Assessment of Risks and Uncertainties in CCS

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1 Executive Summary

In this deliverable the interplay between the Competent Authorities and the operator of a prospective storage site is addressed. The main conclusions are:

- The risk assessment and characterization procedure is best viewed as a common learning process of the two parties.
- Formal as well as informal moments of contact are necessary between the two parties, so as to decide which activities have to be performed, and to communicate where the process is going.
- The Competent Authorities have to be represented by technical experts with sufficient understanding.

This deliverable also contains a technical discussion of uncertainties and modelling, and their interplay. This is to be viewed as complementary to the description of the activities as described in CATO2 deliverable D 4.1_D01, Chapter 3. Dealing with uncertainties is best performed in a Bayesian framework. This is particularly important when in the end one model is to be chosen as the model against which monitoring data are to be compared. This becomes relevant when transfer of responsibility is to be transferred to the Competent Authorities.

- Good communication on a regular basis is advocated between the (heterogeneous) group of technical experts performing the characterization and assessment. One should avoid “loose ends” in the process.
- Special “officers” should be appointed to “streamline” this communication.

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2 Applicable/Reference documents and Abbreviations

2.1 Abbreviations

(this refers to abbreviations used in this document)

CA	Competent Authorities
CCS	Carbon capture and storage
EU	European Union
pdf	Probability Density Function

3 Introduction

In the EU Directive on the geological storage of carbon dioxide (Directive 2009/31/EC)[1] it is stipulated that safe site selection has to be performed whenever CO_2 storage is planned. The actions undertaken in concordance with this Directive have to serve one ultimate goal: a storage site may only be selected if the likelihood of leakage, and risks for human health or the environment are not significant. Also, it is stipulated that the suitability of a geological formation for CO_2 storage has to be assessed through a process of characterization and assessment. This process has to be followed for each concrete proposed storage site. The basis for the subsequent actions, such as data acquisition and modelling, is formed by a qualitative risk assessment, performed very early in the process, eventually leading to a quantitative risk assessment. In the qualitative risk assessment the data on the underground are brought together to select a series of possibly relevant models of the underground. Based on the models, data will be collected to carry out the quantitative risk assessment. The outcome of this last step should shed light on the central question: is this concrete site a serious candidate for safe CO_2 storage according to the stipulations of the EU CCS Directive, and in accordance with the national law? Once a site is selected, the modelled behaviour of this site is monitored throughout the storage process, in order to further assess possible risks.

Various stakeholders can be discerned as regards to CO_2 storage, but two stakeholders have to be singled out here as the leading ones as regards the characterization and assessment activities. These are the Competent Authorities (CA), so addressed in the EU CCS Directive and the operator of the site. The site operator will do the work of characterization and assessment, while the CA or their representatives will pass judgment over the results put forward by the site operator. The decision on the suitability of the storage location is not the only decision in the permitting process to deal with risk assessment, the use of models and the uncertainty that goes with that.

Central in this deliverable is the assessment of risk through modelling. “Risk” is a concept that has a central role in the EU CCS Directive. Unfortunately, in all-day life the word is used both for “probability” and for something that can be described loosely as “probability times effect”. In the EU CCS Directive the second meaning is the intended one. In this deliverable we comply with this usage, and a more formal definition will be given later on. The following example will show how risks, models and uncertainty are connected.

The site operator is responsible for characterizing and assessing the site’s potential consequences in case of a leak, and for assessing the probability of such leakage to occur. Despite all existing and available information and despite any new data acquisition planned, the operator must always concede that there are many things that will remain unknown or uncertain. In short, the operator is confronted with various kinds of uncertainties. For instance, the operator can apply well-logging tools to get a high-resolution picture (of order of one foot) of a small part of the subsurface. This data can be assumed indicative for the direct environment of the well scrutinized (up to 10m in radius, say). For a more global picture the operator can apply seismic methods of the subsurface extending to many km, but with a low resolution (25 m, say). At the same time it is known that small details may have an appreciable effect on fluid flow (e.g. a low-permeable horizontal streak with a thickness of one foot, never discernible on seismic tests, may hamper vertical flow effectively). Thus the operator cannot dispense with this uncertainty, and must take it into account somehow. Hence, uncertainty handling must play a vital role in his activities.

Modelling is one of the activities that are vital in site characterization and assessment. This activity is addressed explicitly in the EU CCS Directive. For this moment –a discussion follows later- modelling is loosely defined as the activity in which processes and events in the subsurface or the atmosphere are “mimicked” with the help of a computer.

[1] For readability this Directive will be referred to as the EU CCS Directive for the remainder of the document.

3.1 Research questions

The tools to investigate reservoir behaviour are well-known in the hydrocarbon production industry, and they can be used in the context of CO_2 storage – possibly with some modifications (e.g. PVT relationships for CO_2 and properties of possible substance mixes within flow computations). Commercial software packages are readily available in relevant fields as 3D Earth model building, geomechanics, reservoir engineering, geochemical modelling, pollution and gas dynamics. But for each of them the results will be as reliable as the input on which they will operate. For each of the software tools it is known what input is required, and what output can be delivered (standard or otherwise). The workings of the tools themselves are clear, but in connection with the above there are a number of questions that need answering before the tools can be sensibly operated in the intended context. These issues mentioned are in the realm of the technical experts.

For the policy makers, on the other hand, there are entirely different questions of interest. These are questions on how the process of assessment and characterization is to be structured. The steps to be taken are mentioned in the EU CCS Directive, and implemented in national law. But the CA have the obligation to see to the proper execution

The questions can be summarized as follows:

1. What are models for? How should models deal with uncertainty? Which problems might arise?
2. Which practical consequences do modelling and uncertainty have for the decisions to be made by the competent authority in terms of procedure?

3.2 Build-up of this deliverable

This deliverable is meant for two distinct groups of readers. First of all it is addressed to policy makers/lawyers. Then it is also addressed to the operator and technical specialists. The needs for these two groups are as different as are the environments in which they work. This makes it necessary to put forward different kinds of information to each group.

We have tried to comply with this desideratum by writing separately for these two groups. A first chapter is written for use by the policy makers. Emphasis is on the formal demands in the EU CCS Directive and the business process. In this chapter results detailed in the following chapters will be used, so as to provide a comprehensive chapter for use of policy makers/lawyers. Question 2 is addressed in this chapter.

The next two chapters detail issues of uncertainty and modelling. They are intended for the specialists. These chapters are targeted at answering the above questions 1. Technicalities on risk and model comparison are described in the appendices. Finally conclusions and recommendations are given.

4 Formal requirements and process of Storage Site Assessment for CCS

4.1 Introduction

The EU CCS Directive prescribes the decisions to be made by the competent authority in order to facilitate CCS. For some of these decisions the use of models is prescribed. This section analyses which decisions are relevant for this study and which further requirements are set out in the CCS Directive. The chapter will conclude with a list of the most relevant decisions in which models are used and in which uncertainty is likely to play a role. Furthermore the business process is commented on from a practical angle.

