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SENSITIVITY ANALYSIS IN NUMERICAL SIMULATION OF MULTIPHASE FLOW FOR CO_2 STORAGE IN SALINE AQUIFERS USING THE PROBABILISTIC COLLOCATION APPROACH

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Summary. Injection of CO2 in geological formations has been proposed as an effective strategy to reduce the emissions of greenhouse gases. The understanding of interactions and the design of operations at an aquifer scale require the use computationally intensive numerical simulations. These simulations require the specification of flow and transport parameters of the formation that in general are poorly known leading to uncertainty in the calculated response. Therefore it is very important to determine which of these input variables have most influence on the predictions; this is called Sensitivity Analysis (SA). In general these methodologies require multiple runs of the original model becoming computationally intensive in even simple problems. In this paper, an efficient Sensitivity Analysis using polynomial chaos expansion along with the probabilistic collocation method is used in a simple problem of the numerical simulation of injection of CO_2 in geological formations

1 Introduction

Injection of CO2 in geological formations has been proposed as an effective strategy to reduce the emissions of greenhouse gases. The CO2 is injected in the geological formation as a supercritical fluid and the understanding of its interaction with the residing brine is critical for estimation of the effectiveness of the trapping mechanisms, the design of the injection operations, the study of interactions with fresh-water aquifers and the likelihood of leakage. In general, these interactions can be studied through laboratory experiments, but at the aquifer scale, numerical simulations are in many cases the only option. These numerical simulations require the specification of flow and transport parameters of the formation as well as the geometry of the domain and boundary conditions. The lack of information about these parameters, conditions and geometry leads to uncertainty in the calculated response of the aquifer; this lead to a natural question: which input variables have most influence on the estimated response of the aquifer. This is the role of sensitivity analysis (SA)[4], and its application requires the execution of the numerical model multiple times, becoming a serious problem in the case of computational expensive models. A possible solution to this problem is the use of a metamodel that is inexpensive to evaluate but captures the dependence between the original input and the actual output. Examples of these metamodeling methodologies include non-parametric regression, artificial neural networks, gaussian processes, orthogonal polynomial bases, etc. A special class of orthogonal polynomial bases called Polynomial Chaos expansion[1,2] approximates the response of the system in terms of Generalized Fourier Series of the random input variables. The coefficients in this expansion are determined using the probabilistic collocation method (PCM)[3] that only requires deterministic model evaluation. In this paper, the PCE and PCM are used for efficient model evaluation in a SA of numerical models of multiphase flow of CO_2 in saline aquifers.

2 Efficient Sensitivity Analysis

2.1 PCE and PCM

The polynomial chaos expansion (PCE) is a series expansion used to express the dependency of a random variable on some set of orthogonal input random variables [1,2]. In general, these input random variables correspond to a set of orthogonal polynomials with respect to some probability measure or distribution. For example, in the case of a Gaussian RV the Hermite polynomials are used, or in the case of a uniform RV the Legendre polynomials can be used. In general, the polynomial chaos expansion of a random variable $Y_i(\boldsymbol{x}, t)$ (model output) is expressed as:

$$Y_i(\boldsymbol{x}, t, \xi) = \sum_{j=0}^{P} c_j(\mathbf{x}, t)\Psi_j(\xi) \tag{1}$$

where c_j are the coefficients, and $\Psi_j(\xi)$ are functions comprising the orthogonal polynomial basis. The coefficients are obtained taking advantage of the orthogonal nature of the polynomials involved[3]:

$$c_j(\boldsymbol{x}, t) = \frac{\int Y(\boldsymbol{x}, t, \xi)\Psi_j(\xi)\varphi_M(\xi)d\xi}{\int \Psi_j(\xi)\Psi_j(\xi)\varphi_M(\xi)d\xi} = \frac{\int Y(\boldsymbol{x}, t, \xi)\Psi_j(\xi)\varphi_M(\xi)d\xi}{< \Psi_j^2 >} \tag{2}$$

where $\varphi_M(\xi)$ is the PDF of the RV ξ, and the term in the denominator can be calculated analytically. In general, the integral in the numerator of equation 2 is approximated numerically and if quadrature methods are used, then the output of the model $Y()$ is required at some specific points ξ_i called *collocation points*. The number and location of these points depend on the degree of the polynomial $\Psi_j(\xi)$ and this in turn defines the number of times the model $Y()$ is evaluated. For high-dimensional problems, the number of model evaluations can be large requiring the use of specialized techniques for the integration such as sparse grids[3]. Once the coefficients in the expansion are obtained, then the moments of the RV such as the mean and variance of $Y()$ can be calculated as:

$$\begin{aligned}\overline{Y} &= c_0 \\ \sigma_Y^2 &= \sum_{j=1}^{P} c_j^2(\mathbf{x}, t) < \Psi_j^2 >\end{aligned} \tag{3}$$

