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To cite this version:

Jean-Charles Manceau, Jeremy Rohmer. Ranking importance of uncertainties for the assessment of residual and dissolution trapping of CO2 on a large-scale storage site. 12th Greenhouse Gas Control Technologies conference : GHGT12, Oct 2014, Austin, United States. pp.3658-3664, 10.1016/j.egypro.2014.11.395 . hal-01003160

HAL Id: hal-01003160

https://hal-brgm.archives-ouvertes.fr/hal-01003160

Submitted on 17 May 2022

Available online at www.sciencedirect.com

ScienceDirect

Energy Procedia 63 (2014) 3658 – 3664

Energy Procedia

GHGT-12

Ranking importance of uncertainties for the assessment of residual and dissolution trapping of CO_2 on a large-scale storage site

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Abstract

We propose an approach to assess the importance ranking of uncertainty sources, with regards to the behavior of the mobile CO_2 during the post-injection period: a variance-based global sensitivity analysis is performed on three output parameters characterizing the location and the quantity of mobile CO_2, considering residual and dissolution trapping. The use of advanced meta-modeling techniques of ACOSSO-type allows circumventing two major difficulties: 1. The large number of computationally intensive reservoir-scale flow simulations; 2. The different nature of uncertainties whether linked to parameters (continuous variables) or to modeling assumptions (scenario-like variables). The feasibility of the approach is demonstrated using a potential site for CO_2 storage in the Paris basin (France), for which the amount, nature and quality of the data available at disposal and the associated uncertainties can be seen as representative to those of a storage project at the post-screening stage. A special attention has been paid to confront the results of the sensitivity analysis with the physical interpretation of the processes.

Peer-review under responsibility of the Organizing Committee of GHGT-12

Keywords: Residual trapping; dissolution trapping; variance based sensitivity analysis, ACOSSO metamodeling

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1. Introduction

The behavior of the injected CO_2 on the long term is of primary importance and numerous authors have pointed out the essential role of trapping mechanisms in the evolution of the storage (Gunter et al., 1997; Juanes et al., 2006; Ennis-King and Paterson, 2005). In terms of safety and more specifically of CO_2 containment, two of the greatest issues concerns the location of the plume – in comparison with the potential leakage pathways – and the quantity of

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1876-6102
Peer-review under responsibility of the Organizing Committee of GHGT-12
doi:10.1016/j.egypro.2014.11.395

mobile CO_2 in case of unwanted upward migration. The migration of the injected plume has therefore been the subject of numerous studies (Hesse et al., 2007; MacMinn et al., 2010 and 2011; Manceau and Rohmer, 2011; Doughty, 2007 and 2010). All these studies highlight the site- and condition-specificity of the evolution of the trapped plume fraction. Particularly, the structural characteristics of the geological formations, the initial hydrogeological conditions and absolute flow properties of the reservoir, as well as the multiphase flow parameters (relative permeability and capillary pressure) relatively to the CO_2/brine system have been shown to influence the pressure evolution and the behavior of the mobile gaseous plume after the injection (Goater et al., 2013; Doughty, 2010; MacMinn et al., 2010 and 2011; Mathias et al., 2011).

Knowledge of these parameters is often limited especially in the early stages of a storage project (before or in the first years of injection); the assessment of the fate of the injected CO_2 is therefore associated to several sources of uncertainties. The improvement of the knowledge on a specific site, before and during the life-time of the storage operations is essential as it may allow a decrease of the uncertainty on the outputs. However, additional data acquisition is likely to be expensive and time consuming, and the parameters to be characterized might be numerous. Thus, under time and budget constraints, ranking the parameters to be estimated according to their impact for the long term assessment of the CO_2 fate seems necessary. Such an importance ranking (aka sensitivity analysis) has been advocated by regulators in the European directive on CO_2 storage for instance (EC, 2009: Annex I Step 3.2 Sensitivity characterization).

However, performing such a sensitivity analysis might be challenging in the context of CO_2 storage. First, assumptions in the modeling procedure can be strong, because data can be scarce and might not be well-defined on a specific site. This is particularly the case for multiphase flow parameters (relative permeability and capillary pressure including hysteresis effects) curves specific to the CO_2/brine system and to the storage conditions; most of the time they do not benefit from previous studies of the site, even in sedimentary basin that are historically well-characterized with regards to intrinsic hydraulic properties (Mathias et al., 2013). Secondly, a robust sensitivity analysis requires a large amount of simulations, which might not be feasible when using computationally intensive simulations of the CO_2 fate on long term at reservoir-scale. Meta-modeling techniques (aka response surface or reduced order models) can be developed to circumvent such a difficulty (Rohmer and Bouc, 2010; Ashraf et al., 2013).