4.2 Risk in the EU CCS Directive

The CCS Directive is designed to facilitate CCS, but also guarantee safety. The competent authority has responsibility for approval of storage permits, and making sure that sites are suitable for CO_2 storage, with appropriate operating plans. This is in effect part of the overall risk management process and a vital aspect of ensuring that suitable sites are selected. The approach adopted in the EU CCS Directive and in the accompanying Guidance Documents[2] is that a risk assessment of the site is to be carried out, that this assessment should lead to monitoring plans, that the site's actual performance is related to the predicted results and that, if necessary, the plans are adapted to the new results. During the lifecycle of the storage, the competent authority shall assess the way in which the operator uses and adapts these plans.

Important decisions for the competent authority related to the assessment of risk based on the EU CCS Directive are:

- The selection of the storage location (art 4)
- The storage permit including the monitoring plan, the corrective measures plan, the closure plan, the post closure plan (art 9, 13) and the way in which the operator updates these plans (art 11)
- The transfer of responsibility, whereby the operator proves the safe and permanent storage (art 18)

In all of these decisions, the competent authority validates the way in which the operators deal with the possible risks that might occur in the storage process. The following section will examine to which extent the EU CCS Directive prescribes or refers to the use of models for these decisions.

4.3 Requirements of the EU CCS Directive on these decisions

4.3.1 Selection of the storage location

Article 4.3 of the EU CCS Directive states that the suitability of a storage location shall be determined through a characterization of the site using the criteria as specified in Annex 1 of the EU CCS Directive. Annex 1 thus might contain further information on the use of models. Article 4.4 indicates the norm by which the competent authority should assess the information based on the analysis: only if under the proposed conditions of use there is no significant risk of leakage, environmental risk or risk to health, a location may be selected. The assessment of a location should lead to a conclusion on the absence of significant risks for leakage, damage to the environment and damage to health.

Annex 1 describes three steps that must be taken according to the best practice at the time of the assessment, and provides for specific criteria. The Annex gives the competent authority the discretion to deviate from these steps, if the operator is able to demonstrate all the necessary characterizations of the location. The steps to be taken are:

- Data collection in order to build a static 3D earth model, including

[2] Available from http://ec.europa.eu/clima/policies/lowcarbon/ccs/implementation/documentation_en.htm

- Intrinsic characteristics such as geology, geophysics, geochemistry etc
- Characteristics of the vicinity of the complex such as natural resources, activities nearby etc.
- Building the static 3D earth model (or a set of such models)
- Characterization of the complex, possible fractures, faults etc
- The uncertainty for each of the parameters should be taken into account, by developing a range of scenarios and calculating the appropriate confidence limits
- Characterization of the storage's dynamic behavior, sensitivity characterization and risk assessment (assessment of simulations of the dynamic model)
- Characterization of the storage's dynamic behavior and that of the overburden.
- Sensitivity characterization
- Risk assessment
- Hazard characterization (possible leakages and effects)
- Exposure assessment (to humans)
- Effects assessment (to the environment)
- Risk characterization (short term, long term, proposed use, worst case scenario, including a description of the possibilities to reduce risks to acceptable levels)

The EU CCS Directive thus prescribes the steps to be taken in order to create and run the models that can be used for the selection of the storage location. It prescribes the steps needed to build the first static model or series of models, a quantitative risk assessment, and it describes which possible risks should be covered by the dynamic modelling of the site, the qualitative risk assessment. Based on the results and possibilities of these models, the competent authority assesses whether or not there is a significant probability of leakage. Significant risk in the EU CCS Directive is defined as a combination of the probability of occurrence of damage and a magnitude of damage that cannot be disregarded without calling into question the purpose of the Directive (art 3 (18) EU CCS Directive). Furthermore, the Directive obliges the operator to describe how he deals with possible uncertainties in the models.

4.3.2 Monitoring plans

Following the decision to determine the suitability of a storage location, a next decision for the competent authority dealing with uncertainty is the granting of the storage permit. The conditions for the storage permit are listed in article 7 of the EU CCS Directive. They contain at least the storage characterization, the proposed quantity of CO_2 to be injected, the measures to be taken in case of irregularities and the different plans as required by the EU CCS Directive (monitoring plan, corrective measures plan, provisional post closure plan), an impact assessment and the financial security. Article 8 determines how the competent authority should assess the application for the permit: it grants the permit when all relevant requirements (CCS and other directives) are met, the operator has proven to be financially sound, and potential effects of interaction with other activities are determined. The requirements to be met are specified in the various articles of the EU CCS Directive (article 12 on CO_2 stream, article 13 on monitoring, article 16 on measures and article 17 on closure). As the decision is also based on the models as described in 2.3.1, this decision deals with the same uncertainties in the predicted model's performance.

Furthermore, article 13.2 prescribes the use of a model as laid out in Annex 2 for assessing the monitoring plans. The essence of the Annex is that based on the dynamic model or series of models a monitoring plan is made. This plan is to meet the requirements of the Annex:

- For each phase of the storage process the plan specifies which observable parameters are monitored, which technologies are used on which basis, how locations are selected, and the frequency of the monitoring
- Elements that should be monitored are the fugitive emissions, the volumetric flow, pressure and temperature, chemical analysis, and reservoir pressure and temperature
- Assurance that the best available techniques are used (some of which are already prescribed in the Annex)
- The way in which the monitoring plan will be updated based on the collected data

- How this information will be transferred into the post- closure plan

The EU CCS Directive thus prescribes the use of models in monitoring, and prescribes – albeit at a rather high level - the techniques that are considered “best practice”. Any time there are leakages or significant irregularities the operator must notify the competent authorities thereof. The latter may then review the storage permit and subject continuation of the permit to new conditions. A “significant irregularity” is defined as any irregularity in the injection or storage operations or in the condition of the storage complex itself, that implies a probability of leakage or risk to the environment or human health (article 3(17) EU CCS Directive). The Guidance Document 2 refers to significant deviation between observed and predicted behaviour. Besides the regular reviews, the data collected by monitoring thus might lead to a review of the storage permit.

4.3.3 Transfer of responsibility

A final decision for the competent authority dealing with uncertainty is the decision on the transfer of responsibility from the operator to the national state. This decision is based on, inter alia, the models that have been used to support previous decisions and that have been updated following the mandatory post-injection monitoring phase. The norm by which the possible transfer is assessed is different. The competent authority should eventually assume the responsibility for the storage location from the operator if the operator can demonstrate convincingly (based on the models, inter alia) that the injected CO_2 is completely and permanently stored in the targeted reservoir(s). Article 18.2 of EU CCS Directive states that, at the end of the mandatory monitoring phase, the operator shall prepare a document in which it is demonstrated that:

- the injected CO_2 behaves according to the models
- there is no detectable leakage
- the storage site is evolving towards a situation of long term stability

The model thus should be used to predict the future development of the CO_2 plume. Based on this prediction the level of monitoring after the transfer can be reduced by the authorities. A minimum amount of monitoring for leakages is necessary. Based on the models and monitored behaviour, this minimum level of monitoring can be determined. If there has been fault on the side of the operator for example in case of deficient data, the operator can be held liable, even after the transfer.