2.2 Global Sensitivity Analysis (GSA)

Sensitivity analysis (SA) is defined as the determination of how *uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input*[4]. Saltelli et al. [4] have proposed and tested a methodology called variance decomposition approach to GSA which assumes a generic model $g(\boldsymbol{Z})$ can be decomposed as:

$$\begin{aligned}g(\boldsymbol{Z}) = g_0 &+ \sum_{i=1}^{n} g_i(Z_i) + \sum_{i<j} g_{i,j}(Z_i, Z_j) + \ldots \\ &+ \sum_{i<j<k} g_{i,j,k}(Z_i, Z_j, Z_k) + \ldots + g_{1,2,\ldots,n}(Z_1, Z_2, \ldots, Z_n)\end{aligned} \tag{4}$$

where each one of the $g_{i,\ldots}$ are orthogonal components. This decomposition is unique only when the input variables are independent and is called the Sobol decomposition[6]. Given the independence of each component in the decomposition in equation 4, the variance of the model output is given by:

$$V[Y] = \sum_{i=1}^{n} V_i + \sum_{i<j} V_{i,j} + \sum_{i<j<k} V_{i,j,k} + \ldots + V_{1,2,\ldots,n} \tag{5}$$

and from this, two importance measures are defined:

- First order index: fraction of variance associated with Z_i alone, which can be interpreted as the highest expected reduction in variance when fixing Z_i.

$$S1_i = \frac{V[Y|Z_i]}{V[Y]} = \frac{V[E[Y|Z_i]]}{V[Y]} \tag{6}$$

  This measure can be easily estimated fixing the values of the input variable Z_i using a Monte Carlo Simulation approach.

- Total effect index: this is a measure of total contribution of the factor Z_i to the output including first order and all higher order effects and it gives information about the non-additive effects of the model (i.e. interactions).

$$ST_i = \frac{S1_i + \sum_j S2_{ij} + \sum_{j,k} S3_{i,j,k} + \dots}{V[Y]} = 1 - \frac{V[E[Y|Z_{\sim i}]]}{V[Y]} \qquad (7)$$

where $Z_{\sim i}$ indicates fixing all input variables Z_j except variable i. Again this measure can be estimated using Monte Carlo Simulation.

2.3 Sensitivity Analysis using PCE and PCM

There are two ways to obtain the sensitivity indices or importance measures using the PCE with PCM:

1. Monte Carlo simulation using the original model and the application of definitions given by equations 6 and 7.
2. Analytically using the variances for the terms of a meta-model (such as results of the Polynomial Chaos Expansion, see equation 3)

In this paper, the second approach is followed due to computational efficiency and it depends on the expansion given in equation 4. The Sobol decomposition of the model output is dependent on the input variables $\boldsymbol{Z}$ and these variables can be expressed in terms of the random seeds $\boldsymbol{\xi}$. This implies that the PC expansion of the model output can be defined as:

$$g_{\mathrm{PC}}(\boldsymbol{x}, t, \xi) = g_0 + \sum_{i=1}^{n} \sum_{\boldsymbol{\alpha} \in \Im_i} g_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\xi_i) + \sum_{1 \le i1 \le i2 \le n} \sum_{\boldsymbol{\alpha} \in \Im_{i1,i2}} g_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\xi_{i1}, \xi_{i2}) \qquad (8)$$

where $\Im_{(\cdot)}$ is the set of valid indexes for each one of the terms where the each one of the is variable appear:

$$\Im_{i1,i2,\dots,is} = \left\{ \boldsymbol{\alpha} : \begin{array}{ll} \alpha_k > 0 & k \in \{i1, i2, \dots, is\} \\ \alpha_k = 0 & k \notin \{i1, i2, \dots, is\} \end{array} \right\} \qquad (9)$$

The variance of the PC expansion can be obtained using equation 3, and therefore the single effect index can be estimated as:

$$S1_i = \frac{\sum_{\boldsymbol{\alpha} \in \Im_{i1,\dots,im}} c_{\boldsymbol{\alpha}}^2 < \Psi_{\boldsymbol{\alpha}}^2 >}{\sum_{k=1}^{P} c_k^2 < \Psi_k^2 >} \qquad (10)$$

