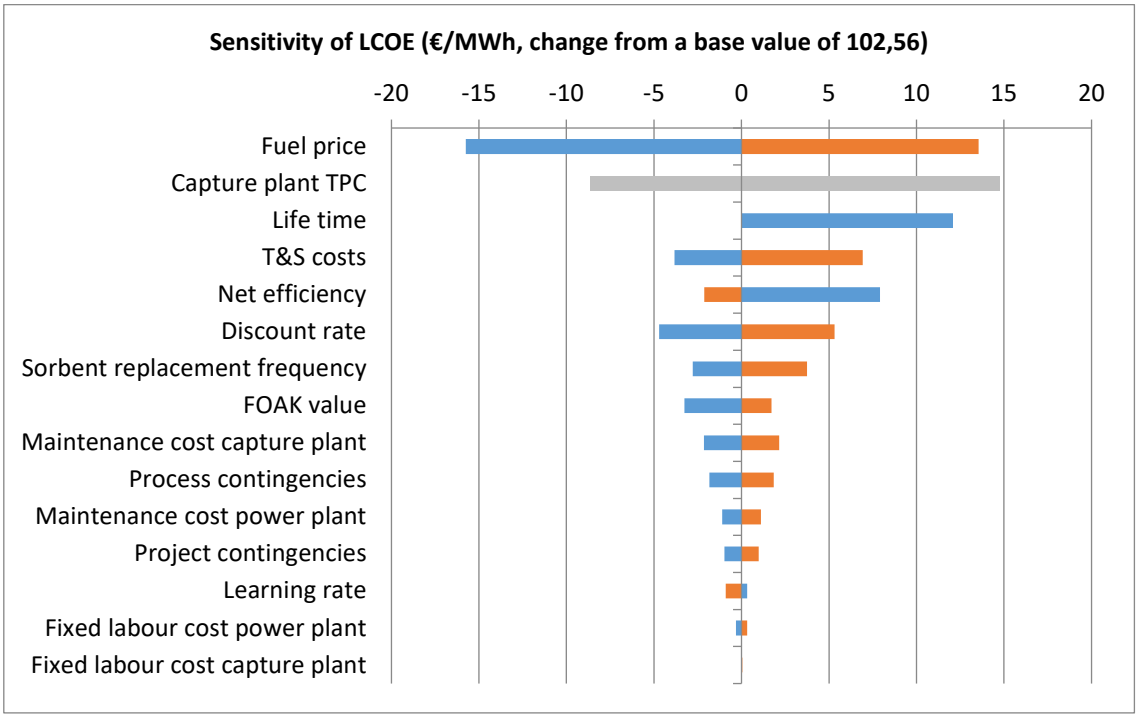

Figure 1. Illustrative example of OAT local sensitivity analysis: Tornado diagram representing the OAT sensitivity of the levelised cost of electricity to economic input parameters. The case study represents an NGCC plant equipped with postcombustion capture with solid sorbents using an electric swing adsorption cycle [33]**. Capture plant TPC ranges (grey colour) include simultaneous variation of the engineering, procurement and contracting (EPC) costs, process and project contingencies, FOAK value, and learning rate, proving a lumped contribution of these capital cost elements.**

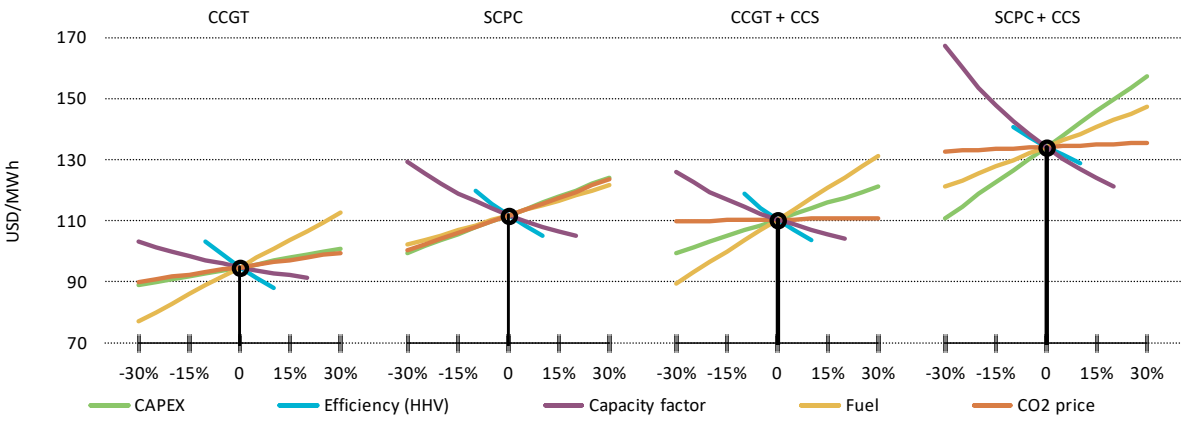

Figure 2. Illustrative example of one-way local sensitivity analysis showing the effect of CAPEX, Efficiency, capacity factor, fuel costs and CO_2 price on the LCOE of power plant with and without CCS: Figure 5.8 from the IEA Energy Technology Perspectives 2014 [32]**. The parameters were varied independently, leading to the typical spider webs of lines. Note the non-linearity of some parameters, e.g., capacity factor, making one-way analysis more suitable for this parameter than OAT analysis.**

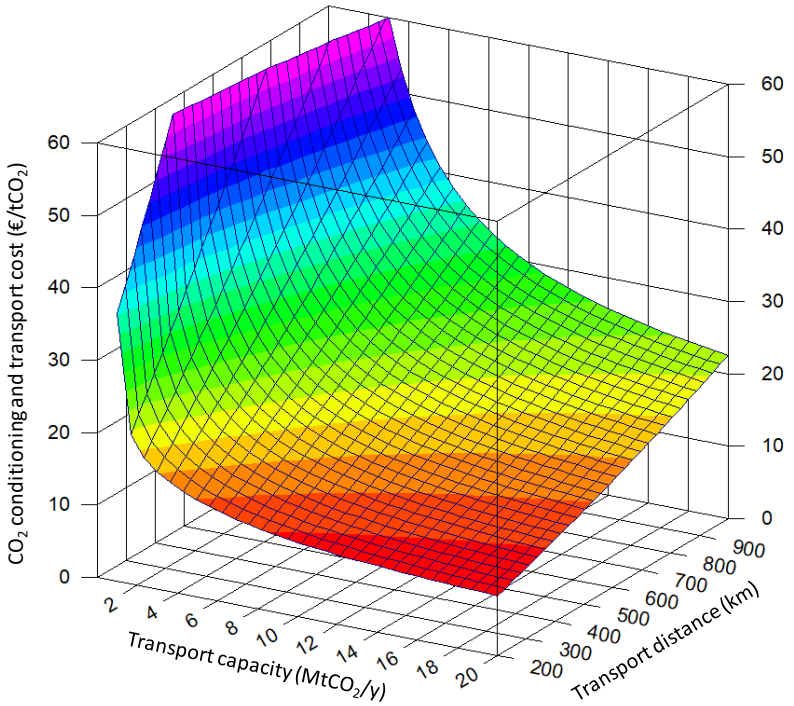

Figure 3. Illustrative example of N-ways (here: 2-ways) local sensitivity analysis, based on [34]**, showing the impact of transport capacity and distance on the cost of CO_2 conditioning and transport for an offshore pipeline infrastructure. This figure is based on the following considerations: 1) CO_2 comes from an MEA-based CO_2 capture unit; 2) Pipeline costs are calculated according the CO2 Europipe cost model** [35] **and an electricity cost of 55.5 €/MWh is assumed; 3) Pipeline diameter is optimised for each combination of transport capacity and distance; 4) A constant utilisation rate of 85%, a project duration of 25 years with an 8% discount rate are considered in the cost calculation.**

3.3.2. Probabilistic uncertainty analysis

What: Probabilistic (global) uncertainty analysis is a step up from simple one-way or n-ways sensitivity analysis because it assigns a probability to the range of values that a parameter can have [3], [28], [36]. It not only tells something about which values the model outputs $\mathbf{y}$ may take on as a function of changes in model inputs $\mathbf{x}$, but also how likely a certain output may be (for e.g. see Figure 4). Global uncertainty analysis can also be used to find the *global* sensitivity of the outputs $\mathbf{y}$ to the input vector $\mathbf{x}$. This is different from *local* sensitivity in the way that the sensitivity indicators are estimated for the whole range of possible inputs and outputs (thus global), while the local sensitivity indicators only apply around the selected base value. Apart from the advantage of understanding the model input-output relationship over the whole range of parameter space, global uncertainty analysis also allows to identify the synergistic effects between model inputs.

How: Probabilistic uncertainty analysis requires assigning to each or some of the input parameters a probability density function. These functions are typically fitted on measured (but often assumed) data. Mathematically, $\mathbb{P}_{\mathbf{X}}$ are the probability distribution functions of the random vector of input parameters $\mathbf{X} = (X_1, \dots, X_n)$ and $\mathbb{P}_{\mathbf{Y}}$ the PDFs of the random vector of output parameters $\mathbf{Y} = (Y_1, \dots, Y_m) = g(\mathbf{X})$. This results in a cumulative distribution function $F_Y(y) = \int f_Y(y)$ over the range of output realisations. Preferably, $F_Y(y)$ and $f_Y(y)$ are evaluated analytically, because of low computational cost. Practically, this is often impossible, because the mapping between $\mathbf{X}$ and $\mathbf{Y}$, denominated $g(\cdot)$, is unavailable (i.e., there is no analytical solution for $g(\mathbf{X})$). In such case, the probability of $\mathbf{Y}$ can be evaluated by repeated sampling using Monte Carlo methods.

From the PDFs of inputs and outputs, global sensitivity measures can be calculated (i.e., the measures that rank the sensitivity of model outputs to each model input), which is now also often done in CCS research. There are different methods to do this and the calculation of these measures is a separate research field (the underlying mathematics can be quite complex and sometimes not transparent). It is beyond the scope of this work to address this in detail, but there are good standard works on calculation of global sensitivity indicators in literature, e.g. [28], [30].

