

# HIGHLY EFFICIENT TOOL FOR PROBABILISTIC RISK ASSESSMENT OF CCS JOINT WITH INJECTION DESIGN

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**Summary.** The potential of large-scale industrial CO<sub>2</sub> injection as an interim solution will vastly depend on our ability to quantify its uncertainties and risks. Current numerical simulation models are inadequate for stochastic simulation techniques, because they are too expensive for repeated simulation. Even single deterministic simulations may require parallel high-performance computing. Because the involved multiphase flow processes of CO<sub>2</sub> in porous media have a significantly nonlinear character, the problem is too non-linear for quasi-linear and other simplified stochastic tools. As an alternative approach, we propose a massive stochastic model reduction which is based on the probabilistic collocation method. The model response surface is projected onto a orthogonal basis of higher-order polynomials, allowing for non-linear propagation of model uncertainties onto, e.g., the predicted risk of CO<sub>2</sub> leakage back to the surface. The variable parameters include uncertain model parameters, such as porosity, permeability, etc., and a list of design parameters (injection rate, depth, etc.). The chosen degree of the polynomial balances between computational effort and accuracy. The proposed stochastic approach was validated through Monte Carlo simulation using a common 3D Benchmark<sup>2</sup>. The reasonable compromise between computational efforts and precision was reached with 2nd order polynomials. In this case study, our proposed approach yields a computational speed-up of 100: 1000 Benchmark runs for Monte Carlo evaluation are comparable to 10 Benchmark runs using the probabilistic collocation method. At the same time, our collocation methodology is an integrative powerful tool for optimizing design variables under uncertainty in one approach (via integrative response surfaces). This leads to robust designs with minimum failure probability over the entire range of uncertainty.

## 1 INTRODUCTION

### 1.1 Uncertainty analysis of carbon dioxide storage

It is highly likely that carbon dioxide (CO<sub>2</sub>) emissions are influencing the global climate<sup>3</sup>. Modeling underground CO<sub>2</sub> storage involves many conceptual and quantitative uncertainties<sup>6</sup>.

The lack of information about distributed properties leads to model uncertainties up to a level where the quantification of uncertainties becomes the dominant question in application tasks and may override the influence of secondary physical processes. In the development of CO<sub>2</sub> injection as a large-scale interim solution, our ability to quantify its uncertainties and risks will play a key role. Unfortunately, only sensitivity analyses<sup>1,7</sup> and no probabilistic risk assessment for carbon capture and storage (CCS) has been applied up to the present. Fault-tree analyses have been used to identify risks through different factors<sup>10</sup>, but have not yielded quantitative risk information.

The multiphase flow and transport processes involved are strongly non-linear, including phase changes about the supercritical state and effects such as gravity-induced fingering, convective mixing etc. This eliminates quasi-linear and other simplified stochastic tools from the list of reliable options. Current numerical simulation models are inadequate for stochastic simulation techniques based on brute-force Monte Carlo simulation and related approaches, because even single deterministic simulations may require parallel high-performance computing. Thus, the necessity for reasonably fast and non-linear stochastic approaches for modeling CO<sub>2</sub> sequestration poses a research task that needs to be investigated as soon as possible. In the current study, we suggest and apply a massive stochastic model reduction technique based on non-intrusive polynomial expansion, as explained below.

## 1.2 Purpose of the paper

This paper has two principal purposes. The first is to develop a reasonably accurate probabilistic risk-assessment method at acceptable computational costs. Considered risks are the risk of CO<sub>2</sub> leakage back to the surface and risk of exceeding of a critical caprock pressure. The challenge here is to find a compromise between computational effort and a reasonable approximation of the physical processes. To this end, we apply for the first time the probabilistic collocation method to the problem of CO<sub>2</sub> sequestration, obtaining an accurate high-order tool for probabilistic risk assessment. The second purpose is to develop a tool for the optimal design of CO<sub>2</sub> injection regimes. To this end, we present a novel framework, which projects all design parameters and uncertain parameters onto a single integrative response surface. This integrates the design task into the stochastic model, as presented in section 2, allowing us to find robust designs with controlled failure risks. We also draw attention to the significant impacts of incorporating uncertainty into model predictions and design tasks, in comparison to deterministic modeling approaches of CO<sub>2</sub> injection (section 3.3).