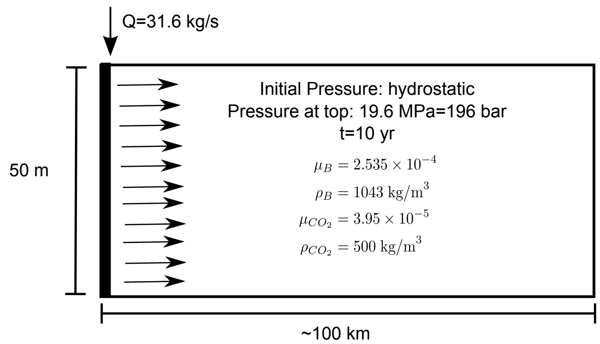

Figure 1: Schematic diagram of the model considered in this problem

where the numerator is the variance of the terms involving only the single variables ξ_i (and hence the variables Z_i), and the denominator is the total variance of the output $g(\cdot)$. The same procedure is used to estimate all $S2_{i,j}, S3_{i,j,k}$ and so on to obtain a numerical approximation of ST_i.

3 Test case

This section gives the definition of the test case for the application of the SA methodology. In this problem, CO_2 is injected in a saline aquifer displacing brine with the corresponding development of a CO_2 plume and an increase in total pressure. A graphical depiction of the problem is given in figure 1. The domain has a lateral extension of 100 km with a constant thickness of 50 m. A radial 1D model is used with 450 cells defined in logarithmic increments from the injection well. The injection well is assumed fully penetrating.

The initial pressure distribution is assumed constant with a value of 20 MPa and temperature of 50 C degrees, typical conditions of a saline aquifer at 2000 m in depth. The lateral boundary condition is assumed dirichlet, while the top and bottom are non-flow boundaries. The injection rate of CO_2 is of 31.6 kg/s (equivalent to 1 Mton CO_2/year). The injection is maintained for 10 years. The random input variables are the hydraulic properties of the aquifer and the residual saturation of brine and their properties are shown in table 1. The output of interest are the formation pressure and the saturation profile. of CO_2 at 10 years after the injection started. The saturation profile can be used to define the position of the plume front and therefore its lateral extent. All the numerical simulations were done using TOUGH2[8] with the equation of state specified in the ECO2N module[9].

Parameter	**Distribution**	PDF Parameters
φ Porosity	Lognormal	$\mu_\varphi = 0.1, \sigma_\varphi = 0.25$
k Permeability	Lognormal	$\mu_k = 10^{-12}\ m^2\ , \sigma_k = 10^{-12}\ \ m^2$
S_B^{RES} Residual satutation of brine	Uniform	$S_{low} = 10^{-4}, S_{up} = 0.25$
ceff Rock compressibility	Uniform	$\text{ceff}_{low} = 5 \times 10^{-11} Pa^{-1}, \text{ceff}_{up} = 5 \times 10^{-9}\ \ Pa^{-1}$

Table 1: Distribution types and parameters *assumed* for the input variables of the problem of the injection of CO_2 in a saline aquifer

4 Results

The estimation of the PCE of the input RVs require a transformation from the original PDFs to uniform PDFs using the quantile transformation and the use of the Legendre polynomials of 3th order. Figure 2 shows the typical results for the position of the plume front and formation pressure after 10 years of injection. The results of the SA are shown in Figure 3.

The results of the SA for the saturation of CO_2 are shown in figure 3a, in which three different regions can be identified:

1. Injection front (0-50m): Permeability and its interactions with other variables are the influential variables for saturation of CO2 in this area. This suggests that saturation is controlled by the flow of CO2 injected at the well.

2. Displacement Area 1 (50-80m): this is area for the maximum extention of injection front. Porosity and its interactions are influential for saturation indicating that CO2 is quasi-static and the horizontal flow is not longer an active process in this area.

3. Buoyancy Area (80-950m): Residual saturation of brine is the influential variable in saturation of CO2 indicating that capillarity effects are dominant. In this region the dominant flow process is the vertical movement of CO2 due to buoyancy.

4. Displacement area 2 (950-2000m): This area shows the maximum extension of the CO2 plume. Porosity and its interactions are the influential variables of saturation of CO2. Again, the CO2 is static and horizontal flow of CO2 is not longer active.

The SA for the Pressure shows a variation in importance in four different regions (figure 3b):

1. Plume zone(0-950m): Permeability and its interactions are the influential variables in the pressure response of the aquifer, suggesting that flow of CO2 is the controlling factor.

2. Transition zone 1 (950-2000m): This zone marks the maximum extent of the CO_2 plume, and shows a slight increase in the importance of the porosity and its interactions (similar to the saturation of CO_2).

3. Transition zone 2 (2 km -30 km): The pressure response in this area is controlled by is a smooth decrease of the importance of Permeability/interactions with an increase in the importance of the compressibility. In this area, the pressure disturbance created by the injection of the CO_2 still has some observable effect.