The characterization or quantification of input parameters with PDFs is arguably the most challenging part of global uncertainty analysis and therefore we elaborate a little further on this, without the intention to provide an exhaustive overview of PDF selection. We identify three possible approaches:

1. Hawer et al., [37] developed a guideline based on a flowchart that contains questions to be answered by the user with “yes” or “no”, as shown in Appendix B. The flowchart leads the user to a recommendation for a representative uncertainty characterization method for each individual case. The guideline aimed at an audience with little to no knowledge on the terminology and or modelling in the field of uncertainty quantification.
2. In another publication [38], the principle of maximum (information) entropy was suggested. The principle of maximum entropy seeks to choose a PDF that maximizes the amount of information that a distribution can provide, subject to known constraints, as summarized in Table 3. This means, for instance, that when only an upper and a lower bound of a range are known, the uniform distribution is the PDF that provides the most information.
3. A third technique for obtaining a PDF is to use a ‘subjective’ probability distribution, that is a PDF that is based on *knowledge* of the process/parameter rather than *data*. Generally, this is accomplished by the application of formal expert elicitation following a systematic procedure. Examples of formal protocols for expert elicitation can be found in Morgan and Henrion [39], developed for the field of quantitative risk and policy analysis and the IPCC tool linking probability with linguistic descriptions of uncertainty [38].

Table 3: Choosing a distributions function using the principle of maximum entropy. Adapted from [38]**.**

Available information	Assigned PDF
Upper bound, lower bound	Uniform
Minimum, maximum, mode	Triangular
Mean, standard deviation	Normal or lognormal if the value physically cannot be below zero
Range, mean, standard deviation	Beta
Mean occurrence rate	Poisson

When: Because of its stochastic nature, probabilistic uncertainty analysis is very capable to answer prognostic, or "what will" type of questions, as well as provide the audience with an answer on how likely such an outcome could be (see also Figure 4). It is therefore helpful to policy and decision makers for strategic decisions and can come to good use in techno-economic analysis of CCS. There are however two large drawbacks that limit the use of probabilistic methods as uncertainty analysis tools. The first relates to the need to describe the variability of the input parameters in probabilistic terms. It requires as a minimum a description of minimum and maximum, but preferably a full PDF. The problem, however, is that the exact values of parameters are often not known (recall the difference between uncertainty and variability, where in the latter case we often do have a good grasp of the variation of values). Randomly assigning probability distributions to inputs can result in misleading outputs. As a result, this would therefore not only not reduce uncertainty, but possibly generate a false sense of certainty and thereby lose its value for answering prognostic questions [1], [4]. It could however still be useful for answering diagnostic questions or for calculating global sensitivity indicators. Given this consideration, we argue here that probabilistic uncertainty analysis is better suited to deal with *variability*, than with true *uncertainty*.

A second large drawback of, especially, Monte Carlo simulation is that it needs a large amount of runs to become a) statistically significant, and b) to estimate sensitivity indices[2], see e.g. [3], [40]. Such large amounts of runs could be feasible for simple and/or analytical models - like most economic models used in techno-economic analysis - but are a large obstacle for highly non-linear numerically solved models - like rigorous process models.

Common pitfalls in probabilistic uncertainty analysis

For probabilistic uncertainty analysis, the following additional pitfalls apply:

- Basic Monte Carlo simulation methods assume that input variables are independent of each other, which is often not the case in reality. Ignoring the correlation between dependent variables may lead to a false ranking of influential parameters. To address this issue, a dependence structure (known as a copula) can be created prior to sampling individual uncertain variables [28]. Alternatively, this problem can sometimes be avoided by explicitly modelling the relationship between two variables (e.g., depth and pressure or temperature in a subsurface reservoir model).

[2] For instance, when using a brute force method, the number of model runs N required to calculate variance based sensitivity indicators (like the conditional mean) $E(Y|X_i) = 1000$, then $N^2 = 1000^2$ runs would be required to calculate the sensitivity indices. Even with smart computational methods like Saltelli's [28], the amount of runs required is still $N(k+2)$ where k is the number of variables to be varied. Linear regression on the Monte Carlo mapping generates sensitivity indicators at lower cost $C = N$, but only calculates univariate (first order) sensitivity indicators (there are other post-processing methods that have this low cost but they have the same drawback, see e.g. [4]).

- The PDFs of input variables are poorly defined, or are insufficiently definable [1], [4]. Monte Carlo simulation will compile seemingly reliable PDFs of model output regardless the quality of the input distributions. It may therefore create a false sense of certainty for the user of the sensitivity study, that could lead to wrong decisions being taken.

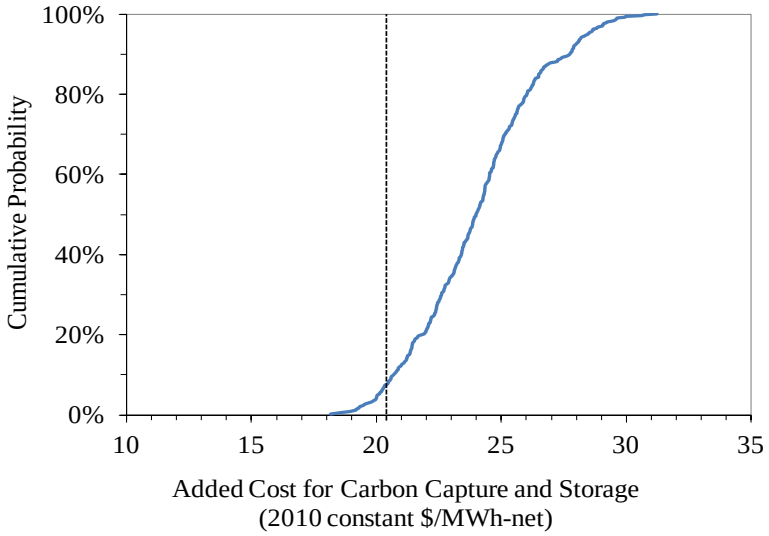

Figure 4. Illustrative example of Monte Carlo simulation. Output of a Monte Carlo uncertainty analysis from [36]**. The figure shows both the deterministic (vertical dashed line, no uncertainty) and the probabilistic (solid line) values of the added cost of CO_2 capture for a supercritical coal power plant under the constraint of a 1000 lb of CO_2/MWh gross emission (US) performance standard. For the assumptions of this study there is less than a 10% likelihood of realizing the nominal (deterministic) value of added cost. The most likely cost (50% probability) is $24.5/MWh (about 4 $/MWh more than the deterministic value).**

3.3.3 Recommended practices for sensitivity analysis and probabilistic uncertainty analysis

As the above sections have shown, sensitivity and probabilistic uncertainty analysis require the rational selection of parameters to vary, how to treat them, and which values, ranges, or PDFs to apply, to perform the uncertainty analysis in a meaningful and efficient manner.

A first good practice then, is to rationally choose the parameters to vary. Initial screening of parameter sensitivity can help reducing the number of varied parameters *k* and makes the sensitivity analysis more efficient. Alternatively, one can find influential parameters for similar problems in academic or grey literature. When planning to run a Monte Carlo simulation for instance, local SA can be used to discard parameters that are not influential, reducing the required number of Monte Carlo runs. Care should be taken though to also test the sensitivity of parameters when interacting with others, before discarding them altogether. It is good practice to find a balance between the number of parameters to vary and their range. If the range is too wide and/or too many parameters are varied, the results may be less useful and relevant observations may get lost in the mass of output variance, apart from putting too much effort to answering the research question. Especially for probabilistic uncertainty analysis, when the chosen range is too small and/or too few parameters are varied, the results may not be global, thus inconclusive [28].

A second good practice is to explicitly distinguish between different types of input data (e.g. physical properties versus operational/design conditions/choices, measured data versus expert opinions, economic data versus technical data) or how to cluster them (e.g. a measured value times its weight) [28].

Finally, defining a good "sampling scheme" up front can save a lot of hassle and unnecessary repetition. Sampling means the amount and values (or positions in a range) of the input data points that are chosen. Sampling can for instance be done by picking random values from a range of possible values, but this may lead to clusters of points and gaps. The modeller can also use random values within subintervals (called stratified sampling) or using particular values within subintervals (also stratified sampling) [28]. Especially for multiparameter sensitivity analysis, several sampling schemes have been developed, focussing on reducing the amount of points that need to be evaluated, while remaining a required level of predictive power of the sensitivity analysis. Such sampling schemes are addressed elsewhere, e.g., [28] and include full factorial (only two levels of values: -1/1 or min/max); fractional factorial (FF, only two levels of values: -1/1); Latin Hypercube (LH: multiple levels of values, stratified, needs number of simulations to be larger than the number of varied parameters), or multivariate stratified sampling.

3.4. Emerging uncertainty methods

3.4.1. Complementary analysis of qualitative uncertainties with pedigree analysis

What: Pedigree analysis is a systematic and harmonised approach to identify and assess knowledge strength in order to minimise subjectivity and increase transparency. It is part of the NUSAP system (Numeral, Unit, Spread, Assessment, Pedigree) for uncertainty assessment and communication proposed by Ravetz & Funtowicz [41]. Generally speaking, pedigree analysis provides an evaluation of the production process of information (how was it measured, derived, theorised?), and investigates the different aspects of the underpinning of the numbers and scientific status of the knowledge used [27], further explained below. Pedigree analysis has key advantages. For instance, it identifies the different sorts of uncertainty in quantitative information and enables them to be displayed in a standardized and self-explanatory way. It also allows to assess the quality of models by increasing transparency on the assumptions and choices and assessing uncertainties in the underlying knowledge base used for building up a process or cost model. Pedigree analysis is flexible in its use and can be used on different levels of comprehensiveness: from a rough sketch to a sophisticated procedure involving structured informed in-depth group discussions on a parameter by parameter format. Quite often results are used to develop so called diagnostic diagrams, which are a convenient way to view each of the key parameters in terms of two crucial attributes: relative contribution to the sensitivity of the output and their strength. Finally, and possibly one of the key advantages, it fosters an enhanced appreciation of the issue of uncertainty in information.

How: Pedigree is expressed using a set of problem-specific criteria that serve to assess different aspects of knowledge strength. It is basically a systematic multi-criteria evaluation of the production *process* of knowledge, therefore looking not only at parameter data but also to knowledge available when building up a model. For example, commonly used criteria are proxy (is something measured directly, or is it estimated using an indirect indicator?) and theoretical understanding (is the data or model based on a well-established scientific theory, or crude speculation?). The type and number of criteria should be tailored to the specific situation.