## 2 THE INTEGRATIVE PROBABILISTIC COLLOCATION METHOD

### 2.1 Novel integrative concept for analysis

We classify model parameters in two classes: design or control parameters that can be chosen by the operator of a system, and uncertain parameters that describe our (incomplete) knowledge of the system properties. In the CO<sub>2</sub> injection problem, the latter include, for example, permeability, porosity etc. This uncertainty has a non-trivial influence on the model output, like the

spatial distribution of pressure, gas saturation, amount of CO<sub>2</sub> leakage etc. On the other hand, the system's performance and failure probability will also depend on design parameters such as the injection rate or injection depth. Evidently, the decision-making for design parameters will depend on the interplay between the response to injection strategy, system uncertainty and, finally, the probability of failure.

In the present paper, we introduce an integrative concept, in which all parameters group into one integrative, transparent and efficient structure. Actually, we project all design and uncertain parameters onto a single integrative model response surface. It is a multidimensional surface and contains the integral information about the system behavior under all possible conditions at all points in space and time. Thus, we expand the notion of stochastic response surfaces<sup>5</sup> to integrative response surfaces forming an effective basis for robust design under uncertainty.

## 2.2 Approach

The current work provides a massive stochastic model reduction via the polynomial chaos expansion<sup>9</sup>. We employ the collocation method<sup>8,11</sup> to project the model response surface onto the polynomial chaos. This technique allows for non-linear propagation of uncertainties in the risk analysis at low computational costs. Our variables of interest (see section 3.1) include uncertain parameters such as porosity, permeability etc., and a list of design parameters (injection rate, depth etc.). No technical detail will be presented in current paper, however let us note that the number of model evaluations  $P$  depends on the total number  $N$  of input parameters of the model (uncertain and design) and the order  $d$  of the expansion, according to the combinatorial formula  $P = (N + d)! / (N!d!)$ .

We validate our proposed approach by Monte Carlo simulation in section 3.2, using a small version of the 3D benchmark study defined by Class et al.<sup>2</sup> using the DuMuX simulation soft<sup>3</sup>. Further, we apply the integrative probabilistic collocation method (IPCM) to the optimal design of a CO<sub>2</sub> injection regime based on the same scenario.

## 3 CASE STUDY: ROBUST DESIGN AND RISK ASSESSMENT FOR CO<sub>2</sub> STORAGE

### 3.1 Modelling description

We consider the 3D benchmark leakage problem of injected CO<sub>2</sub> into overlying formations through a leaky well defined by Class et al.<sup>2</sup> We consider two scenarios within the described benchmark: case 1, validation on a small test problem (section 3.2), and case 2, application to a large problem combined with the design task of finding an optimal injection regime (section 3.3). The first case study focuses on the validation of the proposed collocation approach by Monte Carlo simulation. With this in mind, we consider a small version of the benchmark problem where the simulation time is equal to 30 days, and the numerical grid is coarse (1183 nodes). This simplification is imposed by the expensive Monte Carlo approach. The second case study demonstrates our integrative approach for robust design under uncertainty on the original-size benchmark problem with a fine grid (65985 nodes) and a simulation time of up to 1000 days.

In both cases, we consider three uncertain parameters: reservoir absolute permeability, reservoir porosity and permeability of a leaky abandoned well. Their distributions were considered around the corresponding benchmark values<sup>2</sup>. The assumed probability distribution functions for the uncertain parameters. The correlation between absolute permeability and porosity was reconstructed from the U.S. National Petroleum Council Public Database (more than 1200 reservoirs), like in previous study<sup>7</sup>. For case 2, we also included two design parameters for describing the injection strategy: the CO<sub>2</sub> injection rate (fluctuating around 8.87 kg/s) and the length of the screening interval (up to 30m). The choice of the design parameters in this study is only exemplary and serves to demonstrate how engineering decision-making can be supported by the approach presented here. Both the injection rate and the length of the screening interval directly affect the ratio of forces in the reservoir during the injection.