In this work, we propose an approach to assess the importance ranking of uncertainty sources, with regards to the long term fate of the mobile CO_2 on a specific case, considering notably solution and residual trapping.

2. Method and materials

2.1. Flow simulator, input parameters and output of interest

In this study we focus on the fate of the mobile gaseous plume on the first hundreds years after the injection. Mineral trapping has been shown to be low at that time (especially in a clastic context, see for instance Audigane et al., 2007) and therefore only structural, residual and solubility trapping modes are considered. We chose to conduct numerical simulation to adequately quantify the evolution of the injected CO_2. All simulations were performed with TOUGH2 simulator (Pruess et al., 1999) including the equation of state package ECO_2N (Pruess and Spycher, 2007), accounting for the properties of brine-CO_2 mixture at classical pressure and temperature of CO_2 storage operations. Dissolution of CO_2 in the aqueous phase is treated by means of local equilibrium solubility, i.e. by considering an instantaneous phase partitioning of water and carbon dioxide between the liquid and gaseous phases

A hysteresis module is utilized (Doughty, 2009) to model residual trapping and to take into account the associated hysteresis effects onto relative permeability and capillary pressure. It follows Land's residual trapping model (Land, 1968) as well as hysteretic characteristic functions derived from van Genuchten's capillary pressure function (van Genuchten, 1980) and based on Lenhard and Parker's relative permeability to brine and CO_2 (Lenhard and Parker, 1987).

Whatever the type of flow simulator (analytical, numerical, semi-analytical, etc.) used, the required input parameters for the modeling of CO_2 injection remain quasi-similar. A structural model should give insight on the geometry of the formations that are considered. It is completed by the values, heterogeneous (spatially varying) or homogeneous, of the absolute flow properties (porosity, permeability, compressibility) and of the temperature, pressure and salinity of the formation. The evolution of relative permeability to CO_2 and water and of capillary pressure is an additional required input. If hysteresis effects are accounted for, this evolution should be estimated for drainage and imbibition processes. The CO_2 storage operations characteristics (injected rate, duration, potential fluid extraction…) are also required.

Depending on the information at disposal, the confidence regarding these input parameters is different and the way to consider them in the sensitivity analysis needs to be different as well. Some of them may be directly fixed if they are judged sufficiently reliable. Otherwise, the uncertainty must be adequately represented with the level of information, for instance by a probabilistic law. For this work on two-phase flow simulations, different types of variables can be encountered and a distinction can be made between continuous variables such as petrophysical properties (permeability, porosity) and discrete/categorical variables associated to scenarios like different structural models, two-phase flow laws, or to alternative design choices.

In a risk assessment and management perspective, the evolution of two different characteristics of that plume over time appears to be of interest: the evolution of the quantity of mobile gas (indicator of how much gas might leak) and the evolution of the mobile gas plume footprint (indicator of the zone where gas can potentially migrate). We therefore propose to assess the input parameter importance on the evolution over time of three different output parameters (OPs):

- OP 1: mass of the injected CO_2 that remains mobile and in free-phase;
- OP 2: distance between the injection point and the center of mass of the mobile free-phase CO_2 plume;
- OP 3: surface of the mobile free-phase CO_2 plume directly in contact with the caprock formation.

2.2. Sensitivity analysis strategy

We propose a procedure combining variance-based sensitivity analysis VBSA (Saltelli et al., 2008) relying on the Sobol' indices (Sobol', 1993) and the ACOSSO-like meta-modeling technique (Storlie et al., 2010 and 2013), which allows jointly accounting for continuous variables (parametric uncertainty) and categorical variables (assigned to different model choices).

In the first step, a limited number n (say 100 – 500 depending on the total number of affordable simulations) of the input parameters' vectors (learning samples) are randomly generated to cover the domain of variation of the input parameters. These configurations are randomly generated with a Latin hypercube sampling (McKay et al., 1979) approach (with the uniform distribution) for the continuous variables, and sampling with replacement (with the discrete uniform distribution) for the discrete variables. A computationally intensive flow simulation is performed for this limited number of input parameters. The ACOSSO-type meta-model is then constructed using the training data before validating the meta-model quality (approximation and predictive quality).

3. Case study

3.1. Presentation, data available and uncertainty representation

We consider the case of a large-scale storage site where the amount, nature and quality of the data available at disposal and the associated uncertainties can be seen as representative to those of a storage project at the post-screening stage. We consider in this paper the injection of 30 Mt of CO_2 during 30 years in the lower Triassic sandstone formation based on a potential project in the Paris basin (France).