Assessment of pedigree requires qualitative expert judgment. Expert elicitation systematically makes explicit use of unwritten insights 'in the heads of experts' (e.g., the modeler, or a group of experts), focusing on limitations, strengths and weaknesses of the available knowledge base. To minimise subjectivity and arbitrariness in the evaluation, a pedigree matrix is used to systematically and transparently transform expert judgment into a numerical scale. A pedigree matrix (Table 4) is basically a table with the criteria as columns, and strength scores (typically 0 (weak) to 4 (strong)) as the rows (note that also other scales can be used). In each cell of the table a linguistic description is provided with the requirements that should be met to receive a particular score. These descriptions therefore

serve as yardsticks. Note that these linguistic descriptions are mainly meant to provide guidance in attributing scores to each of the criteria for a given parameter, and as such the descriptions should be tailored to the focus of the study. How clear, explicit and tailormade to the problem the linguistic definitions are, is a key component of the proper and successful application of pedigree matrices. A total score can be then produced for a given parameter or (sub)model (see Figure 6). This, however, requires that the modeler (or the experts) weighs the different criteria of the pedigree matrix, for instance by deciding that all criteria are equally important or that some criteria are more important than others. Furthermore, when a group of experts is scoring, total scores of each expert can be aggregated using the median of the expert respondents' scores. Interquartile ranges can then be used as an indicator of inter-expert heterogeneity (degree of consensus/disagreement in the strength of the knowledge base for a given parameter/model). Table 4 provides an example of a typical pedigree matrix used to assess the strength of data in a cost assessment of CO_2 capture technologies.

Table 4. Example of a pedigree matrix used in the EDDiCCUT project to assess the strength of data input for cost assessment [42]**.**

SCORE	Proxy	Reliability of source	Completeness (only for equipment list)	Completeness (all other parameters)	Validation process
4	A direct measure of the desired quality	Measured/official industrial, vendor, and/or supplier data[3]	Representative data for all line items (processes, instruments, electro, civil, mechanical, etc.)	Complete data from a large number of samples over a representative period	Compared with independent data from similar systems that have been built
3	Good fit to measure	Qualified estimate by industrial expert supported by industry data	Representative data for all process equipment (equipment list, heat and mass balance, PFD)	Complete data from a large number of samples but for unrepresentative periods or from representative periods but for a small number of samples	Compared with independent data of similar systems that have not been built
2	Correlated but does not measure the same thing	Reviewed data derived from independent open literature	Representative data for most important process equipment (equipment list, heat and mass balance, PFD)	Almost complete data but from a small number of samples or for unrepresentative periods or incomplete data from adequate number of samples and periods	Validation measurements are not independent, include proxy variables or have limited domain
1	Weak correlation but commonalities in measure	Non-reviewed data from open literature	Data from an adequate number of process parameters eat and mass balance, PFD)	Almost complete data but from a small number of samples and unrepresentative periods	Weak and indirect validation
0	Not correlated and not clearly related	Non-qualified estimate or unknown origin	Only high level or incomplete data available	Incomplete data from a small number of samples for an unrepresentative period	No validation performed

Proxy: refers to how good or close a measure of the quantity that is modelled is to the actual quantity one wants to score. *Reliability of source:* evaluates the origin of the collected data. *Completeness:* this criterion assesses the coverage of the data, taking into account the information reported for process inputs, outputs and associated stressors. It considers not only the amount but also the specific relevance of the presented data. *Validation:* refers to the degree to which data and assumptions used to produce the numeral of the parameter has been cross-checked against independent sources.

[3] Note that vendor or supplier data was in this example score the highest regarding reliability. This of course does not need to be the case, and while carrying out the scoring the modeler (or expert) should take into account whether the data comes from an offer or from a performance guarantee in a contract, the letter being much more reliable.

Results of the pedigree analysis can be combined with those of a sensitivity analysis in a diagnostic diagram. The diagnostic diagram (Figure 5) is based on the notion that neither spread alone (as obtained from a sensitivity analysis) nor strength alone (as obtained from the pedigree score) is a sufficient measure for assessing the quality of a model output. Robustness of model output to parameter strength could be good even if parameter strength is low because the importance of that parameter for the final results may be minor. Alternatively, robust conclusions can be derived for parameters that have large impact on output spread and high parameter strength. Mapping components of the knowledge base in a diagnostic diagram thus reveals the weakest spots and helps in the setting of priorities for improvement.

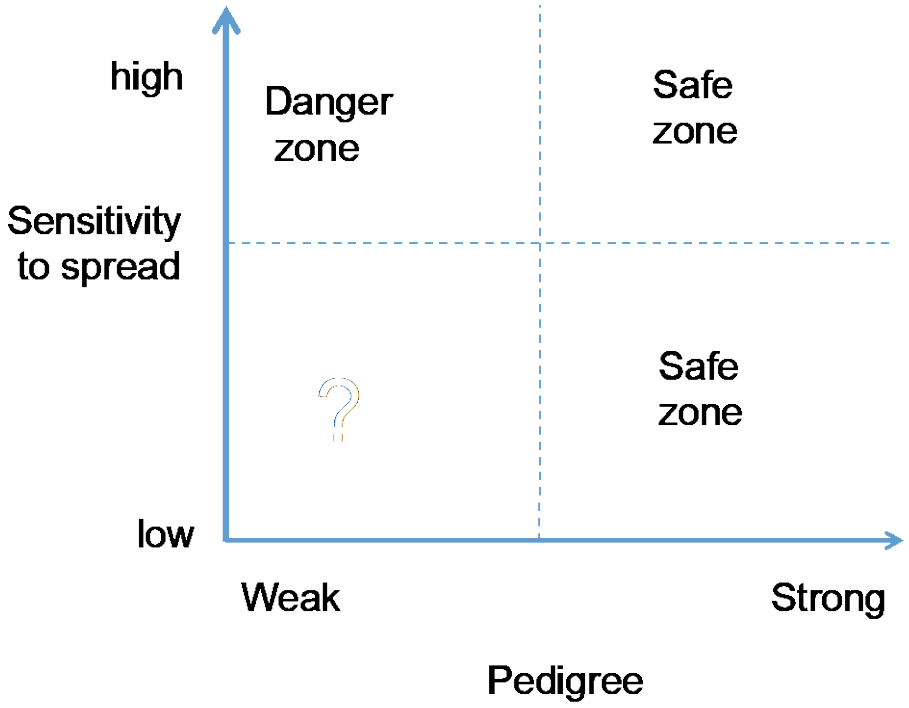

Figure 5. Example of a diagnostic diagram for the evaluation of the robustness of the model and model parameters. The so-called danger zone is the quadrant containing parameters to which the model output is highly sensitive, but which have a weak pedigree, i.e., the results are dependent on a parameter that is characterized with a weak knowledge base. The safe zones are the two quadrants containing parameters that have a high pedigree. Parameters in the zone characterized with weak pedigree-low sensitivity should be further examined as the low sensitivity to spread could be caused by the assumptions in the knowledge driven by a weak knowledge base.

When: Pedigree analysis can be used for any process or cost evaluation as it increases transparency in the reporting of quality of the data and models used in a given assessment. Such information is important for understanding the robustness of model outcomes as well as to facilitate discussion in expert groups. Furthermore, the use of, e.g., diagnostic diagrams allows for easier representation of the quality and importance of uncertainties. The added value of the approach is especially significant for assessments where there is a weak knowledge base. For instance, technology and costs assessments of technologies that are currently at low TRL level, for which only partial information is available, and significant number of assumptions need to be made regarding performance and scaling.

Pedigree scores for technical input data	Proxy	Empirical basis	Theoretical understanding	Methodological rigour	Validation process
SA 2a: H_2 unit without CO_2 capture					
Feed streams	4	3	4	3	-
Design parameters	3	3	4	4	3
Boundary conditions	4	2	4	3	3
Other physical properties	4	4	4	4	3
SA 2b: CO_2 capture unit					
Feed streams	4	3	4	3	3
Design parameters	3	2	3	3	2
Boundary conditions	4	2	4	3	3
Other physical properties	4	4	4	4	3
SA 4a: Conventional polyol					
Feed streams	4	3	4	3	-
Design parameters	3	3	3	2	1
Boundary conditions	4	2	4	3	3
Other physical properties	4	3	4	3	1
SA 4b: CO_2-based polyol					
Feed streams	4	3	4	2	-
Design parameters	3	2	3	2	1
Boundary conditions	4	2	4	3	3
Other physical properties	4	2	4	2	0

Pedigree scores for economic input data	Proxy	Reliability of source	Completeness (only equipment)	Completeness (other parameter)	Validation process
SA 1: Naphtha production and transport					
Capex	-	-	-	-	-
Opex	4	4	-	3	0
SA 2a: H_2 unit without CO_2 capture					
Capex	4	2	2	3	3
Opex	4	3	-	2	0
SA 2b: CO_2 capture unit					
Capex	4	2	2	3	2
Opex	4	3	-	2	0
SA 3: CO_2 transport and storage					
Capex	4	2	1	3	1
Opex	4	2	-	2	1
SA 4a: Conventional polyol					
Capex	4	2	1	3	1
Opex	4	3	-	2	0
SA 4b: CO_2-based polyol					
Capex	4	2	1	3	1
Opex	4	3	-	2	0
SA 5: Chemicals					
Capex	-	-	-	-	-
Opex	3	3	-	2	0

Figure 6. Illustrative example of the use of pedigree analysis. In [42]**, pedigree matrices were used in the evaluation of the techno-economic and environmental performance of carbon capture at a hydrogen unit in a refinery combined with CO_2 conversion into polyol synthesis. As illustrated, the figures above show pedigree matrices for input data (for the technical model and the cost assessment). The information is provided at the aggregated level of a System Area (each representing group of processes that are part of the value chain under study). Note that the criteria selected for each matrix has been tailored to each type of assessment, for instance capex and opex when assessing data used for costing, and feed streams, design parameters, boundary conditions and other physical properties for technical input data. Together with the matrix, the article describes the reasoning behind the choice of scores (which was done by the authors).**

3.4.2. Pseudo statistical approach

What: This approach has been developed in the realm of Life Cycle Assessment (including life cycle costing, see e.g., [43]) but it can be applied to other fields including TEA. The methodology aims to enable the use of Monte Carlo analysis to assess the propagation of uncertainty and/or variability

introduced by both uncertainties in data *and* methodological choices into the final results. An example of a methodological choice relevant to this guideline is the allocation of the costs of capture when more than one valuable product is produced in a given system (e.g., polygeneration systems). The key feature of this method (compared to others) is that it explicitly acknowledges large choice related uncertainties on top of parameter uncertainties.