The Commission has adopted guidelines on this issue; in Guidance Document 3 for the implementation of the EU CCS Directive, the Commission further elaborates the requirements. The guidance document states that the conformity with the models might be demonstrated by the fact that the 3D static or dynamic model does not need recalibration for at least 5 years before the transfer and that the results of the model simulations over the entire life of the project are within the confidence interval of the monitored parameters (as established by the steps in 2.3.1). The absence of detectable leakages should be based on consultation between the operator and the competent authority and are dependent on the site- specific characterizations. The guidance document lists a series of metrics that can be used by operators to assess the absence of leakage.

The evolution towards long term stability may be indicated when the models project stability (i.e. lack of migration) of the CO_2 plume, the monitoring parameters (pressure, temperature, saturations, groundwater pH, etc.) are within the predetermined range of values and in line with historical monitored parameters, the rate of change in key monitoring parameters is small and declining. The Guidance Document 3 proposes a list of required documentation from the operator to demonstrate the permanent and complete storage.

4.3.4 Summary

The assessment of risk in the EU CCS Directive is visible in three main decisions:

- In determining the suitability of the location
- In approving the monitoring plans
- In accepting the responsibility for the storage location

In Guidance Document 1 the European Commission emphasizes risk assessment as being an on-going and iterative process throughout the CO_2 storage life cycle. In all of these decisions the operator has to provide the information, based on the use of models. In essence a final model must be chosen as representative of the subsurface and the on-going physic-chemical processes. Finally, a prediction based on this model is the basis for the decision to transfer responsibility. How these models assess the residual risk and which uncertainties may still remain will be addressed in the following chapter.

4.4 The process

The requirements that have been described in the previous sections have consequences for the interplay between the CA and the operator. It is clear from the last sections which topics have to be addressed, but not how they are practically implemented. In the next part of the deliverable the topics of uncertainty and modelling will be described. They constitute the back-up for the claims of the operator as to the site's suitability for CO_2 storage or the lack thereof. Although these topics are within the realm of so-called hard science it is naive to think that things are ever clear-cut. Different backgrounds of scientists involved invariably lead to different personal (subjective) assessments, and that is certainly the case when the investigations have to begin. Therefore the following maxim is all-important: During the process an common picture has to develop, first of all among the working scientists themselves, but this picture must then be shared with the CA. So, not only the operator, but also the CA must take part in this process, but their roles are obviously different.

Nevertheless, the CA must be able to engage in a discussion with the operator on both a procedural and a technical level. Procedures may have to be adapted as a result of content, as will be discussed in the next chapters. The uncertainties of all kinds, to be detailed in the next chapter require a process of measuring and modelling, and of communication between the different partners. As will be indicated in the next chapter, the modelling part is not free of subjective judgment. This judgment has to develop by the modelling process itself. One must learn by doing, modelling and discussing results.

The assessment and characterization process is to be viewed as a learning route with combined forces. It is a joint enterprise between CA and operator. Operator and CA should work together to go this route towards fuller understanding of the (pre-selected) storage site. The modelling practice and its careful monitoring is a well-suited aid to go this route. But, as will be detailed in the next chapters, it is a far from easy and obvious route, where joint decisions must be taken. There is another reason why the view of a "learning route" is important: the CA has the authority to derogate from the criteria laid down in the EU CCS Directive under provisos laid down in Annex I of that Directive. However, the CA must be fully informed and must have developed an understanding before they can responsibly exercise this right. Since the operator and the CA have different goals / perspectives in such a project (somewhat simplified as "commercial" versus "communal" interest) it is all-important to develop mutual trust. These considerations lead to the following main conclusions:

1. Formal and informal regular contacts between Competent Authorities (CA) and site operator are deemed necessary. The CA should have a body of technical experts to its disposal with legal status. These experts make communication possible on a technical level, when needed. Before and during the characterization and assessment activities it should be discussed what has to be done in the assessment and characterization activities for each concrete case. All relevant uncertainties and risks should be addressed. Those circumstances that do not seem to present any real risk should be discussed as well. It is in the authority of the CA to tailor the work to the actual concrete circumstances (EU CCS Directive Annex I, prologue). During the investigations regular contacts are very much desirable. The site operator should communicate any novelties and unexpected developments. The CA then can respond and may suggest deviations from the original plan of actions if this is deemed appropriate. The CA and the site operator will discuss which models (in broad outline) are to be investigated. Also, it can be determined which models are carried along during the different phases (injection, closure, post-closure.) In so doing none of the parties will meet with unpleasant surprises of a

process nature at the time that formal reports must be handed in, or formal decisions are to be taken.

2. The various fields of expertise should have organized ways of communication before and during the research activities, since a lot is going on at the same time. For instance, every sub-model that is defined should be "drawn" through the evolution sequence covered by the various realms of expertise. Hence it is important to know the "status" of each sub-model at any time. Moreover, if sub-models show unexpected behaviour this information should be shared among all researchers in order to define appropriate re-iterations within the workflow. Since many (sub)-models will have to be scrutinized organized information sharing among the researchers is vital. In view of these It would seem appropriate to appoint (a small group of) persons responsible for the communication and for the administration of the activities.

5 Uncertainty

This chapter is intended for the "working scientist". A general background into uncertainty is provided that may sketch the framework in which the detailed expert investigations on assessment and characterization of a storage site are brought together. This chapter is certainly not superfluous as the subject matter is (usually) not addressed extensively in formal courses for natural scientists, where pure technicalities as error propagation dominate. This chapter provides a link with modelling work as well.

5.1 Dealing with uncertainty

In a previous deliverable CATO2-WP4.1-D01 issues are described concerning the implementation of the EU CCS Directive into national law. Notably, in chapter 3 the necessary scientific investigations for the assessment and characterization are listed. This chapter has been written mainly, though not exclusively, with an eye on the needs of the site operator, emphasis being put on the strictly geo-scientific elements in the process. The step towards risk determination, however, has not been made in any explicit way. Yet this is important, as the proper goal of safe site selection as formulated in the EU CCS Directive shows.

In the activities of characterization and assessment of the storage risks the subsurface plays a prominent, though not exclusive, role. It is for that reason that the activities stipulated in the EU CCS Directive are overwhelmingly targeted at the subsurface. In this chapter, the discussion will be confined to the subsurface plus the effects in the atmosphere and water surfaces, if CO_2 were to escape. In this "playing field" the discussion of uncertainty is important.

The EU CCS Directive per se does not impose any way in which the results of the investigations by the different domain experts should be combined. In Article 4 sub 4 of the Storage Directive it states that, "a geological formation shall only be selected as a storage site, if under the proposed conditions of use there is no significant risk of leakage, and if no significant environmental or health risks exist". It is not specified how this is to be determined. Whereas Annex I just stipulates which (geo)scientific investigations should be conducted it is not mentioned how these should be combined to yield responsible statements as to the envisaged risks.

Our task, then, in this deliverable is to make the problems arising when using predictive models explicit, and formulate solutions.

It is to be noted that the EU CCS Directive defines other "technical" items to be delivered by the site operator seeking a storage permit (e.g. monitoring and mitigations plans), but characterization and assessment are the very backbone of the necessary activities.