The site has been classically characterized: a 3D geological model of the storage formation is available (built after wellbore and seismic lines databases). The data at disposal are characterized by different degrees of uncertainty. The number of porosity and permeability data (from wellbore measurements) is relatively significant and we therefore considered their empirical cumulative probability distributions for the sensitivity analyses. No relationship between these two parameters was considered given the low correlation between them. The permeability anisotropy is unknown in the reservoir. We therefore considered several anisotropy scenarios: an isotropic case ($kv/kh = 1$), a laminated case ($kv/kh = 0.1$) and one scenario in-between ($kv/kh = 0.5$).

The range of salinity being relatively narrow, we consider that the uncertainties on this parameter are low and use a mean value corresponding to 20 $g.l^{-1}$. In a similar way, the CO_2 migration after injection is limited and therefore the temperature variations are planned to be low in the area of interest: the temperature is therefore considered constant with a value of 45 °C (estimation of the temperature at 1,000 m).

The hydrogeology of the region has been studied on a large scale. However, in the specific area of injection the local pressure gradient is not precisely known: two extreme scenarios have been considered to overcome the lack of data, one with initial hydrostatic conditions and another one with a strong hydraulic gradient in the injection area (0.01 m/m equivalent to 1050 kPa/km). The direction of this groundwater gradient was chosen towards the outcrops.

Contrary to intrinsic parameters such as porosity and permeability, no available information has been found on the multiphase flow parameters of this sandstone formation. To date, few data have been published regarding brine and CO_2 relative permeability curves. Recently, two exhaustive reviews of published relative permeability laws on sandstones with regards to the CO_2/brine system have been provided by Akbarabadi and Piri (2013) and Mathias et al. (2013). From the papers reviewed in these studies, we selected the data on sandstones (carbonate reservoir rocks and low permeability rocks were not taken into account). Moreover, as our study is focused on long-term assessment, both drainage and imbibition laws should be considered, which are even scarcer in the literature. Ten different datasets from published works have thus been taken into account (Akbarabadi and Piri, 2013; Bennion and Bachu, 2008; Krevor et al., 2012; Perrin and Benson, 2010; Berg et al., 2013; Pentland et al., 2011). These experimental data were fitted using the model of relative permeability mentioned in section 2.1: the fit was performed for the first drainage relative permeability laws; the successive imbibition and drainage laws were computed, based on this first drainage law and on the maximum residual saturation. Given the differences among the data and their low number, it was judged more relevant to consider these datasets as sets of limited number of scenarios rather than using a continuous range of coefficients' values for the relative permeability model. In the present study, all the different modeling scenarios are considered equally adequate, and therefore the relative permeability uncertainty is represented by a uniformly generated discrete random variable. Conversely, if the confidence weights were different, they could have been used to constrain the random generation (see an example in Rohmer et al., 2014).

Data regarding capillary pressure for CO_2/brine system are even more limited than relative permeability ones, as noticed by Pini et al. (2012): two extreme cases are considered: 1. a case of significantly low capillary pressure (equivalent to no-capillary pressure) and 2. a case of strong capillary pressure (using the same magnitude as Alkan et al. (2010) (case n°2 named high capillary pressure in this paper). No change (hysteresis) between drainage and imbibition was considered.

We also integrated in this importance ranking analysis the influence of the gridding in the dynamic modeling: four different meshes were built: 1/ Coarse mesh named Mesh1 (4,030 cells); 2/ Mesh2: Mesh1 with refinement in horizontal directions (11,477 cells); 3/ Mesh3: Mesh2 with refinement in the vertical directions (15,822 cells); 4/ Mesh4: Mesh3 with additional refinement in the vertical direction (19,671 cells).

3.2. Results and discussion

This strategy is applied by using 300 large-scale complex dynamic 3D model runs. The OPs were assessed for each run, every 30 years for a total running time of 250 years (including the 30 year-CO_2 injection). Based on these training data, an ACOSSO-type meta-model was constructed for each OP at these different times. The approximation quality was considered satisfactory with coefficients of determination all being superior to 90 %. The coefficient of determination computed to assess the predictive quality (performed through a 10-fold cross-validation procedure) were all over 75 %, which can also be qualified as satisfactory. Two different indices were assessed with the VBSA: 1. the 'main effect' (S_i) which is used for prioritizing the input parameters in terms of effort needed to decrease the OPs uncertainty range (it corresponds to the expected proportion of the total variance of the model output that would be removed in average if we were able to fix the true value of the given uncertain parameter i); 2. the 'total effect' ($S_{t,i}$) useful to highlight the non-influential input parameters that can be fixed and therefore to simplify the model (it corresponds to the expected proportion of the total variance of the model output if we were able to fix all the uncertain input parameters but the parameter i).