Compared to the natural variability of data, which could be represented through a probability distribution, there is not natural variability in a discrete choice (such as allocation). Although the methodology treats both data and methodological choices in a similar way, the use of the term "pseudo statistical" has the goal of tacitly acknowledging that the use of terminology (e.g. probability, statistical) is not entirely suitable for all cases.

How: To be able to introduce pseudo-statistical propagation of a methodological choice, a variable called *methodological preference* (p) (as percentage) is introduced. If there is only one methodological choice, p equals 100%, but if there are different choices (for instance allocating the capture costs based on energy (method 1), mass (method 2), price of the products (method 3)) then each choice is assigned different p values (each between 0 and 100%), with the condition that the sum of all p values equals 100%. In this respect, the pseudo statistical approach is very similar to assigning weights in multi criteria analysis. As the p values reflect preferences, they are inherently subjective. The methodology therefore allows to explicitly include values (preferences) of stakeholders or to include values that represent trends found in e.g., literature. Compared to other methods, the main advantage is on selecting p values that reflect stakeholder preference or preferences. If literature is used instead, other methods could be used (e.g., analysing discrete cases). The methodological values provided by the experts define the ranges of methodological preferences, such that for each range one methodological choice takes place. The value of a random number from a uniform distribution between 0 and 100 is then generated and evaluated for the ranges of preferences. In mathematical terms, this can be represented as follows:

$$Methodological\ choice = \begin{cases} method\ 1\ if\ x\ \in\ [0, p_1] \\ method\ 2\ if\ x\ \in\ [p_1, p_1 + p_2] \\ method\ 3\ if\ x\ \in\ [p_1 + p_2, p_1 + p_2 + p_3] \\ \dots \\ method\ n\ \ if\ x\ \in [p_1 + p_2 + p_3 + \cdots + p_{n-1}, 100] \end{cases} \qquad 2$$

$$x \sim U\ (0{,}100)$$

After the parameters are defined, Monte Carlo analysis can then be used for the random sampling to propagate the uncertainty. In the results, the uncertainty introduced by different combinations of methodological choices can then be included. This approach accounts in a pseudo-statistical manner for a representative sample of combinations of methodological choices.

When: The method is particularly recommended when a large number of methodological choices are required (for instance in process modelling and/or costs assessment) thereby avoiding the need for developing one-at the time scenario modelling for choice-related uncertainties, which depending on the number of methodological choices in a given analysis, can become easily very time and resource intensive.

3.4.3. Reduced order models for global uncertainty analysis

What: As mentioned above in section 3.3.2, probabilistic uncertainty and sensitivity analysis comes at the expense of many thousands (or more) of model realisations. This may severely hamper their use for computationally heavy models, such as most first principles process models, especially when high performance computing is unavailable. Therefore, the discipline of global uncertainty analysis has

moved towards the use of reduced order models $\hat{g}$ (ROMs, also meta-models or surrogate models) as a representation of heavy numerical models:

$$\mathbf{y} = g(\mathbf{x}) \approx \hat{g}(\mathbf{x}) = \hat{g}(\mathbf{v}, \boldsymbol{\theta}) \quad 3$$

Where, $\mathbf{v}$ is a vector of deterministic input parameters and $\boldsymbol{\theta}$ is a set of stochastic input parameters.

Different methods of model reduction have been studied and some have found their way to the CCS field of research: Hanak and others have used Artificial Neural Network (ANN) models as surrogates for full physical calcium looping models, and have used these to perform integrated global uncertainty analysis of the economics of calcium looping systems [8], [44]. [45] used Polynomial Chaos Expansion (PCE) to produce surrogate models of physical models for CO_2 storage well leakage and combined those with risk and cost analysis tools to retrieve stochastic integrated leakage risk and cost information.

How: The reduced order model types for global uncertainty analysis vary, but they all rely on the same approach:

1. Run a limited number (typically several hundreds) of realisations of the full physical model, with uncertainty and/or variability assigned to its inputs (i.e. running different realisations for different combinations of model inputs from predefined parameter ranges).
2. Fit an analytical (e.g. polynomial, ANN, linear regression) reduced order model based on this limited set of model runs.
3. Perform a full Monte Carlo simulation on the ROM. Given that the ROM is analytical, this should take a fraction of the time of a full physical model.
4. Calculate the sensitivity indicators, either directly/analytically when possible or based on the Monte Carlo runs.

The methods to produce some reduced order models and to calculate sensitivity indicators from their probabilistic uncertainty analysis can be quite mathematical and therefore can easily seem daunting to the general techno-economic analysis practitioner. But since the basis of these methods is now well established, also more accessible, ready to use kind of tools are coming available (see section 5), which should open up these methods to a wider audience.

When: Previous studies have shown that the used reduced order models are very accurate in describing the input-output combinations of the original physical model within the specified ranges of application [3]. They are therefore very useful when reliable representations of uncertainty and variability are necessary to answer *what will* kind of questions using Monte Carlo simulation, while the original model would be too heavy (computationally intensive) to allow this. They are especially helpful to perform global sensitivity analysis of heavy models, and to aid in factor priorisation and factor fixing. Like with any probabilistic method however, they are best suited for the variability of input parameters, and less for real uncertainty, given that there may not be a reasonable basis for probability density functions of truly uncertain parameters.

Tables 5 and 6 and Figure 7 exemplify the use of reduced order models for global sensitivity analysis and the calculation of Variance based (Sobol) sensitivity indicators. The example is based on a series of papers [46]–[48] in which surrogate models of an MEA capture plant were built based on a full process model and compared with process data from the National Carbon Capture Center (NCCC) in Alabama, USA [49]. Table 5 shows the names of the varied parameters along with sources that contain more details of the submodel development and uncertainty quantification.

Table 5. List of parameters for MEA model considered in uncertainty analysis

Parameter Number	Parameter Name
Thermodynamic Model (Aspen Plus names in brackets) [47]	
1	Gibbs energy of formation at infinite dilution (DGAQFM) for MEA+
2	Gibbs energy of form. at infinite dilution (DGAQFM) for MEACOO-
3	Enthalpy of formation at infinite dilution (DHAQFM) for MEA+
4	Enthalpy of formation at infinite dilution (DHAQFM) for MEACOO-
5	Henry parameter A (HENRY/1) for MEA-H_2O
6	Henry parameter B (HENRY/2) for MEA-H_2O
7	NRTL binary interaction parameter A (NRTL/1) for MEA-H_2O
8	NRTL binary interaction parameter A (NRTL/1) for H_2O-MEA
9	NRTL binary interaction parameter B (NRTL/2) for H_2O-MEA
Holdup Model [48]	
10	H_{L1} (liquid holdup)
11	H_{L2} (liquid holdup)
Mass Transfer/Interfacial Area Model [48]	
12	A_1 (interfacial area)
13	C_L (liquid mass transfer coefficient)

A total of 23 steady-state data sets were generated during the test campaign at NCCC; the propagation of uncertainty was demonstrated for three cases in the previous work [49] and for two additional cases in this paper. Table 6 shows the key absorber operating variables for the two cases; the case labels are consistent with the previous work.

Table 6. Key operating variables for absorber simulation for two cases

Variable	Case K2	Case K7
Lean Solvent Mass Flowrate (kg/hr)	11794	11791
Flue Gas Flowrate (kg/hr)	2243	2233
Lean Solvent Loading (mol CO_2/mol MEA)	0.247	0.399
Lean Solvent MEA Weight Fraction (g MEA/g [MEA+H_2O])	0.312	0.288
CO_2 Mole Percent in Flue Gas	11.40	9.18
Percent Capture of CO_2	99.49	54.76

The main advantage of developing surrogate models, is the lower computational effort, and therefore the ability to calculate variance based sensitivity indicators. In this example, this was done in the software platform PSUADE ([50], more information in section 5), which allows to calculate Sobol indices [51], which represent a decomposition of variance technique for determining the relative influence of each parameter on the model output. The development of the surrogated model required 1000 runs in Aspen Plus, taking 2-3 hours on a normal desktop machine. Based on these full model realisations, the reduced order model was fitted with Multivariate Adaptive Regression Splines (MARS) [52]. This reduced order model was then run to calculate the normalised Sobol indices in Figure 7 for the contributions of the parameters listed in Table 5.

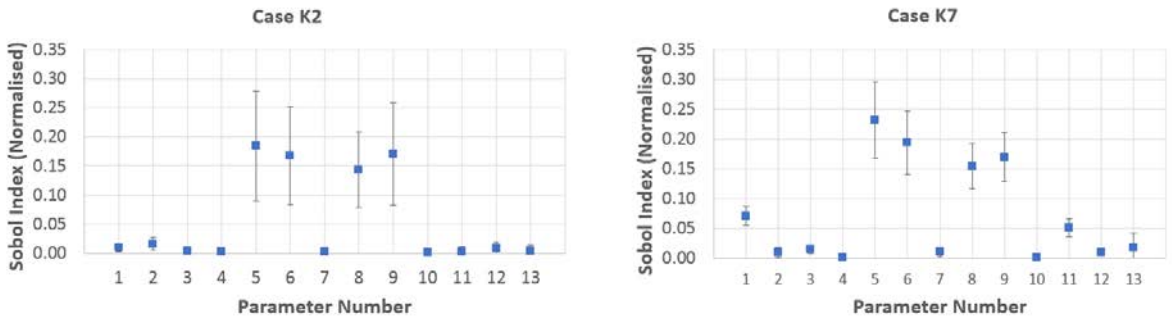

Figure 7. Normalised Sobol indices for contributions of individual parameters for two model simulation cases. Points represent mean values and error bars ± 1 standard deviation (n=100 replications performed). Parameter numbers are consistent with those given in Table 1

Although the results demonstrate some spread in the values of Sobol indices that results from replicating the calculation, the relative importance is shown to be predicted consistently; for both cases parameters 5-6 and 8-9 are shown to have the highest effect on the CO_2 capture prediction. For Case K2, the packing-related parameters (No. 10-13) are shown to have very minimal effect on the prediction of CO_2 capture. For Case K7, this is not so due to the much higher loading of CO_2 in the inlet solvent, which results in inefficient absorber operation. Although some of the thermodynamic model parameters still have the highest Sobol indices, some of the packing dependent parameters have higher values in comparison to Case K2. As a result, the calculated value of CO_2 capture percentage is not insensitive to the parameterisation of the packing models (mass transfer, interfacial area, hydraulics).