5.1.1 Types of uncertainty

Van der Sluijs wrote a Ph.D. thesis on the management of uncertainties in risk assessment related to anthropogenic climate change (Van der Sluijs,1997). In this work he cites no less than 12 different proposed classifications of uncertainty. Perusing the various classifications one can establish a set of uncertainties that apply in the more limited context of CO_2 storage. A broad classification is as follows:

- Data uncertainties
- Modeling uncertainties
- Completeness uncertainties

Data uncertainties arise from the quality of the data (i.e. their precision) as input for the models. These uncertainties relate to measurement errors and also to inherent variation. For instance, the measurement of the permeability of a chunk of matter sampled from a well is subject to measurement error. It is also subject to an error due to the chosen method to actually determine this value, especially if assumptions and theory necessarily enter this determination process.

Such a measurement is usually taken as an indication of the value of a certain volume, but this assumption neglects the fact that permeability may vary substantially within that volume. Inasmuch as the measured value is taken as an indication of the permeability it is subject to inherent variability. No number of data will ever suffice to describe the volume exhaustively. On account of the inherent variability the investigator is bound to formulate a probability density function (henceforth pdf) for the permeability for the given volume, and this will always require subjective judgment.

In principle there is also the question of the “appropriateness” of the data. When data are used on input for an investigation it should be clear that it is those data one needs. This is linked to the description one chooses in the investigation. For instance, if one adopts Darcy’s law for the fluid flow in a reservoir, data on the permeability are appropriate. It is, however, also a question of scale which data are deemed “appropriate”. In a reservoir flow simulation, for example, one must usually resort to an up-scaling procedure which requires more than just using permeability values as obtained by direct measurement. Uncertainties here are intimately linked with the following type of uncertainties.

Modelling uncertainties

Theories in the natural sciences are quantitative. This holds obviously for physical and chemical theories, but it holds for a “softer” expertise like geology as well. In physics, conservation laws give rise to equations describing the evolution of “state variables”. However, in “descriptive” geology static properties of the subsurface are ultimately described (“translated”) in quantitative terms and, hence, geological static models do not compute state variables.

The first modelling uncertainty thus arises as regards the choice of a theory that adequately describes phenomena on a desired scale in space and time. This entails the choice of appropriate (process) descriptions. In case different viable descriptions are available this choice represents a very basic uncertainty. The appropriateness of available data, touched upon above will play a role here. An “engineering” approach is often necessary to accommodate the description to data as available. This is, for instance, clear in reservoir modelling where permeability up-scaling is sheer necessity. However, there are various ways to do this, each with different underlying assumptions. Thus this “engineering” process is fraught with uncertainty.

The second modelling uncertainty arises as regards the technical implementation of a chosen description into a numerical scheme. For instance, in numerical flow simulations one may resort to implicit or explicit matrix solver schemes, and each of such concrete schemes have their pros and cons.

In any case one should be fully aware of numerical errors related to gridding in space and time. This might be especially an important issue as the computations will have to comprise long time spans and, likely, many time steps to perform. The accuracy of the computed results is clearly at stake. [For some deep-searching information one might wish to consult the time-honoured standard texts by Potter (1977) and Ames (1977).]

The third modelling uncertainty, highly specific for subsurface modelling, is connected with the initial situation that forms the starting point of any modelling activity. The geologists design a 3D static Earth model (explicitly referred to in the Annex I of the Storage Directive) from which all other modelling activities (geo-mechanical, fluid flow, geo-mechanical) are derived. The basic uncertainty here is governed by the fact that, no matter how many data are available, geologists have to draw on general knowledge or general models, and have to fill the remaining gaps. However vast this general knowledge, geologists have to make choices that might well have been different, and are hence uncertain.

Completeness uncertainties are present on different levels again. When a certain description has been chosen as the basis for further investigation it is usual that additional simplifications are needed. For instance, in a reservoir flow simulation the temperature of the subsurface, once specified, might be left unchanged in the computations. There may be very down-to-earth reasons to do so, for instance related to computational effort. In such cases one might wish to have cogent arguments showing this neglect to be warranted. In flow calculations the assumption of constant temperature might be warranted, in geochemical calculations it might not. If an assumption is dubious, we are left with uncertainty on the validity of the results due to our “shortcut”.

A second completeness problem, at the very heart of our task, is governed by the attempts, early in the process, to define the scenarios that must be investigated. This qualitative phase of risk assessment involves experts of several scientific branches. But even so, there is always the possibility of an oversight. One can never be absolutely sure that nothing relevant has been overlooked. Our understanding and available data are always incomplete, and this will always remain that way.

A further completeness uncertainty deals with the state-of-the-art of knowledge. At the forefront of scientific research one deals with both abstract problems and those that present themselves in practice. It is likely that in the modelling practice issues are involved that are actively investigated and have not, as yet. , yielded unambiguous results.

Occasionally there is also mention of the slogan “we don’t know what we don’t know”. This may very well be true, but this statement does not help us in any way, and this generic type of uncertainty will be discarded in the further discussion. The “unknown unknowns” cannot be taken into account in risk analysis.

5.1.2 Treatment of uncertainty

The task of characterization and assessment of a prospective storage site entails the obligation to deal with uncertainty. In the last paragraph a distinction was made between types of uncertainty. The following questions impose themselves upon us:

- What is the goal of taking uncertainties into account in characterization and assessment? Perhaps more specifically, why is it important for the results?
- Which methods are available for a proper treatment of the uncertainties in this context? This is a technical question, but certainly one of great practical importance.

When after a pre-selection phase a potential storage site is deemed “promising” it is still clear that lots of things are not precisely known as yet. The subsequent collection of additional data intends to diminish uncertainties(and hence risks, ultimately), but can never remove them in full measure. We have to do a characterization and assessment exercise based upon a collection of data and must put forward a judgment whether the various identified risks are deemed small enough to warrant starting an injection phase.

We can formulate the following maxim for the first question above: “The goal of taking uncertainties into account is: obtaining overall results consistent with these uncertainties”. This maxim tells us that the uncertainties must somehow “propagate” via the characterization and assessment activities to the final judgment of the risks. In Chapter 3 of the deliverable CATO2-WP4.1-D01 attention was paid to the tasks to be performed in the various fields of expertise involved, but no attention was given at all to the overall coordination with respect to uncertainty handling. In fact, the Storage Directive, leading as it is for subsequent developments, does concentrate on the fields of expertise, not on their coordination as may be seen from Annex I therein. It is appropriate, then, to address the second question above in some detail.

The list of types of uncertainty in paragraph 5.1.1 reveals that not all uncertainties are of a simple numerical type. For example, the uncertainty regarding the appropriate initial situation for all subsequent modeling exercises is of a “hypothesis” type. Indeed, we can choose more than one feasible structural build-up of the subsurface in the light of the knowledge available when the characterization and assessment activities begin. Our uncertainty treatment must be able to encompass both the “simple” numerical uncertainties and the uncertainties of the latter “hypothesis” type. It might be thought that statistics as usually taught to social and natural science students at the universities will provide the obvious and appropriate vehicle for our uncertainty propagation problem. However, this overlooks a rather unpleasant limitation of the standard practice. A salient feature of the characterization and assessment activities is that a good deal of background knowledge is present that must be taken into account. Standard statistics, however, is not designed to do this. It is based on the so-called “frequency interpretation” of probability which makes it impossible by definition to attribute a probability to a hypothesis. What we need is a vehicle that can use prior knowledge in the process, knowledge that may itself be –and generally is- fraught with uncertainty. That vehicle should obviously be based on a different interpretation of probability, one that allows to speak of a probability (or plausibility, but we will stick to the use of the word “probability”) of a hypothesis and allows mathematical operations in a self-consistent manner. Such a vehicle is available, and has become rather prominent in the last four or five decades in quite some disciplines. This vehicle will now be described.