Our model *outputs of interest* are: (a) Physical characteristics of flow: spatially distributed pressure and saturation as a function of time and the CO<sub>2</sub> leakage through the leaky well as a function of time. CO<sub>2</sub> leakage rate is defined in the benchmark study as the CO<sub>2</sub> mass flux midway between the top and bottom aquifer divided by the injection rate, in percent. (b) Stochastic characteristics of flow: mean values, variances and cumulative distribution functions of all quantities form (a).

### 3.2 Case 1: Validation on a small test problem

First, we validate the PCM method against traditional Monte Carlo simulations. We performed a Monte Carlo simulation with 1000 realizations and P simulations (see equation 2.2) for the collocation approach within the simplified benchmark problem. We repeated the comparison study for different degrees of chaos expansion, such as first order (4 samples), second order (10 samples), third order (20 samples) and fourth order (35 samples).

The strongest CO<sub>2</sub> infiltration processes occur between the injection well and the leaky well. Therefore, we show the mean values of CO<sub>2</sub> saturation after 30 days in the 2D section for  $y=0$ [m] (Figure 1). The bottom plot in Figure 1 illustrates the reference mean value which was calculated on the basis of 1000 Monte Carlo samples. The other plots were obtained by the PCM with different degrees of expansion. The most integrative characteristic of the overall process is the total leakage of CO<sub>2</sub>. Figure 2 shows the

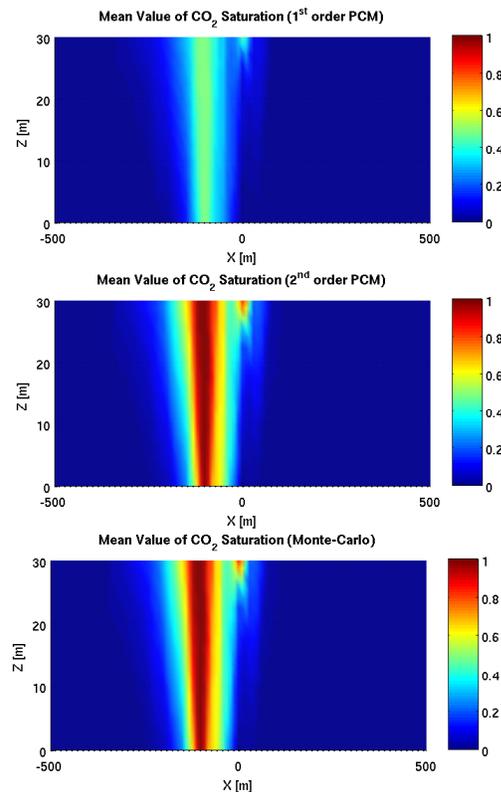


Figure 1: 2D section plot ( $y=0$ [m]) for mean value of CO<sub>2</sub> saturation

mean value and standard deviation of CO<sub>2</sub> leakage rate as functions of time, respectively. Evidently, the linear approximation is not adequate to represent the non-linear behavior of multi-phase flow. The second-order expansion shows high accuracy at very low computational costs. The higher orders of chaos expansion show even better accuracies, but the convergence is not uniform (see the third order), because of a special property of the collocation method which we will not discuss here.