3.5. Strengths, weaknesses and applicability of uncertainty methods to TEA

The previous sections discussed a selection of uncertainty analysis methods available to the CCS techno-economic practitioner aiming to provide basic information on their use. Here, we synthesise this discussion into guidelines on choosing from these methods.

The choice for an uncertainty method depends first and foremost on the purpose of the uncertainty analysis. Recall that we divided these into diagnostic, prognostic, or factor prioritisation/factor fixing and model testing. Additionally, the choice will depend on such criteria including:

- The computational cost of running the model and uncertainty analysis
- The number and type of input factors that need varying
- The context of the analysis including the audience

Note that selection criteria will differ for each user, and also depend on the purpose of the uncertainty analysis, as well as on their experience. Table 6 summarises the uncertainty analysis methods in terms of possible selection criteria and suggests TEA areas to which a method may be more or less applicable, while Figure 8 provides a general workflow for selecting uncertainty analysis methods.

For diagnostic, or “what if” type of questions, local sensitivity analyses often suffice. They present a simple and clear picture of how an output might change as a result of varying one, or multiple parameters, e.g. how the performance and cost may vary as a result of changes in ambient conditions. We recommend the use of one-way or N-way sensitivity analysis, because they provide more information (on non-linear responses) than a standard OAT analysis.

For prognostic, or “what will” type of questions, we strongly recommend global uncertainty methods, provided that the input parameter probability can be quantified satisfactorily. If this is not the case, it

is recommended to avoid prognostic analysis altogether, because there is a danger of creating a false sense of certainty (i.e., the receiver of the model output will see a carefully compiled probability density function, adding to the perception of certainty). However, if the probabilistic output is based on a poor description of input uncertainties, the result is still very weak and may be misleading. The requirement of quantifiable input PDF's implies that what will type of questions should preferably only be answered for CCS technologies and systems that have reached a certain level of advancement, arguably beyond the large pilot plant stage.

For both diagnostic and prognostic questions, we recommend complementing the quantitative uncertainty analysis with a qualitative one, like pedigree analysis. This is especially the case when the model and its results are used for policy and/or decision making, because it provides decision makers with information on how robust the model results are, which is indispensable for making informed decisions.

In case of factor priorisation or factor fixing, sensitivity analysis is required. In the case of very simple (mostly linear) models without many parameter interactions, a local sensitivity method could suffice, where it is arguably advisable to go beyond OAT. However, factor prioritisation and fixing are often most needed in complex models, in which case a global (probabilistic) sensitivity analysis is essential, to also account for second or higher order effects of an input parameter on model output.

If the purpose of the uncertainty analysis is model testing, we recommend using single (OAT) or multiple (NAT) parameter local uncertainty analysis. Preferably, the model is subjected to (combinations of) an extreme value of input parameter(s), that should trigger an extreme output (think e.g., of an extremely high cost of energy, which should lead to a very high cost of CO_2 avoided).

Finally, for a non-specialist audience and sometimes even for a specialized audience, it is arguably a poor idea to show results of uncertainty analysis in very advanced (complex) graphs. To best convey the results, simple plots like tornado or spider plots may be more useful than more complex and less commonly used visualizations, e.g., scatter clouds.

Table 7. Uncertainty analysis selection guide.

Possible selection criteria	OAT sensitivity analysis	One-way sensitivity analysis	N-ways sensitivity analysis	Global uncertainty analysis (incl. Monte Carlo)	Pedigree analysis	Pseudo statistical approach	Reduced order global uncertainty analysis
Purpose of uncertainty analysis	Understand first order relative ranking/importance of parameters, understand response to extreme input values for single parameters (model testing)	All of OAT plus understand break points, non-linearities	All previous plus investigates interactions and response to extremes of multiple parameters	To quantify the probabilistic variability/uncertainty in the knowledge base and how that impacts an outcome. To foster an understanding of the distribution of uncertainty and/or variability. To quantify the chance of a certain event of happening. To quantify the global sensitivity to input parameters	To foster an understanding of the strength of the knowledge base underlying data or a model	To understand the significance of value-laden choices compared to parameter variation on the model outputs.	To quantify the probabilistic variability/uncertainty of computationally heavy models in our knowledge and how that impacts an outcome. To foster an understanding of the distribution of uncertainty and/or variability. To quantify the chance of a certain event of happening. To quantify the global sensitivity to input parameters

Relative computational cost/time	Low	Low	Medium	Medium - Very High	Not applicable, but requires substantial time for expert elicitation	Medium - Very High	Medium
Pre-processing data	low	low	Low	high	medium	High	High
Type of uncertainty method	quantitative	quantitative	Quantitative	quantitative	qualitative	qualitative & quantitative	quantitative
Able to cope with interactions	No	No	Yes	Yes	Not applicable	Yes	Yes
Able to cope with non-linearity	No	Yes	Yes	Yes	Not applicable	Yes	Yes
Target user/ reader	General public	General public	Depends on number of investigated parameters N (the larger the number the more specialized knowledge is required to interpret the results)	Specialist	General public	Specialist	Specialist
Prior knowledge required on parameters to conduct the assessment	Low	Medium	Medium	High	Understanding the knowledge base is the goal of this type of assessment	High	High

Example TEA areas applicable to	Linear cost models, e.g., capital cost factor models	Simple technical and cost performance models without strong interactions between parameters, e.g., exponent models for capital costs	More complex technical and cost models where there are known parameter interactions and non-linearities, e.g. rigorous/first principle process models	More complex technical and cost models where there is enough data to make/select PDF's, e.g., NPV and LCOE models	Any, particularly TEA studies used for policy and decision making and where knowledge is contested or inherently limited (low TRL)	Situations where contextual choices are expected to have an impact.	Highly complex and non-linear process models that are to be directly linked with economic estimates
Limitations (preferably not to be used for)	When strong non-linearities and interactions are expected	When strong interactions between parameters are expected	When the process models are computationally very heavy	When there is too little information on the shape and potential values of PDF's. When the model is computationally heavy	When a large set of input data needs to be analysed	When there is too little information on the shape and potential values of PDF's. When the model is computationally heavy. When there is a limited (or non-existing) number of value-laden choices.	Models that do not need reduction to become computationally feasible

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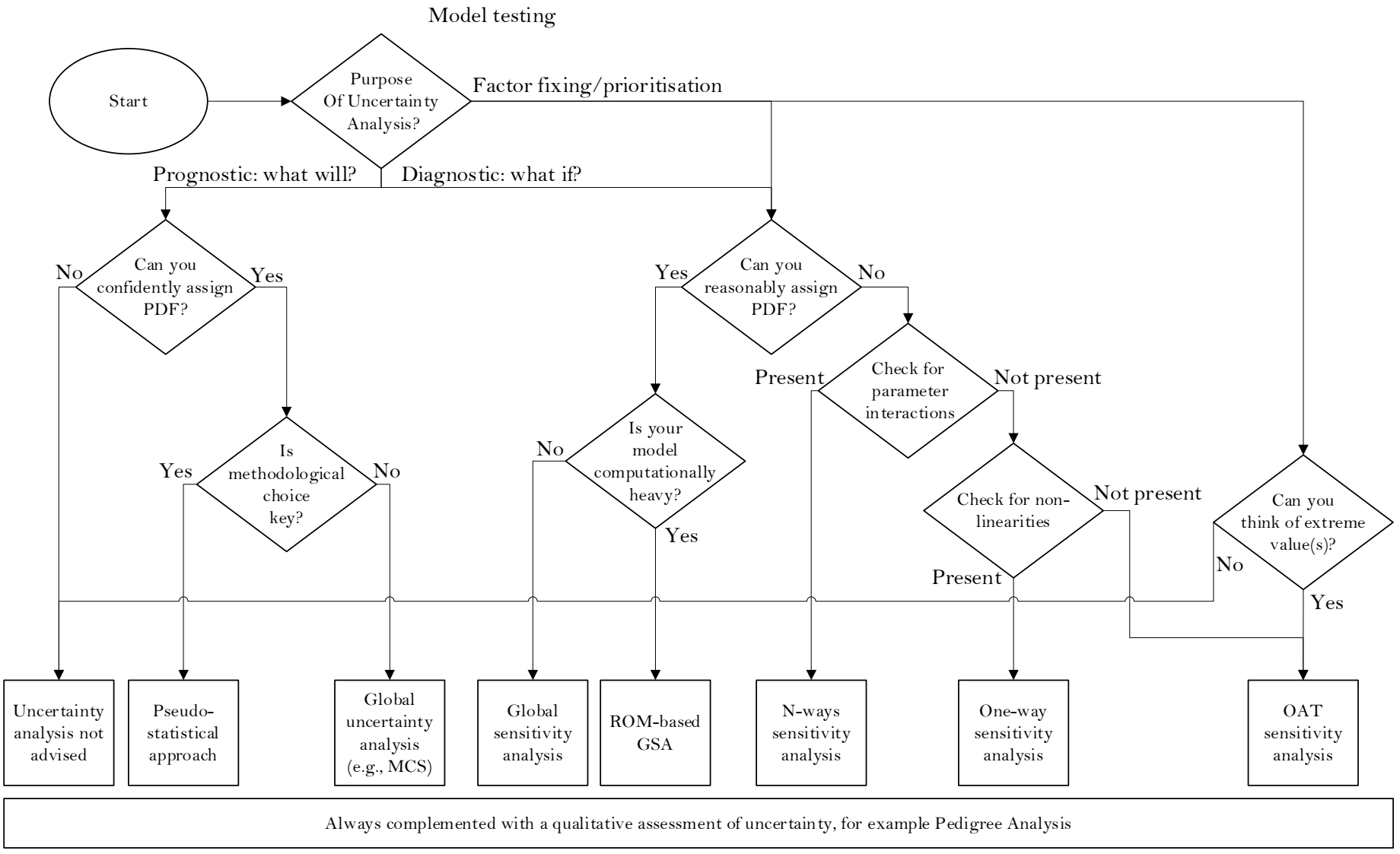

Figure 8. Scheme for initial uncertainty analysis selection guidance.