4. Unaffected zone (from 30 km to the boundary of the model). This is the zone with brine where original aquifer conditions are present. The interactions of the compressibility and other variables are influential in the pressure response in this area as expected.

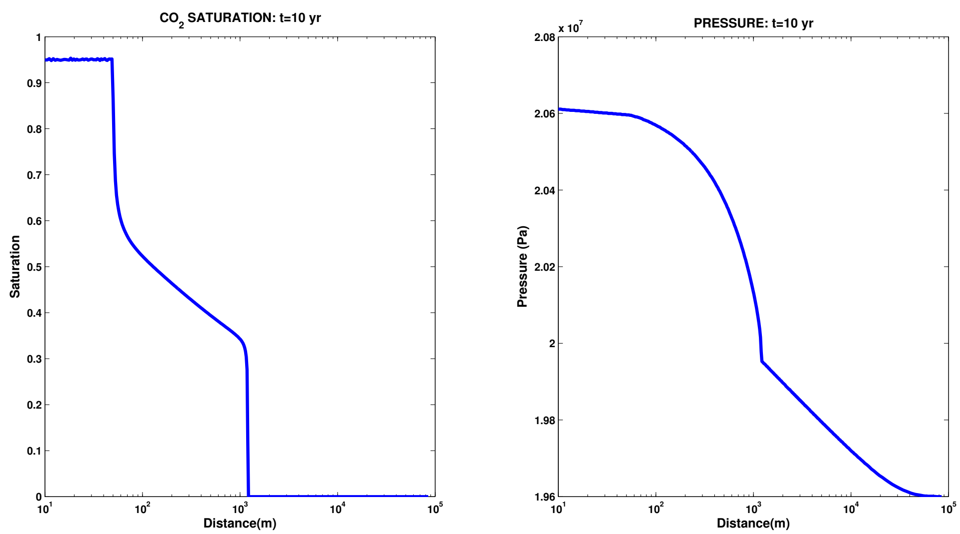

Figure 2: Typical results for saturation profile of CO_2 and formation pressure after 10 yrs of injection.

5 Preliminary conclusions

The combination of the polynomial chaos expansion (PCE) and probabilistic collocation method (PCM) allowed an efficient sensitivity analysis (SA) of a numerical model of the pressure response and position of the plume front due to injection of CO_2 in a saline aquifer. The variance decomposition approach to SA identified the regions in which permeability porosity and residual saturation of brine are the influential variables for saturation of CO_2. The variation in pressure is driven by the variability in absolute permeability combined with interactions with other variables, and the interactions of rock compressibility beyond 30 km from the injection well.

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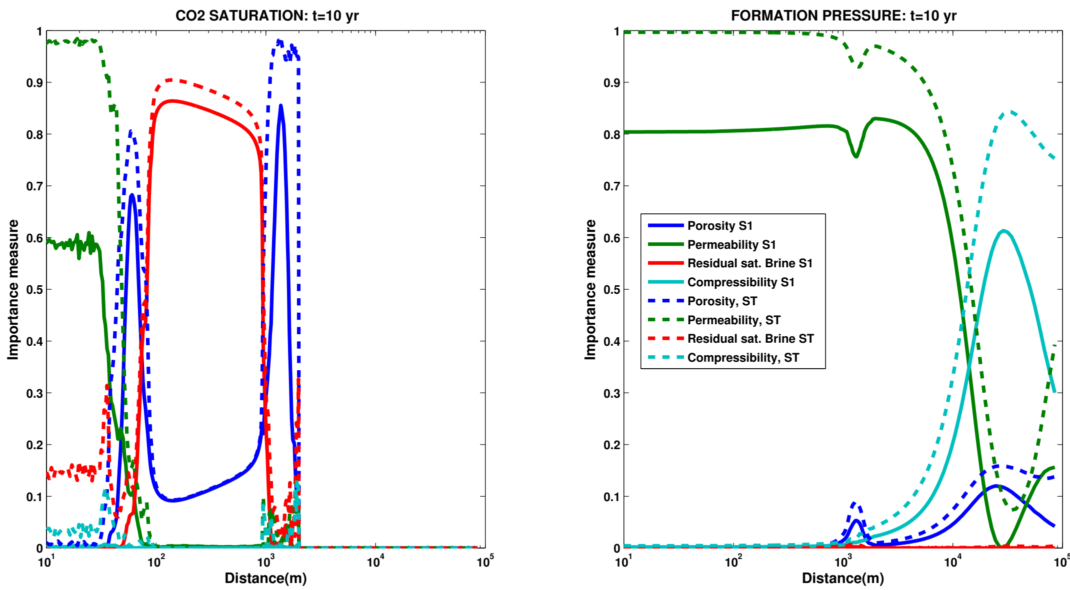

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