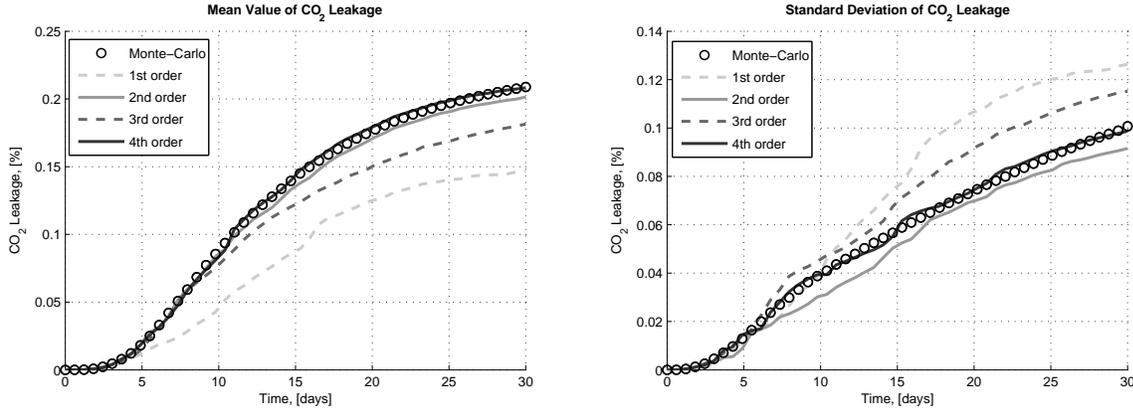


Figure 2: Mean value (left plot) and standard deviation (right plot) of CO<sub>2</sub> leakage rate

In summary, the probabilistic collocation method provides an effective tool for a probabilistic risk assessment of CO<sub>2</sub> storage; this risk assessment is based on a knowledge of probability distributions, in this case on the distribution of the parameters: porosity, reservoir permeability, permeability of leakage well. For our purposes, the second degree of expansion turned out to be sufficiently accurate and can be considered the cheapest reasonable approximation for non-linear transport processes in CO<sub>2</sub> storage.

### 3.3 Case 2: Application to a large problem and robust design of injection regimes

We now consider the original-size benchmark problem and additionally include design parameters. Using our novel IPCM conception, we construct an integrative response surface (section 2.1) of the model output in the combined 5D parametrical space (porosity, reservoir permeability, permeability of leakage well, injection rate, screening interval) and 4D physical space ( $X, Y, Z, t$ ). Figure 3 illustrates probability of unacceptable CO<sub>2</sub> leakage back to the surface and can be explored to quantify the probability of punishment actions when the CO<sub>2</sub> leakage towards the surface exceeds acceptable limits.

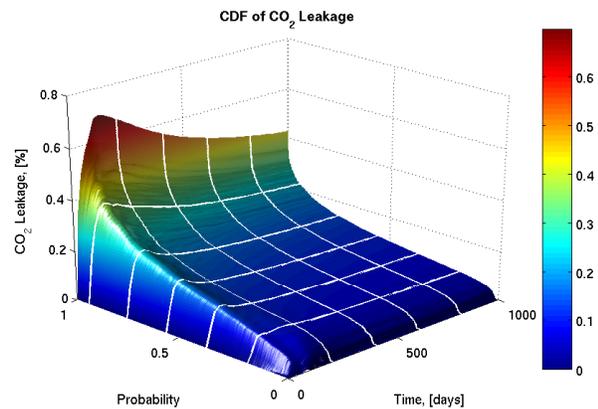


Figure 3: Time dynamics for the cumulative distribution function of CO<sub>2</sub> leakage rate

All the above results had the values of design parameters fixed to their original benchmark values when information was extracted from the integrative response surface. Figure 4 demonstrates how the injection rate and the screening interval influence the leakage rate of  $\text{CO}_2$ . An important advantage of IPCM is that parameter uncertainty is easily included in such predictions. The top surface in Figure 4 is the  $\text{CO}_2$  leakage rate expected after 100 days as a function of the design parameters, averaged over the uncertain parameters. The bottom surface in Figure 4 is the  $\text{CO}_2$  leakage rate using the expected values of the uncertain parameters, i.e. as in deterministic simulations. It is easy to see that the impact can be extremely important for non-linear systems (here, a factor of about two), especially in long-term simulations.