4. Advanced uses of uncertainty analysis in CCS TEA

The previous sections discussed guidelines to select and apply methods for sound uncertainty analysis. These methods not only aid the critical analysis of the techno-economic potential of a CCS technology but also points towards specific areas that are candidates for further investigation. There are also, what can be called, advanced uses of uncertainty analysis, for instance in multi-scale modelling for material and system design, design of experimental campaigns in pilot plants that are very expensive, design of CCS supply chains, CCS risk and safety analysis and use of existing infrastructure in CCS value chain. Two such examples will be discussed here.

4.1. Using uncertainty analysis for design of experiments

Bayesian inference is the theoretical foundation upon which intelligent experimental design can be leveraged to inform the models used to characterize a process [53]. When model precision is considered unacceptably low for a process that needs to be further understood, measures should be undertaken to improve understanding of the process [54]. The technique of Bayesian inference, coupled with collection of experimental data, provides a means for reduction of model uncertainty, and thus refinement in understanding for a process systems application of interest. Sequential Design of Experiments (SDoE) is a framework that incorporates uncertainty-based criteria for selection of operating conditions for data collection and the use of the data for refining a stochastic process model in a cyclical manner. The SDoE procedure was previously summarized in Soepyan et al. [55], and demonstrated at pilot scale for a solvent based CO_2 capture system in Morgan et al. [56].The SDoE process is represented schematically in Figure 9.

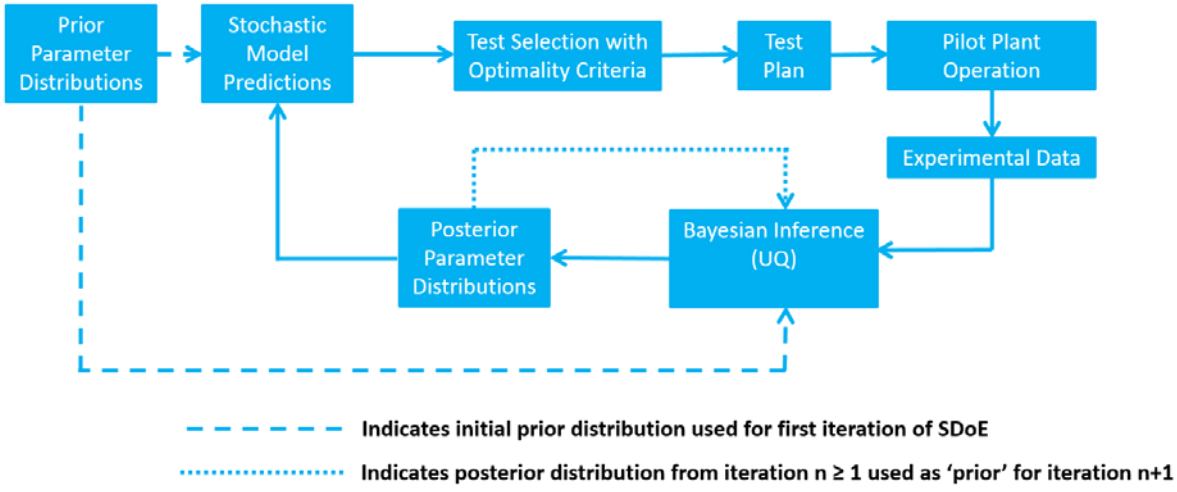

Figure 9. Schematic of Bayesian SDoE implemented for pilot plant campaign

The SDoE methodology requires an initial process model, or a reduced-order surrogate model of the process, in which some of the parameters are characterized by probability density functions (PDFs), representing the parametric uncertainty. For the example of a solvent-based carbon capture system, uncertain parameters may include those related to the physical properties the system, reaction kinetics, and mass transfer and hydraulic models for the packing used in absorption and stripping columns [46]–[48]. Accurate characterization of mass transfer, interfacial area, and hydraulics, with quantified uncertainty, is necessary for representing the rate-based column models with a specific packing type. For chemical solvent systems, including the traditional amine-based systems, characterization of reaction kinetics is also essential. Physical properties such as viscosity, density, and surface tension are independent of packing type, although their uncertainties propagate through the

mass transfer and interfacial area models, which are dependent upon the property models. However, previous work on physical properties uncertainty quantification for the MEA system for the aqueous monoethanolamine (MEA) system [46],[47] has demonstrated that the most influential source of property model uncertainty is the thermodynamic framework. Accuracy in the thermodynamic framework is necessary for characterizing the vapor-liquid equilibrium in column packing, heat of absorption, heat capacity, and reaction equilibrium constants for chemical systems.

The prior distributions on these uncertain parameters represent initial beliefs about the parameters before collection of data. At various process conditions covering the full operating space of interest, the process model is evaluated stochastically by sampling from the prior distribution of the parameters and calculating the model output for each point in the sample. At each process condition, the model output calculated from all samples may be used to estimate statistics (e.g. mean, variance, prediction intervals) for the model output. For the solvent-based CO_2 capture system example, the operating space of interest represents feasible combinations of input variables including but not limited to solvent flowrate, flue gas flowrate, CO_2 loading in solvent, and CO_2 concentration in the flue gas. Some output variables of interest may include CO_2 capture efficiency in the absorber and reboiler duty requirement in the stripper [49].

Along with the model prediction of uncertainty as a function of the process operating conditions, some optimality criteria [57], which are chosen based on specific experimental goals, are used to select a subset of the candidate set to be included in a test plan for data collection. For example, If a goal of a test campaign is to refine a model by reducing the parametric uncertainty, it may be desirable to collect data in operation conditions where the initial predicted uncertainty is relatively high.Experimental data are collected according to the test plan, and Bayesian inference is used to estimate posterior distributions of the parameters, which represent refined distributions of the parameters conditioned on the data observations. The model prediction of uncertainty is updated (generally reduced) as a result of refinement in the parameter estimates, and this information is used to determine a new test plan for further data collection. This results in the sequential nature of the SDoE process, in which the model is refined over multiple iterations. The decisions regarding the amount of data to collect in each iteration and the criteria for terminating the SDoE loop are left to the experimenter. In practice, however, these decisions may be dictated by limitations in time and money available for pilot-scale test campaigns.

A recent example [58] of SDoE execution for a large pilot-scale test campaign at Norway's Technology Centre Mongstad (TCM) is summarized in the following. In the example here, a Bayesian DoE was applied to an MEA baseline test campaign at Technology Centre Mongstad (TCM). Solvent flowrate, gas flowrate, and lean loading were variables in the test plan, serving as inputs to pre-existing fundamental models which are targeted for refinement using the experimental results. The objective of this experimental campaign was to minimize the maximum uncertainty in the operational space under consideration.

Figure 10 below illustrates the results of one DoE iteration for parametric refinement, which results in the following computationally projected improvement in the 95% confidence interval width of the capture percentage projection. Parameters targeted for refinement in this design of experiments related to, among other things, mass transfer characterization which directly affects equipment size and thus cost. Therefore, improving our understanding of these parameters also improves cost projections.

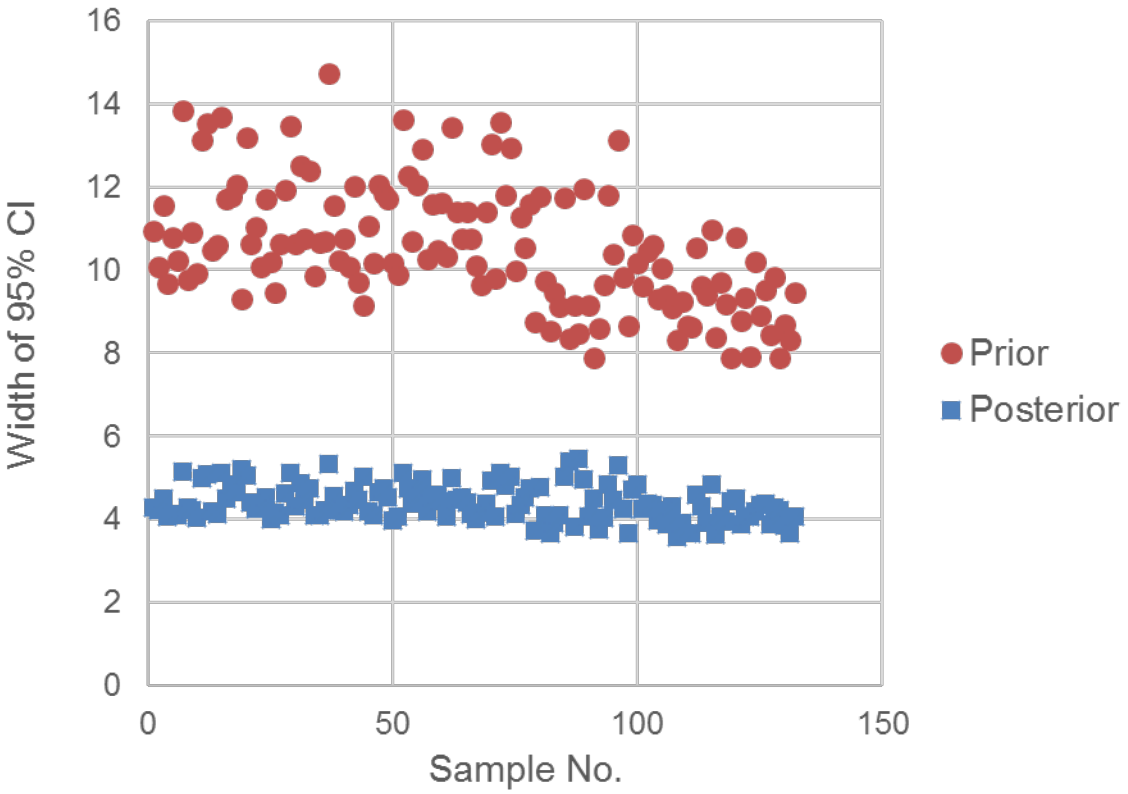

Figure 10. Example of results from Bayesian SDoE implemented for an MEA pilot plant campaign at Technology Centre Mongstad (TCM). The reduction in uncertainty (i.e. width of the 95% confidence interval) before and after the campaign is clearly visible.