5.1.3 Probability theory as the logic of science

We want to be able to scrutinize models on the basis of a comparison of model predictions and measured data. Each model is to be considered a hypothesis, a proposition. Propositions would be expressions as: “Model M describes the state of affairs best given new data ”, “Model M describes the state of affairs best before considering any of the recently acquired data.”
We want to be able to attribute a probability to a proposition. Not any proposition, but propositions of which can be said that they are true or untrue. Remarkably enough, a few simple desiderata are sufficient to set up a complete system, called Bayesian Probability Theory (Jaynes 2003, van Horn 2003). Remarkably enough, the rules of applicable mathematical operation turn out the same as for the standard probability theory, but the big difference is that the Bayesian probabilities apply to propositions, whereas standard probability applies to sets as axiomatized by Kolmogorov in 1933. (Grimmett, Stirzaker, 2003). Jaynes (2003) writes:

“Our system of probability, however, differs conceptually from that of Kolmogorov in that we do not interpret propositions in terms of sets, but we do interpret probability distributions as carriers of incomplete information.“

The last part of this excerpt is crucial, it brings the state of information into the probability theory, which now turns into a kind of logic taking into account uncertainty. Jaynes follows up the above sentences with a particularly revealing statement:

“Partly as a result, our system has analytical resources not present at all in the Kolmogorov system. This enables us to formulate and solve many problems – particularly the so-called “ill-posed” problems and “generalized inverse” problems – that would be considered outside the scope of probability theory according to the Kolmogorov system. These problems are just the ones of greatest interest in current applications."

The following example may illustrate this. When geologists construct a 3D earth model they may envisage that a number of conceptual models are consistent with their background knowledge and the data available at the moment they start their activities. They may attribute a so-called a priori probability to each of these models. When further data become available they ascertain the likelihoods of the new data in the light of each model. By multiplying the a priori and the likelihood (and normalizing) we get the posterior probability of each of the models. This is the content of Bayes' theorem. Thus the initial probabilities are updated in the light of new information, and the "verdict" is contained in the posterior probability. This enables us to perform further enquiries which remain in the realm of probabilities. Note, that reasoning about data and models is now brought into the realm of a mathematically coherent framework, and we may dispense with the "ad hockeries" (Jaynes) of "standard" statistics. The present situation is that Bayesian probability (or Bayesian Updating or Bayesian Statistics, two alternative names also coined for this framework) is accepted within the statistics community, and widely used in the exact sciences (Gregory, 2010). For further information, see Jaynes (2003).

5.2 Risk

The word "Risk" used in an expression like "Risk Assessment" has a very definite meaning. One should be aware that the word is used in a rather sloppy way in ordinary speech. Also, it is sometimes used in a rather vague way in a management context. (This is apparent, for instance, in CATO2, WP4.5 where a definition is claimed based on ISO. But also in the EC Storage Directive Art.4.4 some confusion seems to appear, where two different meanings seem to feature!.) In the present context one must insist on a definite operational definition. If we attribute a probability of occurrence to a so-called effect, called E, the associated risk is by definition the product of these two. For example, if E stands for "3 injured persons per year" and the probability of this is taken as 0.06 the risk is "0.18 injured persons per year." However, this definition is usually too simple. Usually, we must assume that the severity of the effect is a function of some parameters q1, q2, … These parameters depend on features (properties) in the subsurface system, events (man-induced or otherwise), and physical or chemical processes. Within a Bayesian framework an exact definition can now be given. The interested reader is referred to Appendix I for details.

5.2.1 Qualitative risk assessment

Qualitative risk assessment has to take place at an early stage of a characterization and assessment project. The best moment seems to be when the geologists have composed a provisional (?) earth model, or when they have produced several models consistent with their background knowledge and the available data. Experts will make an inventory of relevant Features, Events and Processes (FEPs) that may have a potential contribution to "risk" The experts will define effects that may be adverse to human health or the environment within this geological context. They will then also define scenarios which may lead to such adverse effects. In the subsequent activities these effects and scenarios play a dominant role. Some will turn out real, others more of an academic nature. In any case, subsequent quantitative treatment will be based on their collective findings. Even though this is a qualitative phase, it is possible to make some non-trivial quantitative predictions on the probability of occurrence of the various risks as well as the time scales involved, based on a branch of probabilistics known as Markov Chain theory (Nepveu et al., 2009). The information from such an exercise can be used to highlight the relative importance of the risks and this helps shaping the subsequent activities. In the light of the somewhat formal discussion above one might say that risk assessors determine prior probabilities. This is most conspicuous in their discussion of the Boolean variables connected with the presence or absence of potentially adverse features, like faults penetrating a reservoir, etc. The guiding role of qualitative risk assessment demands that utmost care is taken not to overlook relevant effects. Experts from different fields are brought together, and participation of stakeholders is important, also for the sake of furthering public acceptance of the results. Nevertheless, choices will be made as to what is a realistic risk or a realistic risky scenario, but these choices are never “cast in iron”. That is to say, in the quantitative phase revision of these choices might turn out to be necessary.

6 Modelling

Modelling activities are explicitly addressed in the Storage Directive, albeit on an abstract (regulatory) level that provides little guidance to modellers. The Annex 1 testifies to this. In our context modelling offers various possibilities for site characterization and assessment, especially when combined with monitoring activities. The issue is how to reduce subjectivity and, hence, manipulability of the modelling process in order to gradually gain mutual trust (and convergence / commitment on the validity of the model) between the operator and the competent authority. Before discussing these aspects it is important to define the words "model" and "modelling". The 3D earth model that is to be constructed at the beginning of the activities will be the backbone for all further activities. It is a so-called static model, a way to describe the subsurface in terms of position dependent geological attributes like porosity and permeability as a function of location xyz. A given earth model- a 3D structural-geological description with its clothing of attributes like porosity and permeability- is what we will refer to as our "model", our view of the initial subsurface situation. The term "modelling" on the other hand, will be reserved for the subsequent activities, connected with process descriptions of what may happen upon injection activities.

6.1 Goals of modelling

Scientific modelling in general has two aims. It is concerned with "obtaining numbers" and "acquiring understanding". If one wants to estimate the effect of a leaky well one wants to know the CO_2 flux from the well bore and other places, so as to be able to assess the possible effects on humans and the environment. Analytical calculations ("pen and paper") are out of the question in any realistic, non-trivial situation. One must numerically "mimic" what happens, follow the evolution numerically to obtain the answers one is looking for. A basic assumption here is that the equations employed capture the processes on the macroscopic level one addresses. This important issue is addressed in the various areas of expertise. Software packages that are used present the state-of-the-art situation, and usually offer various options to adapt equations, etc. There is a third and practical "final" aim of the modelling: determining a limited set of final models that will be used to show that what we see in the monitoring phase after closure conforms to our expectations and to demonstrate that, if necessary, any deviations from our expectations can be adequately addressed by operational mitigation measures (risk management objective). This final set of models defines our understanding of the subsurface with all the knowledge and (injection) data we obtained. Obviously, this set can only be defined after the injection and closure phase. In the very first phase one just wants to ensure with reasonable probability whether the proposed site can be used as a storage site, when one does not yet have the benefit of the data that will be collected during the injection phase.