In a similar fashion, the dependence of the leakage probability or any other statistical characteristics on design parameters can be evaluated, so that the injection regime can be chosen according to a maximum allowable failure probability. Figure 5 illustrates the choice of design parameters based on the caprock pressure after 1000 days. In this test case, a critical caprock pressure equal to 330 bar was chosen at a significance level of 5%, i.e. the maximal acceptable probability of failure is set to 0.05 (solid black line on surface). Figure 5 demonstrates acceptable strategies of injection where the caprock pressure does not exceed the limit of 330 bar, which corresponds to an injection-induced pressure build-up of about 40 bar.

In this way, the proposed approach provides a constructive solution to the problem of robust design under uncertainty and provides valuable support for risk-informed decision making.

#### 4 Summary and conclusions

In this work, we provide a massive stochastic model reduction via the polynomial chaos expansion. We use the collocation technique to project the space and time model response surface onto a orthogonal basis of higher-order polynomials. This allows for the non-linear propagation of parameter uncertainty affecting the predicted quantities, ensures fast computation and provides a powerful tool for joining design variables and uncertain variables into one approach

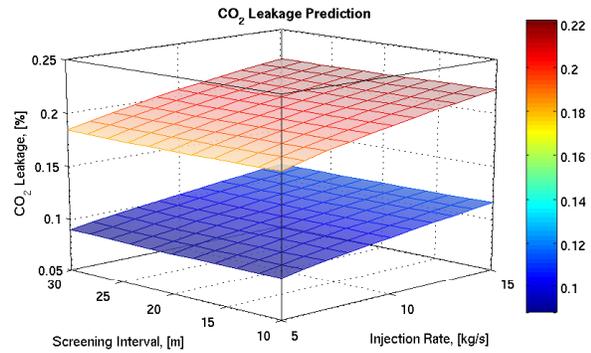


Figure 4: Influence of design parameters on prediction of  $\text{CO}_2$  leakage rate after 1000 days

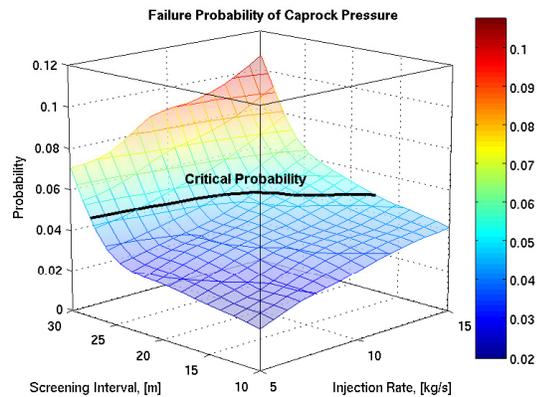


Figure 5: Choice of design parameters based on caprock pressure after 1000 days: critical pressure 330 bar at a significance level of 5 %

based on an integrative response surface in the form of an explicit polynomial expression. This offers fast evaluation for statistical quantities and their dependence on design or control parameters.

We recommend the second order of polynomial expansion as a reasonable compromise between computational effort and accuracy. The proposed stochastic approach was validated on the basis of Monte Carlo simulation using a common 3D benchmark problem. In this case study, our proposed approach yielded a significant speed-up of 100: 1000 Benchmark runs for the Monte Carlo evaluation were comparable in accuracy with 10 benchmark runs using the probabilistic collocation method.

A specific novelty is that we project all the design parameters and uncertain parameters onto one single integrative response surface. Based on this integrative concept, the design task explicitly includes uncertainty, which leads to robust designs with minimum failure probability. Thus, the integrative response surface provides a powerful tool for probabilistic prediction and robust design of non-linear systems and provides valuable support for risk-informed management decisions.

We demonstrated that neglecting parametric uncertainty constitutes a strong simplification for modeling CO<sub>2</sub> sequestration. Due to the non-linearity of CO<sub>2</sub> infiltration, including uncertainty leads to a systematic and significant shift of the predicted leakage rates (here towards higher values), affecting both risk estimates and the design of injection scenarios.

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