4.2. Design of CCS supply chains under uncertainty

Even though uncertainties can be reduced through technology testing, uncertainties remain an inherent and important element of novel systems with limited large-scale industrial experience and must be taken into account to enable the design of cost-efficient energy systems [2]. Advanced uncertainty quantification approaches, often referred to as 'design under uncertainty' in the engineering field [59], [60], have been developed to account for uncertainty already during the design step to achieve better and more robust designs. In practise, an optimisation layer is added to an uncertainty propagation approach, like Monte Carlo simulation, to optimise system variables according to one or several targeted objective(s) related to the output distribution of key performance indicators (KPIs) as shown in Figure 11. The targeted objective(s) can be of different nature. One may want to minimize or maximize the mean value of the probability distribution of a given key performance indicator (KPI). Alternatively, one may aim to minimize the uncertainty range of a KPI distribution or to limit extreme values to reduce associated risks.

While design under uncertainty is being more and more considered in engineering approaches [60]–[62], only few studies have considered such approaches for design of CCS chains or its components. Cerillo-Briones and Ricardez-Sandoval [63] investigated the robust design of an absorber column under process uncertainties such as flue gas flow and temperature, as well as solvent characteristics. Bjerketvedt et al. [64], investigated optimal ship-based CO_2 transport considering uncertainties in sailing time due to weather conditions, seasonal variations, future fuel cost and risk of ship breakdown. Similarly, Knoope et al. [65], investigated the impact of price uncertainties on the decision to

differentiate or expand investment in a CO_2 infrastructure network using real option analysis. Meanwhile, Roussanaly et al. [66] performed an extensive study on the impact of technical, economic and system uncertainties on the cost and design of CCS from a waste-to-energy plant.

In the work by Roussanaly et al. [66], one of the considered cases investigated the impact of uncertainties on the design and cost of a CCS chain based on solvent CO_2 capture and a transport and storage infrastructure shared with nearby industries. An optimal design of this chain was developed considering two uncertainty scenarios: 1) "internal" uncertainties such as uncertainties in investment costs, steam and electricity consumptions; and 2) internal uncertainties combined with uncertainties in the amount of CO_2 captured from the other nearby industries (referred as "external" uncertainties). The evaluation showed that a more robust design could be achieved in the second uncertainties scenario through design under uncertainties. A larger pipeline diameter is optimal in the second scenario although it results in a CO_2 avoidance cost 5 €/tCO_2 avoided higher than in the first uncertainty scenario. Indeed, the optimal design of the first uncertainty scenario has a probability of 35% that it cannot accommodate all the CO_2 captured from nearby industries.

One of the main drawbacks of design under uncertainty is that it requires significantly more computational time than deterministic approaches, due to the combination of extensive Monte Carlo simulations and the optimisation of multiple variables. Furthermore, a robust modelling of the considered system, as well as a good understanding of the potential underlying uncertainties are required if meaningful results are to be achieved. Despite these challenges, design under uncertainty has shown to provide significant advantages compared to deterministic approaches: enabling cheaper designs or designs that can foster a higher value creation, enabling more robust designs, or limiting risks associated with expected uncertainties. It is therefore important to note that while design under uncertainty modelling approaches can be self-developed, several academic and commercial tools such as UQ lab and Oracle Crystal ball also offer this functionality (see also section 5).

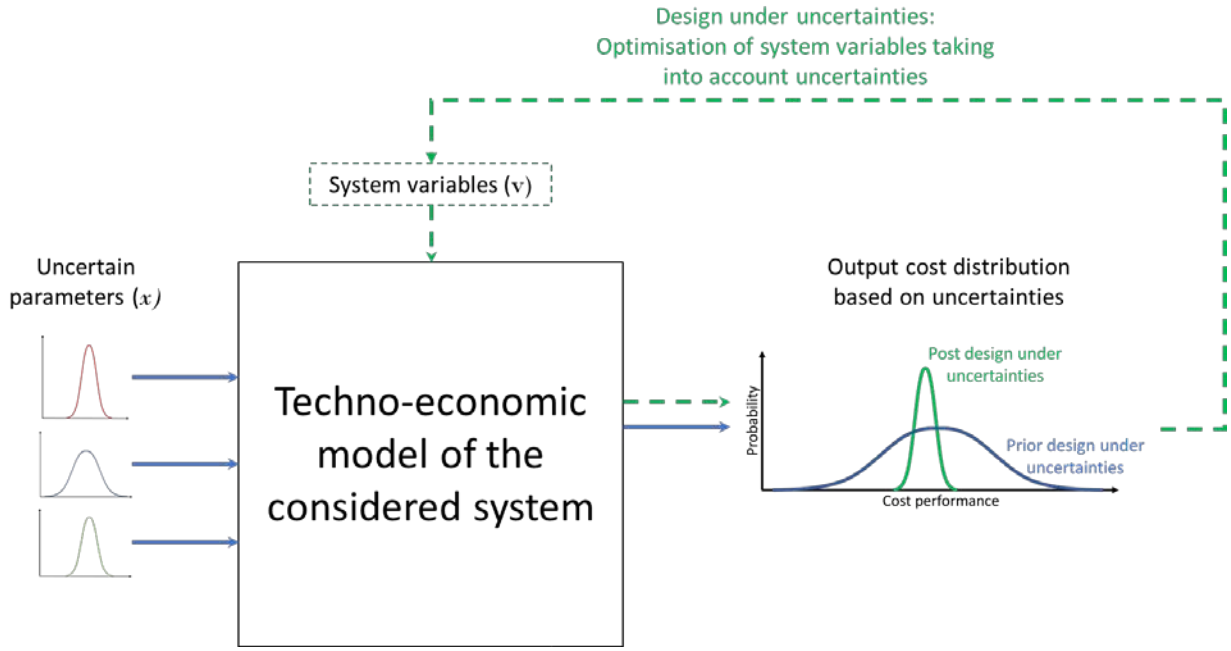

Figure 11: Schematic representation of design under uncertainties. The "classical" Monte Carlo simulation process is shown in blue while the additional design element is illustrated in green.

5. Available software for uncertainty and sensitivity analysis

With recent interest in uncertainty analysis from many researchers, engineers and academic institutions, various software packages have been developed to perform uncertainty analysis in a structured manner. The aim of these tools is to provide more accessible, easy and ready to use software and to facilitate the use of uncertainty analysis to a wider audience. However, selecting a suitable analysis tool for a specific application is not always straightforward: it requires to understand the options' relative merits, features and performance level. We here try to provide a brief review of the current uncertainty analysis tools can be employed in (CCS) TEAs.

Commercially available tools for uncertainty propagation and sensitivity analysis include Crystal Ball, Pallisade's @RISK [67] and RISK AMP [68]. These three tools are Excel add-in's, which makes them easy to use also to practitioners less versed in programming languages. According to a review by Sugiyama [67], Crystal Ball is the easiest to use due to an excellent user guide and reference manuals, and the provision of a number of illustrative models [69]. All three packages include local and global sensitivity analysis methodologies using post processing of the Monte Carlo simulations. A limitation of using excel based software for CCS TEA's, however, could be the integration with external software such as MATLAB, Python, or Aspen, which are often used for the process modelling of CCS technologies (this may especially be a limitation for starting TEA practitioners). It should be noted however, that Aspen includes the capability to perform local SA for process modelling and techno economics, in addition it can be controlled from Excel using the Aspen Simulation Workbook add-in, which then allows the possibility to use these excel based UQ software packages.

In addition to the Excel-based packages, there are number of recently established tools that have advanced capabilities in performing probabilistic uncertainty analysis. They include, e.g., surrogate-modelling methods such as Polynomial Chaos Expansion (PCE) or Bayesian inference with the Markov Chain Monte Carlo (MCMC) method[4]. They also include the calculation of local and global sensitivity indicators such as Perturbation, Morris and Sobol indices and facilitate design optimization under uncertainty. As a starting point, we name some here that are widely used: the Dakota toolkit is a C/C++ based tool developed by Sandia National Laboratories [70]; UQLab is a MATLAB based framework developed by the Chair of Risk, Safety and Uncertainty Quantification of ETH Zürich [71]; and FOQUS (the Framework for Optimization and Quantification of Uncertainty and Sensitivity), developed by the United States Department of Energy's Carbon Capture Simulation [72], is a Python based framework that connects to several flowsheeting software using a graphic user interface the United States Department of Energy's Carbon Capture Simulation [50].

Among the discussed software above, the Dakota toolkit provides the most extensive range of UQ methodologies. It has more functionalities than the other two, including for instance methods for quantifying epistemic kinds of uncertainties. It is, however, easy to get lost in all the options it provides and may not be the best software for starting TEA practitioners. The fact that it is written in C++ may also make it difficult to integrate with TEAs. Although all these tools provide extensive manuals and documentation, their use can seem quite daunting, especially if one does not have an advanced programming knowledge. In general, the choice of tool can be based on the programming language preference and most of the tools provide the advantage of being open source type which allows new methods to be added and integrated. For this reason, it is recommended to start with a tool that provides the best technical guidance, e.g., through the inclusion of interactive procedures or step-by-

[4]A sampling technique to identify the posterior probability distribution of a parameter once the prior probability distribution has been determined.

step checklists. In addition, it is recommended to choose a tool that offers active discussion forums among the user community to help the user with methodological or model implementation issues. Examples include UQLab and FOQUS. Further guidance on the selection of uncertainty analysis tools can be sought for instance through online databases like swMATH. Table 6 summarizes the above considerations.

Table 8. Comparison of available software packages for uncertainty evaluation of (but not specific to) CCS techno-economic models.