"Mimicking" processes in concrete circumstances as presented by the 3D earth model enables the investigators to follow the (geo-mechanical, flow, geochemical) evolution. Usually one will expect certain results: the computer output is qualitatively understandable for the scientist. However, the reverse is possible as well: the output "baffles" the scientist. Then, expressed in an anthropomorphic phraseology, the results try to teach us something. This aspect of modelling is very important in our context indeed. It helps to diminish the completeness uncertainty connected with the qualitative risk assessment. For instance, if CO_2 escaped from the envisaged container it might rise and lead to surface fluxes just above it. However, if the overburden has a layer cake structure, CO_2 might become entrapped against a certain layer, move sideways and only "pop through" when the pressure exceeds some critical value, the entry pressure. This might lead to surface fluxes at lateral distances far from the container. This process -or rather cascade of processes- is easy enough to understand, but equally easily overlooked as it depends on certain details in the subsurface. The "numerics" will simply detect these details and hence their consequences if the physical processes are encompassed in the equations employed. This potential of numerical computations of pinpointing to unexpected effects is important and must have implications for the overall workflow –to be discussed later.

In the context of characterization and assessment the Storage Directive mentions definite roles for modelling. In article 13, comparison of modelled behaviour and actual behaviour as testified by monitoring is demanded. In article 18 again, conformity of actual behaviour of the injected CO_2 with modelled behaviour is put forward as an explicit demand before transfer of responsibility from the operator to the CA can take place. Finally, in both Annexes I, II modelling is mentioned again. The explicit use of modelling in these cases is "verification". In Annex II it is explicitly stated that "…The observed results shall be compared with the behaviour predicted in dynamic simulation of the 3D-pressure-volume and saturation behaviour undertaken in the context of the security characterization pursuant ….". And further: "Where there is a significant deviation between the observed and the predicted behaviour, the 3D model shall be recalibrated to reflect the observed behaviour…". This signifies that the incoming data produced by monitoring have to be used for an updating of the model(s) and the further modelling activities if there is reason to do so. As a result of this updating one must re-iterate steps in the overall workflow. Significant deviations will thus also require a new qualitative risk assessment, as stated in Annex II 1.2 as well.

6.2 The modelling sequence

In a deliverable of EU-project SiteChar, one finds the essential steps in a site characterization and assessment study. The workflow proposed there is reproduced here pictorially in fig.1 (with kind permission by the coordinator of EU-project SiteChar). The blue boxes under the heading "thorough analysis" show a possible sequence of modelling activities. Starting with the 3D earth model quantitative modelling will be conducted, basically in a sequential fashion. This means, for instance, that the output from the flow simulation is used as input for geo-mechanical modelling. This is a slight oversimplification as we will discuss later Nevertheless, quite generally one can formulate a rule of thumb: "Output (n) = Input (n+1)" where the arguments n, n+1 denote the various steps / fields of expertise in the chain. It is obvious from this scheme, then, that regular communication between the investigators in the various fields of expertise is all-important.

At this point it is necessary to introduce a refinement on what we think of as a 3D earth model. A 3D earth model specifies the structural "skeleton" of the subsurface, and this is dressed up with attributes like porosity and permeability. This last step is amenable to quite some variation, as the spatial information the geologist has to go on is incomplete, as already mentioned. Here it is useful to make a distinction between models and sub-models. Models differ in structural make up, sub-models only in attributes. So, to each model many sub-models are attached. The geologists will only make several models in the above sense if there is room to do so. For instance, seismics may not be entirely conclusive as to the presence of a fault in some area in the subsurface. However, faults are possible pathways for leakage, and hence it seems necessary to make a model with the suspected fault and one without. Both structural possibilities are to be considered. In any case, the starting point for the subsequent modelling activities per model (structural realization) is governed by the various sub-models. A large variety is possible here. For instance, well logging in several wells might have indicated the presence of a thin low-permeable streak not indicated on a large-scale seismic picture. This possibility should not be ignored, as this streak may have grave consequences for the flow of CO_2 and other fluids and adequate sub-models must be put to the test.

But even if nothing "special" is found among the data it will still be necessary to run many sub-models (per model) in order to map out the possibilities for undesirable effects. The question then is: how many sub-models (per model) must be run? Properties of the subsurface are described by variables (e.g. length, depth, porosity, correlation length of the permeability field), expressed in physical basis units. The description of the system is completely determined by the number of independent dimensionless quantities that can be formed from them. For instance, if L is the width of a reservoir, h its height, and the permeability correlation length λ, one can describe the system with two independent dimensionless parameters. This result is a special case of Buckingham's PI-theorem which states that if n variables describe a system, involving a total of p different units one can construct (n-p) independent dimensionless variables (Buckingham 1914, Hanche-Olsen 2004) that describe the system. Maybe some will turn out irrelevant, but one does certainly not need more than this number! In any concrete situation one can estimate upper- and lower bounds for each dimensionless variable and make an estimate how many runs should give a good impression of how the results depend on that variable. Thereby an order of magnitude of the total modelling workload is obtained. The number of simulations will become prohibitive in situations whose description demands many dimensionless variables. This problem can be expected to feature in the context of characterization and assessment of storage sites.

6.3 Practical issues

Reducing the numerical workload.
Suppose that the structure and make-up of a static 3D earth model can be encapsulated in m dimensionless variables, each of which one decade in reach (= uncertainty). One might think of 3 runs per decade as an acceptable cover of the uncertainty for that parameter. This would lead to 3m sub-models to be drawn through the complete modelling sequence. If an assessment project is scheduled for a year or so, practical problems might ensue even for moderate m: how could one master all the work during that time given today's computer facilities?. This problem might be enhanced still by unexpected numerical quirks that would necessitate re-iterations, as mentioned earlier. In actual practice it is hoped that the uncertainties in many variables can be narrowed down such that one set of dimensionless variables can be taken as a at least a fair description of the subsurface under investigation. Somewhat more precise: one hopes that one particular sub-model (for each structural model, see above) stands out as a fair candidate for the subsurface description. Sensitivity analysis is subsequently called for, and this is even explicitly mentioned in the Annex I, step 3.2 of the Storage Directive, where such an analysis is explicitly required. The question here is: how extensive should it be made? Over all of parameter space? Or over a certain “delicate” subspace? Sensitivity analysis is also an excellent method to enquire into the question which dimensionless parameters have the strongest / weakest influence on the evolution of injected CO_2 , thereby cutting down on the numerical work really needed.