The results for OP1 are detailed in the following (the full study has been submitted in Computational Geosciences): Table 1 and Table 2 provide the value of the main and total effects of all parameters during the observation period.

Table 1: Main effect over time of the input parameters for OP1

Time after injection starts (years)	60	90	120	150	180	210	240	254
Porosity	0.1%	0.1%	0.1%	0.2%	0.2%	0.2%	0.3%	0.2%
Absolute permeability	33.9%	43.4%	53.7%	53.2%	48.7%	53.0%	50.2%	53.7%
Regional hydraulic gradient	0.6%	0.4%	0.7%	0.6%	0.4%	0.6%	0.6%	0.6%
Relative permeability	30.1%	27.7%	25.0%	26.5%	28.3%	26.5%	26.8%	25.4%
Mesh	1.7%	1.6%	0.0%	1.2%	1.5%	1.5%	1.5%	2.0%
Capillary pressure	27.3%	20.6%	14.6%	12.7%	11.6%	9.9%	10.8%	8.8%
Permeability anisotropy	0.0%	0.0%	0.2%	0.0%	0.4%	0.1%	0.0%	0.0%

Table 2: Total effect over time of the input parameters for OP1

Times (years)	60	90	120	150	180	210	240	254
Porosity	0.1%	0.3%	0.2%	0.3%	0.9%	0.5%	0.5%	0.5%
Absolute permeability	35.3%	47.8%	57.3%	57.0%	53.6%	59.5%	59.3%	61.5%
Regional hydraulic gradient	0.4%	0.3%	0.5%	0.4%	0.5%	0.6%	0.4%	0.6%
Relative permeability	34.5%	30.6%	27.9%	28.9%	33.6%	31.3%	31.9%	31.0%
Mesh	3.4%	2.4%	0.4%	1.8%	4.3%	2.6%	2.6%	3.2%
Capillary pressure	29.3%	21.5%	15.7%	13.7%	12.3%	10.3%	10.2%	8.8%
Permeability anisotropy	0.0%	0.0%	0.0%	-0.1%	0.9%	0.0%	0.0%	0.0%

They show that three main input parameters, absolute and relative permeability and capillary pressure, drive this quantity (S_i respectively of 54 %, 30 % and 27 % at the maximum). Their importance is evolving over time: at the end of the injection, the capillary pressure has a significant main effect, with a non-negligible importance of the mesh. However, these main effects decrease rapidly to low values while the main effect of the absolute and relative permeability increases or are stable compared to their initial value. These evolutions can be explained by the chronology of the occurrence of the different trapping modes: during the injection, almost all the plume is in the drainage process and therefore few residual trapping occurs but a large quantity of the plume has been already dissolved; dissolution appears to be driven at early times by the capillary pressure scenario. Right after the end of the injection, the saturation of a large portion of the plume starts to decrease and therefore an important quantity of CO_2 is in imbibition and is considered as residually trapped (the residually trapped quantity is calculated from Land's model in the cells in imbibition, even if the irreducible saturation is not reached yet). This explains the relatively high importance, even at early times, of relative permeability dataset which includes the maximum residual gas saturation. Then, the two processes occur simultaneously and the residually trapped CO_2 dissolves progressively, increasing the proportion of the dissolved CO_2 in the total trapped quantity. Contrary to early times, this slow dissolution process is shown to be driven by the absolute permeability of the aquifer, rather than by capillary pressure. The interactions effects are low (the sum of the main effects is always higher than 90%): the relationship between OP1 and the input parameters appears to be additive and could be simplified to a sum of univariate functions. The total effects analysis also indicate that the mesh, the porosity, the regional gradient scenario and the anisotropy have a low influence on the mobile gaseous CO_2 mass from 60 years after injection beginning (S_t respectively of 4.3 %, 0.9 %, 0.6 %, and 0 % at the maximum). In the simulation those four parameters (over seven in total) could then be fixed at their nominal values with negligible influence on the values of OP1. Interestingly, for the two other OPs, which describe the geographical footprint of the mobile plume, the results are not completely similar: the absolute permeability value and the capillary pressure scenario appear to drive mostly OP2 (highest main effect), while the porosity, the absolute permeability and the relative permeability dataset are the most influential parameters for OP3. Contrary to what was shown for OP1, the interaction effects between parameters are significant for OP2 and OP3 (the sum of the main effects is around 60 % for both OPs and for all simulation times). As a consequence, almost none of the input parameters can be fixed: only the permeability anisotropy scenario can be considered as non-influential (total effect of less than 1.5 % for both OPs and for all simulation times).

Acknowledgements

The research leading to these results has been carried out in the framework of the ULTIMATE-CO_2 Project, funded by the European Commission's Seventh Framework Program [FP7/2007-2013] under grant agreement n° 281196.

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