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Global sensitivity analysis of the impact of impurities on CO_2 pipeline failure

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ABSTRACT

This paper describes the testing, comparison and application of global sensitivity techniques for the study of the impact of the stream impurities on CO_2 pipeline failure. Global sensitivity analysis through non-intrusive generalised polynomial chaos expansion with sparse grids is compared to more common techniques and is found to achieve superior convergence rate to crude Monte Carlo, quasi-Monte Carlo and EFAST for functions with up to a moderate level of "roughness". This methodology is then applied to the hypothetical full bore rupture of a 1 km CO_2 pipeline at 150 bara and 283.15 K. The sensitivity of the ensuing outflow to the composition of a quaternary mixture of CO_2 with N_2, CH_4 and O_2 as representative stream impurities. The results indicate that the outflow rate is highly sensitive to the composition during the early stages of depressurisation, where the effect of the impurities on phase equilibria has a significant impact on the outflow.

1. Introduction

As part of the carbon capture and sequestration (CCS) chain, pressurised pipelines are considered to be the most practical and efficient means for transportation of the large amounts of CO_2 captured from fossil fuel power plants for subsequent sequestration [22]. It is inevitable that such pipelines will cover distances of several hundreds of kilometres, possibly at line pressures above 100 bar. Given that CO_2 gas is an asphyxiant at concentrations higher than 7% [25], the safety of CO_2 pipelines is of paramount importance and indeed pivotal to the public acceptability of CCS as a viable means for tackling the impact of global warming [22].

The outflow and its variation with time following pipeline failure dictates the resulting atmospheric dispersion of the escaping inventory, an example of which can be observed in Fig. 1. These data govern all the consequences associated with the pipeline failure, including minimum safe distances to populated areas and emergency response planning.

Naturally a great deal of uncertainty is present due to the many possible circumstances in which a failure occurs including failure type, i.e. puncture or full bore rupture, initial failure pressure and temperature and variations in the captured stream composition due to fluid stream sources based on differing capture methods (i.e. pre-combustion, post-combustion or oxyfuel) [12] and post-capture processing. The use of predictive models to examine the sensitivity of the consequences of pipeline failure to these variations is standard within a quantitative risk assessment [23]. Such an analysis is often conducted using a one-factor-at-a-time (OAT) methodology [23,47], but as discussed by Saltelli and Annoni [35] this technique assumes an underlying linear behaviour, which is unlikely to be the case in such complex systems. To avoid such an assumption about the underlying model, a global sensitivity analysis (GSA) is required.

GSA is concerned with quantifying how the variation in the model's output depends on different sources of variation over the entire parameter space, here treated as random input data, by providing quantitative importance measures that relate the variance of the output with each input variable. This form of analysis of model sensitivity has been applied to parts of the CCS chain, to the geological storage of CO_2 by Kovscek and Wang [24] where the effect of porosity and permeability on reservoir performance was assessed, and widely applied in environmental engineering. For example, Cea et al. [10] studied the effects of aleatoric and epistemic uncertainty on a water quality model for evaluating biological pollutant concentration.

Given the complexity of the fluid and thermodynamic behaviour of the flow following a pipeline failure, substantial resources are required for its computation [28], and as a result, the application of GSA has been considered impractical. However, the success of recent work [6,28] to decrease the computational expense of each simulation enables one to calculate the total sensitivities.

In this work GSA is applied using a sensitivity measure proposed by Sobol' [41] to gain a better understanding of the effect of impurities on the outflow following pipeline failure.

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Fig. 1. CO_2 outflow and dispersion during pipeline decompression courtesy of Dalian University.

The Sobol' method is related to analysis of variance (ANOVA) and decomposes the model variation into a number of effects that represent the influence of each input, represented by a probability distribution, and their interactions. Many methods have been proposed to compute the integrals required to calculate these effects, of these the most widely applied are Monte Carlo sampling and the Extended Fourier Amplitude Sensitivity Test (EFAST) [30]. These approaches usually require large sample sizes to provide accurate estimations of the sensitivities, making them impractical when the underlying model is computationally expensive.

Sudret [44] proposed a procedure for the computation of the Sobol' sensitivity measures through the approximation of the model's output by a polynomial expansion, known as generalised polynomial chaos (gPC) [19]. The gPC expansion is a linear combination of suitable global polynomial approximations in probability space, for which the statistical moments, expected value and variance, are known *exactly* from the coefficients of the expansion (see also [13,16]). The family of orthonormal mono-dimensional polynomials is selected in accordance with the general Askey scheme [50] with respect to the probability measure of each random input variable. The gPC expansion may be constructed intrusively by a Galerkin projection reformulation of the underlying problem or through non-intrusive approaches such as projection and regression (see [5,45]).

In recent years stochastic collocation [4,49] has been applied to build *sparse* gPC expansions on tensor grids for high dimensional random input data (see e.g. [9]), to mitigate the so-called "Curse of Dimensionality". This method constructs an approximative function that is a sum of Lagrangian interpolants on a set of points, which is known as a *sparse grid* (see [8]) (originally introduced by Smolyak [39] for multi-dimensional integration). The approximative function can be converted into the form of a gPC expansion. Formaggia et al. [18] applied GSA with gPC expansion derived from the stochastic collocation method to a basin-scale geochemical compaction model and advocated its applicability to models subject to high dimensional random input data. This sparse gPC expansion potentially requires far fewer function evaluations than the other methods identified above, meaning that the use of GSA for complex numerical models, such as that required for modelling the discharge following pipeline failure, may be tractable.