Interplay between fields of expertise
Literally carrying over results (usually quantitative output) from one area of expertise to the next is plainly not possible in some cases. The geologist who composes a 3D earth model has data on various scales. He might be able to “paint” some parts in the reservoir with an accuracy of a few meters or less, and will generally do so. However, the reservoir engineer, responsible for the flow simulations, will generally not be able to handle this kind of detail with the available flow simulators. Not only is there a problem with the number of gridblocks needed to honour the details of the 3D earth model, the accuracy of the numerical results will generally deteriorate when details on a small scale are involved (e.g. numerical dispersion, Potter 1977). As a result of this limitation the reservoir engineer has to lump together large parts of the 3D earth model. It is of no small importance, then, that the geologist and the reservoir engineer communicate about how to do this, so as to avoid erasing the more relevant details. Misunderstandings at this stage may render all further results totally useless. Whereas the above lines of communication are clear beforehand the necessary iterations, required upon unexpected findings are more ad hoc. Structuring any necessary ad hoc communication prior to the start of a characterization and assessment project seems the only remedy against the danger of non-communication and its dire consequences.

Coupled modelling
This is a special form of interplay between fields of expertise. At the beginning of section 5.2 it was stated that the various (sub-) models are treated sequentially. This is not literally true. If processes develop at similar timescales one may have to combine them, i.e. resort to coupled modelling. For instance, during the post-injection phase, water imbibition from wet to dry regions could take place, leading to reactive transport. At time scales of 10,000 years the changes in the subsurface as regards flow are expected to be minimal (the injection phase will most probably take tens, at most hundred years), whereas chemically changes are still possible. In this case the geochemical evolution calculations can be considered decoupled from the flow, and they can be performed in a stand-alone fashion. Reactive transport due to diffusion (e.g. in the caprock) requires a coupled simulation approach (Tambach et al.,2012).

Probability approach vs. worst-case approach
Each chosen sub-model should be dragged through the full modelling sequence. In those cases where leakage of some sort is possible assessment must be done, as stipulated in the Storage

Directive (Annex II, step 3.3.3). The amount of computations where leakage occurs is input for a probability assessment. The tacit assumption is that each concrete computation is an indication for the " leakage sensitivity" of a certain part of parameter space, but this assumption is to be treated with utmost care. Geo-scientific judgment of the specific situation is indispensable, and necessarily subjective. There is a second way in which one can investigate whether a model or a larger set of sub-models is "leakage prone": the so-called worst-case approach. In this approach one chooses parameters such that leakage will show up in the computations, or will at least be facilitated. This method is particularly sensible if certain aspects of the subsurface are difficult to determine with any real certainty. For instance, there may be faults in the subsurface that might offer pathways for leakage. But the question is: are the faults sealing or are they not? The worst-case scenario is to assume they are not, and perform computations. If no such leakage can ever reach the surface this particular leakage scenario can be seen as not realistic. If, however, leakage does occur, one has to perform the effects assessment. It may turn out that the risk is below set boundaries. The worst-case scenario can be seen as computing risk under "probability one" conditions. Again it is important to invoke geo-scientific judgment as to the question whether the chosen case really represents a worst-case scenario. The worst-case approach is a method in which one "cuts corners" in a responsible way.

Communication between Competent Authorities and site operator
It has been said already that communication between the various scientific disciplines involved is a matter of absolute necessity. It is equally important to entertain frequent contacts (both formal and informal) between the site operator responsible for the assessment and characterization activities and the Competent Authorities. In this contacts it must become clear what has to be done by the operator to fulfil his legal obligations in view of handing over responsibility to the CA. This necessity is a direct consequence of the level of abstraction of the Storage Directive, and possibly of its implementation in the national law. The amount of work in the characterization and assessment of a particular site is non-trivial in any case, and hence one does not want to be bothered by investigations that are unnecessary, given the a priori knowledge of the site. The CA has the authority to derogate from the criteria laid down in the Storage under provisos laid down in Annex I. Before and during the research activities contact between the parties mentioned is necessary to establish what has to be done. Indeed, during the investigations new insights may emerge that make a revision of plans necessary. The goal of the frequent contacts is to make the process of site characterization and assessment run smoothly. This seems the more necessary because many prospective sites have to be scrutinized in the next decade or so if large-scale CCS is to take off. It goes without saying that mutual trust and honesty is an absolute prerequisite.

6.4 Model comparison

Modelling activities take place in two distinct phases: prior to obtaining a storage permit and during (and after) the injection phase. In the first phase the modellers possess a given stock of data to work on. These data may have been augmented by exploration drilling, but after this there is no increase in the amount of data. Only when injection activities start the modellers acquire new data. These enable them to modify their pre-injection models (e.g. by history matching). When the injection phase has ended, post-injection monitoring is the activity that informs them about any development of the subsurface system's state variables, and hence on the validity of the models and hence of the (long term) performance predictions. In the EU CCS Directive it is explicitly assumed that the site operator has been able to embrace a final model or a set of final models by the time that Transfer of Responsibility is at stake. For instance, in art.18 sub 2a it is stipulated that the operator has to demonstrate "the conformity of the actual behaviour of the injected CO_2 with the modelled behaviour." Also, in Annex II to the EU CCS Directive dealing with the monitoring plan it is stipulated that "Where there is significant deviation between the observed and the predicted behaviour, the 3-D models shall be recalibrated to reflect the observed behaviour". The big question is, of course, how to do this; there is no generally agreed way, even after 100+ years of experience in the hydrocarbon business. Given this expectation the question boils down to how the best set of models or sub-models from many sets is eventually chosen by the site operator. Within a Bayesian framework this question has a rather elegant and simple solution. It is detailed in Appendix II.

Summary of Chapters 5 and 6

We started with two main questions:

- How does modelling take into account the many uncertainties?
- How does one obtain a final model to be used in the fulfillment of the obligations for the CA at the time that transfer of responsibility becomes an issue?

In Chapter 5 a number of different types of uncertainties were defined that appear in the context of site characterization and assessment. The outlines of a general framework were given for dealing with these uncertainties in a coherent fashion. This framework is known as Bayesian probability theory Within this context risk can be defined in a clear way. Qualitative risk assessment as performed at the start of the characterization and assessment activities was also placed within this general framework. It was thereby seen as the driving force for subsequent quantitative analysis.

In Chapter 6 it was put forward that modelling in general is for obtaining a better conceptual understanding, and also for obtaining “numbers”. In our context “verification” is an extra demand: comparing monitoring data and the results of the modelling activities. Monitoring activities, especially with respect to the behaviour of the CO_2 plume may be in accordance with the chosen model, or must lead to adaptations, or adopting one of the other sub-models that have been constructed and run through the modelling sequence. This plays a role at the transfer of responsibility to the CA, as stipulated in the Storage Directive. Model Comparison should lead to a decision of which model is finally adopted, and to be compared with monitoring results before, finally, a transfer of responsibility to the CA can take place. Finally It was discussed that the (complexity of the) work requires communication on at least two levels: between the experts performing the detail investigations, and between the site operator and the CA.

7 Recommendations for CA and Operators

In Chapters 5 and 6 the roles of uncertainty and modelling have been discussed, and a summary has been given. The relation of the competent authorities and the operator is, however, the main issue in this work package. The main recommendations in this respect are here now summarized.

1. Formal and informal regular contacts between competent authorities and site operator are deemed necessary. In these contacts information is exchanged between operator and CA. Storage sites will be very diverse: abandoned gas fields differ from aquifers, but each of these groups is very diverse in itself. That means that the “to do” list is in all probability strongly site dependent.

