be considered a "black-box", i.e., commercial software can be used without any modifications required.

According to Villadsen and Michelsen (1978), the optimal choice of collocation points corresponds to the roots of the polynomial of one degree higher ($d+1$) than the order used in the chaos expansion (d). This choice adapts the position of collocation points to the involved distribution shape, and is based on the theory of Gaussian integration (e.g., Abramowitz and Stegun, 1965). For one-dimensional problems (i.e., when analyzing only one uncertain model parameter), it allows exact numerical integrations of order $2d$ given $d+1$ values of the function to be integrated.

For multi-parameter analysis, the number of available points from the corresponding Gaussian integration rule is $(d+1)^n$, which is larger than the necessary number M of collocation points. The minimum value of M is equal to the number of coefficients n_c in Expansion (2), according to Eq. (3). The full tensor grid can be used only for low-order (1st, 2nd) analysis of few parameters. For higher-order analysis of many parameters, the tensor grid suffers from the curse of dimensionality (a full tensor grid in n dimensions requires $(d+1)^n$ points, which rises exponentially in n) (Nobile et al., 2008). In that case, a smart choice of a sparse subset from the tensor grid becomes necessary. Then, PCM chooses the minimum required number of collocation points, equal to the number of coefficients n_c, from the full tensor grid according to their probability weight, i.e., according to their importance as specified by the available probability distribution of Θ. This simply means to select the collocation points from the most probable regions of the input parameter distribution (see Oladyshkin et al., 2011).

The weighted-residual method in the random space is defined as (Li and Zhang, 2007):

$$\int \left(\Gamma - \sum_{i=1}^{n_c} c_i \Pi_i(\Theta) \right) w(\Theta) p(\Theta) d\tau = 0, \quad (5)$$

where $w(\Theta)$ is the weighting function and $p(\Theta)$ is the joint probability density function of Θ. Please note that choosing $w_i = \Pi_i$ in Eq. (5) results in the method discussed by Ghanem and Spanos (1991) and Le Maî tre and Knio (2010). In PCM, the weighting function is chosen as the delta function:

$$w(\Theta) = \delta(\Theta - \Theta_c). \quad (6)$$

Θ_c is the set of collocation points. Substituting from Eq. (6) into Eq. (5) gives the following:

$$\Gamma_c - \sum_{i=1}^{n_c} c_i \Pi(\Theta_c) = 0, \quad (7)$$

where Γ_c are the response values corresponding to the collocation values Θ_c. We solve Eq. (7) to find the coefficients c_i.

Hence, in total, n_c detailed runs are required to determine the n_c unknown coefficients. The roots of the data-driven polynomial basis (see Section 2.2) define the positions of the collocation points specific to the distribution of input parameters at hand and, thus, indicate the optimal parameter sets for model evaluation, using all available information about the input parameters. In our study, we have $n=4$ uncertain parameters and we use a polynomial of degree $d=2$. This means that only $n_c=15$ detailed runs are necessary to obtain the expansion coefficients and approximate the response surface.

3. CO_2 storage problem

Here, we describe the injection scenario for which we analyze sensitivities, uncertainties, and risks in Sections 4 and 5. The same flow responses are studied here as in Ashraf et al. (2010a,b). These are CO_2 pressure, CO_2 mobile and residual volumes and leakage risk

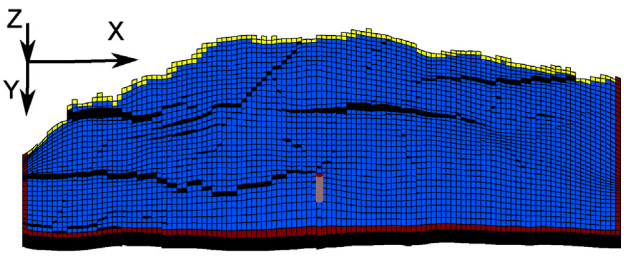

Fig. 1. Boundary conditions and the well location in the designed injection scenario. Red color corresponds to the open boundaries and yellow color shows the closed side on the crest. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

as described below. Then, we describe the uncertain parameters considered in the study followed by a discussion on the uncertain structural aspects of the considered geological settings.

3.1. Modeling scenario

A typical scenario of CO_2 injection is defined in which a volume of 40×10^6 m^3 is injected via one well during an injection period of 30 years. This volume corresponds to 20% of the total aquifer pore volume. After stopping injection, simulation continues for 70 years to study the early migration of the CO_2 plume. For brevity, we omit the detailed model equations here and refer the interested reader to Oladyshkin and Nowak (2012) and Oladyshkin et al. (2011).

In our scenario, we feature an aquifer system that is formed by shallow-marine deposits. There is one closed boundary on the top side of the model and the other sides are assumed to be open (Fig. 1). All the open boundaries are modeled as Dirichlet boundaries, two of which with hydrostatic pressure distribution (the right and bottom boundaries in Fig. 1). The remaining left boundary is also hydrostatic, but modified in order to account for the regional groundwater effect (see below).

The cells on the faces of the open boundaries are equipped with a very large pore volume multiplier, such that they numerically represent a much larger volume and effectively enlarge the domain. This helps to minimize the boundary effects of a computational domain that would otherwise be relatively small compared to the injected CO_2 volume (about 20% of the total pore volume, see above). The pore volume multiplier technique allows for a physically reasonable pressure build-up close to the boundary. Moreover, this allows the CO_2 that has left the domain to re-enter by gravity segregation after the injection has stopped.

A summary of the used parameter values is given in Table 1. The hydrological parameters like permeability and porosity vary within individual realizations due to the considered geological structure (see Fig. 2 for the histograms of porosity and permeability in one selected realization). They also differ between the different realizations, as they are changed to represent different geological features. Although the geological realizations of this model vary in some geological features, but the same total pore volume, grid, and fault

Table 1
Aquifer model information.

Parameter	Value	Unit
Number of active cells in the model	78,720	–
Resolution X, Y, Z	$40 \times 120 \times 20$	–
Scale X, Y, Z	$3000 \times 9000 \times 80$	m
Injection rate	3650	m^3/day
Initial pressure	266.5	bar
Critical CO_2 and water saturations	0.2	–
CO_2 viscosity	0.04	cp
Water viscosity	0.4	cp
Rock compressibility	0.3e−6	1/bar

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