The paper is organised as follows. Section 2 presents a review of a particular decomposition of a multi-variate function (Section 2.2). It is then shown how this expansion is used to define the Sobol' sensitivity indices (Section 2.3) and a number of common methods (i.e. Monte Carlo, EFAST and gPC) for calculating the Sobol' indices are presented. These methodologies are then tested against two benchmark test functions, and a family of test functions constructed to investigate the robustness of gPC (Section 2.4). The test functions constructed exhibit near discontinuous behaviour, and further difficulty is induced with additive artificial white noise. In Section 3 the most efficient of these techniques, in terms of convergence per number of function evaluations, is applied to a pipeline failure scenario. An extensively validated pipeline decompression model is presented in Section 3.1, while the uncertainty in the likely composition of a CO_2 stream is discussed in Section 3.2. Firstly, Monte Carlo simulation is used to estimate the outcome probability distribution and perform a crude sensitivity analysis with scatter plotting. The final analysis serves as a framework for future work on consequence analysis for pipeline failure under uncertainty. Finally conclusions resulting from this work are drawn in Section 4.

2. Global sensitivity analysis

2.1. Probabilistic formulation

Let $\mathbf{y}(\omega)=(y_1(\omega),y_2(\omega),\ldots,y_n(\omega),\ldots,y_N(\omega)):\Omega\rightarrow\mathbb{R}^N$ represent N independent and identically distributed (i.i.d.) random variables, $\Gamma_n\subseteq\mathbb{R}$ the image set of the random variable y_n, and $\Gamma=\prod_{n=1}^{N}\Gamma_n$. Hence the joint probability distribution function $\rho:\Gamma\rightarrow\mathbb{R}$ of $\mathbf{y}$ can be factorised as $\rho(\mathbf{y})=\Pi_{n=1}^{N}\rho(y_n)$, where $\rho(y_n)$ is the marginal probability distribution function of y_n. Let $(\Gamma,\mathrm{B}(\Gamma),\rho(\mathbf{y})\,\mathrm{d}\mathbf{y})$, where $\mathrm{B}(\Gamma)$ is the Borel σ-algebra on Γ, and $\rho(\mathbf{y})\,\mathrm{d}\mathbf{y}$ is the probability distribution measure of $\mathbf{y}$ on Γ. $L^2_\rho(\Gamma)$ denotes the Hilbert space consisting of square integrable functions on Γ with respect to the measure $\rho(\mathbf{y})\,\mathrm{d}\mathbf{y}$.

2.2. Functional ANOVA representation

A function $u\in L^2_\rho(\Gamma)$ can be expanded as a functional ANOVA decomposition

$$u(\mathbf{y})=u_{\mathbf{0}}+\sum_{\mathbf{j}\subseteq\mathcal{J}}u_{\mathbf{j}}(\mathbf{y}_{\mathbf{j}}), \tag{1}$$

for which $\mathbf{y}_{\mathbf{j}}=(y_{j_1},y_{j_2},\ldots,y_{j_{|\mathbf{j}|}})$ is a vector including the components of $\mathbf{y}$ indexed by $\mathbf{j}$, where $\mathbf{j}$ represents a non-empty subset of the coordinate indices $\mathcal{J}=\{1,\ldots,N\}$ with cardinality denoted by $|\mathbf{j}|$. For example, for $\mathbf{j}=\{2,3\}$ and $\{1,3,4\}$, $|\mathbf{j}|=2$ and 3, respectively. Let $\Gamma^{\mathbf{j}}$ denote the $|\mathbf{j}|$-dimensional hyper-rectangle defined as the projection of the N-dimensional Γ onto the hyper-rectangle indexed by $\mathbf{j}$. The ANOVA representation allows one to distinguish between first order effects, low-order interdependence, and high-order interaction. The summands $u_{\mathbf{j}}(\mathbf{y}_{\mathbf{j}})$ can be calculated recursively as follows:

$$u_{\mathbf{0}}=\int_{\Gamma^N}u(\mathbf{y})\rho(\mathbf{y})\,\mathrm{d}\mathbf{y} \tag{2}$$

and

$$u_{\mathbf{j}}(\mathbf{y}_{\mathbf{j}})=\int_{\Gamma^{N-|\mathbf{j}|}}u(\mathbf{y})\rho(\mathbf{y}_{\sim\mathbf{j}})\,\mathrm{d}\mathbf{y}_{\sim\mathbf{j}}-\sum_{\mathbf{k}\subset\mathbf{j}}u_{\mathbf{k}}(\mathbf{y}_{\mathbf{k}})-u_{\mathbf{0}}. \tag{3}$$

The measure $\rho(\mathbf{y}_{\sim\mathbf{j}})\,\mathrm{d}\mathbf{y}_{\sim\mathbf{j}}$ represents the integration over $\Gamma^{\sim\mathbf{j}}$. The ANOVA expansion is an exact projection of u with respect to the $L^2_\rho(\Gamma)$-inner product onto the mutually orthogonal $u_{\mathbf{j}}$, $\mathbf{j}\subseteq\mathcal{J}$, that is,

$$\int_\Gamma u_{\mathbf{j}}(\mathbf{y}_{\mathbf{j}})u_{\mathbf{k}}(\mathbf{y}_{\mathbf{k}})\rho(\mathbf{y})\,\mathrm{d}\mathbf{y}=\delta_{\mathbf{jk}}, \tag{4}$$