Software name	Crystal Ball	Palisade	Risk AMP	Dakota	UQLab	FOQUS
Type	Commercial	Commercial	Commercial	Open access	Open access	Open access
OAT, One-way and N-ways sensitivity analysis	✓	✓	✓	✓	✓	✓
Global uncertainty and sensitivity analysis (Monte Carlo)	✓	✓	✓	✓	✓	✓
Reduced order global uncertainty and sensitivity analysis	X	X	X	✓	✓	✓
Direct linking with external software (e.g. MATLAB, Python)	X	X	X	✓	✓	✓
Linking with Aspen via Excel interface	✓	✓	✓	✓	✓	✓
Availability of supporting documentation/manual/ training materials	✓	✓	✓	✓	✓	✓
Level of programming skills required	None	None	None	Intermediate	Intermediate	Intermediate

6. Conclusions and recommendations

Proper use of uncertainty analysis in the performance of CCS TEAs can provide more robust understanding of technical and cost performance to modelling practitioners as well as policy and decision makers. While there is a growing appreciation over the importance of uncertainty evaluation to both development of models and reporting of results, it remains the case that they are not always evaluated and, when they are, they are often not evaluated using the most appropriate methods. This paper provided a critical review of a selection of existing and emerging uncertainty analysis methods and provided guidelines on their use. It discussed good practices as well as pitfalls, provided guidance on how to select and use methods and pointed to sources of further information when outside the scope of this work. It aspires to be a starting point for an audience getting acquainted with CCS TEA, or that wishes to improve their (knowledge of) TEAs.

The review showed that many different methods and approaches to uncertainty analysis exist. We emphasised that key to starting any uncertainty analysis is to first thoroughly define its purpose, and then to ensure that the most suitable type of uncertainty analysis for that purpose is selected (also in relation to the choice of techno-economic model itself). In addition, a good understanding of the methods' strengths and limitations is imperative. Finally, the choice also depends on the existing

knowledge of the investigated technology and the associated TEA model and its inputs (including potential parameter ranges – and possibly probability distribution).

The simplest method for model diagnostics ("what If" questions), and one that should as a minimum be applied (in the first instance), is one-at-a-time sensitivity analysis, but we recommend one-way or N-ways sensitivity analysis since most TEAs include non-linearities and parameter interactions. OAT has a really very limited use (although it is actually the most used), except in the case of model testing to extreme inputs, and also then it is arguably better to test the model to extreme scenarios (i.e., combinations of extreme inputs, NAT sensitivity analysis). To address prognostic ("what will") questions, probabilistic methods are most appropriate, but caution must be applied in their use as the distribution of results is only as good as the distribution of inputs. If distributions cannot be quantified with good confidence, then probabilistic methods are simply not suitable to answer prognostic questions (but may still be suitable to answer diagnostic questions). Finally, we highly recommend always complementing quantitative uncertainty analysis with qualitative methods, because they provide insights into the kinds of uncertainty that are unquantifiable, especially relevant to policy and decision making.

In addition to the classic uses of uncertainty analysis, advanced uses can come to the advantage of TEA practitioners and CCS developers. We exemplified that iterative uncertainty analysis can aid the design of experimental campaigns by pinpointing regions that need further investigation, allowing the experiments to be more efficient and less costly. Another advanced use is in the development of CCS infrastructure, where integrating design under uncertainty at the planning stage can enable more robust systems.

The (un)availability of suitable software is something that has hampered (and continues to hamper) the use of more advanced uncertainty analysis in CCS TEA. Although possible, it may be difficult for starting practitioners to combine Excel-based (and very user friendly) uncertainty analysis add-ins with process simulation software like Aspen (although Aspen does allow local sensitivity analysis on techno-economics within its suite). Further expanding the capabilities of process simulation software to include advanced global uncertainty approaches would be very helpful (the gProms software has already included this option). For some flowsheeting software, TEA practitioners can link their simulations to existing (and quite elaborate) uncertainty quantification tools in MATLAB or other programming languages, but this requires substantially more knowledge of, and skill in, programming and the software layers underlying process simulation software to make the connection. Easier ways to connect different software would be highly desirable. Also, further improvement of the user friendliness of existing UQ toolboxes (e.g., by including graphic user interfaces) would aid in the further adoption of advanced uncertainty analysis methods. Finally, a key challenge is to fully combine detailed technical and cost models, to allow for integrated (instead of piecewise) TEA uncertainty analysis.

CCS remains a technology that has had so far limited large-scale implementation and therefore inherently large uncertainties. Uncertainty analysis has, thus, an important role to play in TEA of CCS technologies and systems and there are many opportunities to bring our use of uncertainty analysis to a level higher than currently often done. Hopefully, this work inspires the use of the available possibilities and the continued development towards robust and meaningful CCS TEAs.

Acknowledgements

Simon Roussanaly would like to thank Rahul Anantharaman and Jabir Ali Ouassou for their useful inputs and comments.

Appendix A: mathematical representations of uncertainty analysis

In OAT sensitivity analysis, the model output vector $\mathbf{y}$ is only evaluated against a minimum and maximum value of a input parameter x_i. It assumes a base case vector of input parameters $\boldsymbol{x^0}$ and a sensitivity perturbation (min/max, the plus/minus 10%) of the input parameters $\boldsymbol{x}^+$. The difference between the base case and the sensitivity case is then $\Delta^+\boldsymbol{x} = \boldsymbol{x}^+ - \boldsymbol{x^0}$ Δ^+. The output of the sensitivity analysis is the delta between ${y_i}^+$ and ${y_i}^{+0}$:

$$\Delta_i^+ y = g\left(x_i + \Delta x_i^+, \mathbf{x}_{\sim i}^0\right) - g(\mathbf{x}^0) \qquad \text{A1}$$

Where $\mathbf{x}_{\sim i}^0$ is the vector of all inputs other than *i* (i.e., the inputs that are kept constant). A one-way sensitivity function $h_i(x_i)$ can be defined as

$$h_i(x_i) = g(x_i;\ \boldsymbol{x}_{\sim i}^0) \qquad \text{A2}$$

A typical representation of one-way sensitivity analysis is by so-called spider-plots, where the sensitivity of the output values is plotted against changes in the vector of input values. To plot the changes to all input parameters in one graph, they need to be normalised (calculated as a percentage deviation) according to the function

$$h_i^*(x_i) = \ h_i(x_i) - g(\boldsymbol{x}^o) = \ g\left(x_i;\ \boldsymbol{x}_{\sim i}^0\right) - g(\boldsymbol{x}^o) \qquad \text{A3}$$

Appendix B: Guideline for the characterization of probability density functions by Hawer et al.

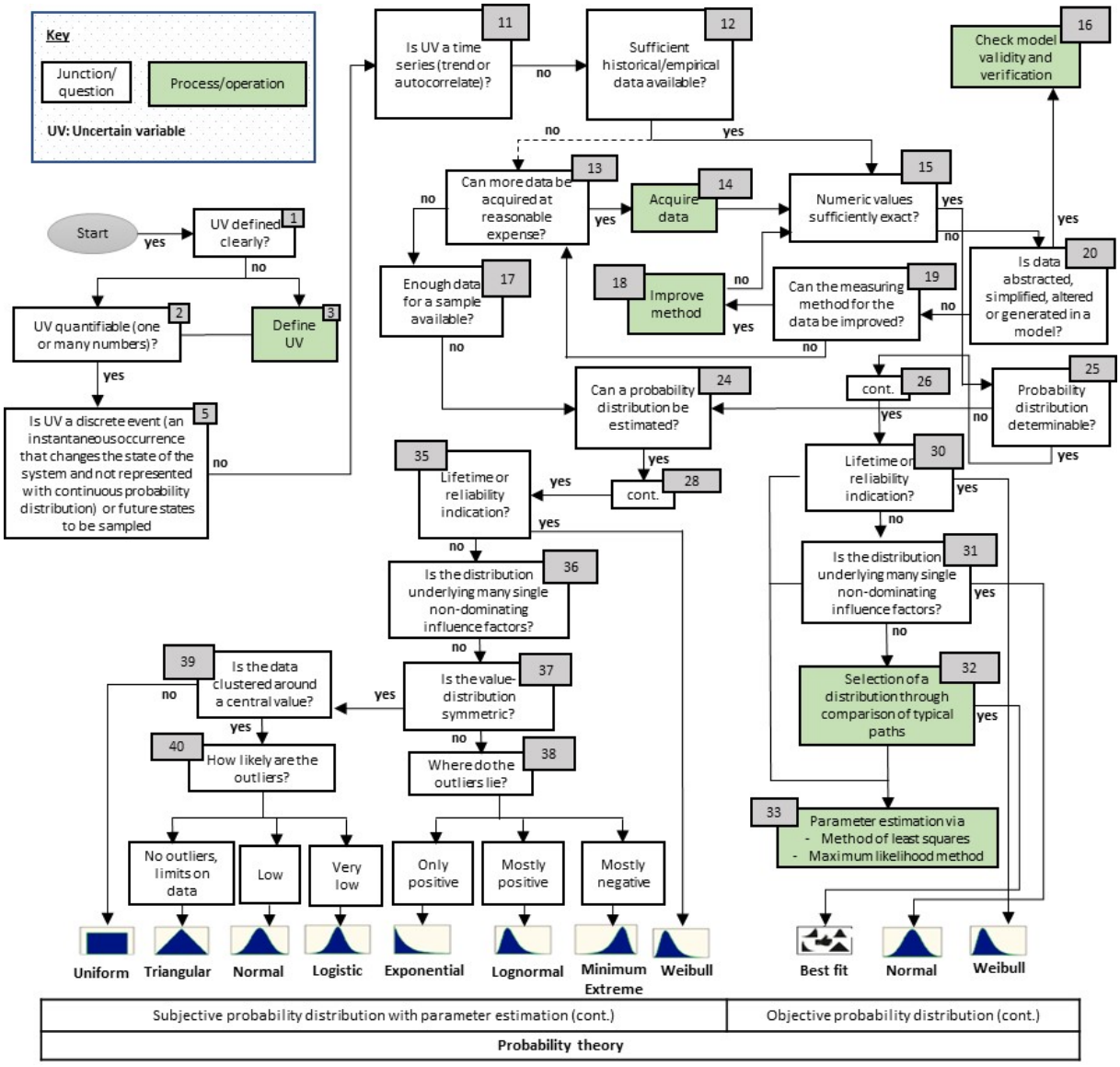

Figure B1: Guideline for the classification and quantification of uncertainty, based on Hawer et al. [37]**. UV is short for Uncertain Variable; the numbers in the boxes refer to the original numbering by Hawer et al, of which we used a subset.**

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