2. The investigations are truly a learning process, not just for one of the parties, but for both. Trust should be built up between the parties as the procedures and methods in the actual modelling activities can still be interpreted in various ways, and shortcuts will be sometimes necessary. Moreover, unexpected features may reveal themselves, necessitating a re-direction of the work. This is all very much a technical matter, where guidelines cast in iron won’t probably work. The actions have to be tailored. For all those reasons the CA should have a group of scientists available that take care of the (informal) communication with the operator. This group should have sufficient know-how as well as a well-defined authority.

3. The experts of the operator should communicate among themselves on a regular basis as the process is complicated and the separate expert activities are intertwined. It is recommended that special “officers” streamline the communication.

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Appendix I: Risk

If there are N parameters identified as in some way relevant for defining "risk" they form a N-dimensional parameter space. If we summarize the parameters symbolically in the parameter vector q, one can define the Risk of a certain effect E as

$$\text{Risk} \equiv \int p(q | D, I) \,.\, E(q)\, dq \qquad (1)$$

The integration extends over all of parameter space, with the understanding that
E (q) may be zero for parts of the parameter space. In this formula p(q | D, I) is the joint probability density function (pdf) of the parameter values summarized in q consequential upon the data "D" and background knowledge "I". In Bayesian parlance this is the posterior distribution. Hence, risk is nothing but the so-called mathematical expectation of E over the posterior probability.
This posterior probability is related via Bayes' theorem to the prior probability that we attribute to the parameters q before we have done all kinds of data processing / computational work. This prior represents our knowledge of the situation when the characterization and assessment activities are just started. Put otherwise, we must define the prior probability in accordance with our initial state of knowledge. The posterior probability featuring in definition (1) depends on both the initial "guess" and the data obtained during acquisition and injection phase according to Bayes' theorem

$$p(q | D, I) = p(q | I)\, p(D | q, I) \;/\; \int p(y | I)\, p(D | y, I)\, dy \qquad (2)$$

where the integration is over the dummy vector y representing values in parameter space.
The denominator is a normalization constant; the real content is in the numerator, being the product of the prior pdf and the likelihood. See also ULTimateCO_2 by Bos, Wildenborg, Wilschut 2012, forthcoming where a like definition is given.

Appendix II: Bayesian model comparison

Suppose we have N sub-models, each of which belonging to one of the structural 3D static earth models constructed by the geologists. At any one moment t we have body of data D(t) consisting of all data obtained prior to time t. We wish to give a probability to each of the sub-models. We consider the set of sub-models "complete", i.e. we attach probabilities to the sub-models such that the total sum equals unity. In principle we can attach a prior probability to each of the models, preferring some over others. Let $p(M_j)$ be this prior probability for sub-model j. The likelihood for this model, given the body of data D(t) is denoted by $p(D(t)|\ M_j)$. The probability of model j at time t, given the data obtained before t, D(t) then is given by Bayes' rule as:

$$p\ (Mj\ |\ D(t)) = p(Mj)\ p(\ D(t)|\ Mj)\ /\ \ \Sigma\ \ p(M_k)\ p(\ D(t)|\ M_k) \qquad (3)$$

The likelihood is determined by $p(\ D(t)|\ M_k) \propto \exp(-\ \chi 2 / 2.)$ with

Chi-squared $\chi^2 \equiv \Sigma$ (measured data value − Mk predicted data value)^2 / σ^2

where the sum is over all data in the set D(t) with their own "sigma ". One needs to know the typical uncertainty in the various data values, the various "sigma's" in usual parlance, and with this quite general information Maximum Entropy considerations lead us to use the chi-squared as the objective function in the likelihoods (Nepveu et al., 2010, Gregory 2010).

A number of general remarks are in order.

- The "sigma's" above must contain both the measurement errors as well as the expected errors in the predicted values of the data. The last ones will depend on the grid sizes and time steps. The usual quadratic addition seems appropriate as the two error sources are independent.
- In the formulation we have explicitly introduced the prior probability p(Mj) for the subjective assessment of model j. It might be wise to give all models the same "start position". This seems the more reasonable as one only wants to deal with acceptable models anyway; initial choosiness seems a bit overdone. On a practical matter, the wealth of data D(t) would very quickly swamp the influence of the prior assessment; notably, initial preferences won't stand up to unfavorable chi-squared values!
- For all models the same dataset must be used. Hence, each model in the comparison set must produce value predictions that can be compared to measured values for all measurements invoked.
- With this comparison method there will always be one or more "winners", even though these winners might perform very badly in an absolute sense. "Quality Control" on the best models is a necessity therefor. For good or at least acceptable models the chi-squared values should be of order of the number of measurements in the set D(t), a standard result from probability theory (Press et al.,1999). If much larger values are found, then there are two possibilities. Either the sigma's used have been underestimated, or the models are truly unacceptable. The chi-squared values thus act as a measure of the appropriateness of each of the models.
- In the formulation the dataset D(t) was introduced. It is thus possible to perform the model comparison dependent on time. It may well happen that those sub-models initially favored in the comparison are later surpassed by others (for an example, see e.g. Nepveu et al.,2010). This evolution in preference given to the various sub-models might give some clues for the construction of new models, if needed.
- In case numerical values of a parameter are to be predicted from the models it is generally not a good idea to just take the value of the very best model. One should rater use so-called Bayesian Model Averaging (BMA). The BMA value of a parameter is the sum of the values of the parameter as obtained in the individual sub-models, weighted with the sub-model probabilities. Expressions for the variance of such a value can be computed as well, taking into account the variance (uncertainty) of the parameter within each sub-model, as well as the variance in the ensemble of all sub-models (Hoeting et al., 1999)

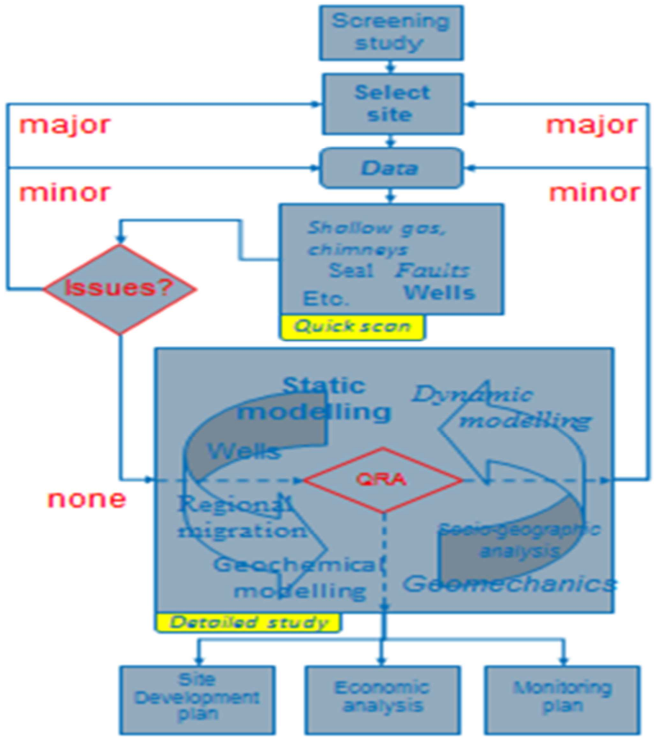

Figure 1. Broad outline of a possible characterization and assessment work flow (By kind permission of the SiteChar management).