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GRS

Comparison of two metamodeling approaches for sensitivity analysis of a geological disposal model

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Motivation

- Comparison of the RS-HDMR and BSPCE metamodeling approaches on the basis of higher order indices

Outline of the Presentation

- Introduction
- Metamodelling Approaches
  - RS-HDMR
  - BSPCE
- Repository Models
  - LILW Test Case
- Results
  - LILW6 Model
    - SI1
    - SIT
    - R^2
  - LILW11 and LILW20 Models
- Summary and Conclusions

Introduction

- Advanced methods of global sensitivity analysis can identify both individual effects of model parameters and parameter interactions by computing Sobol' sensitivity indices
- Better understanding of parameter interactions may help to better quantify uncertainties of repository models, which can behave in a highly non-linear, non-monotonic or even discontinuous manner
- Sensitivity indices may efficiently be estimated by the Random-Sampling High Dimensional Model Representation (RS-HDMR) and Bayesian Sparse PCE (BSPCE) metamodeling approaches
- The RS-HDMR approach also belongs to a wider class of methods known as polynomial chaos expansion (PCE)
- PCE methods are based on Wiener’s homogeneous chaos theory published in 1938
- PCE is a widely used approach in metamodeling

Random Sampling - High Dimensional Model Representation (RS-HDMR)

A metamodel can be built using HDMR considering only low order terms in the ANOVA decomposition. Typically these terms are dominant in ANOVA.

$$f(t,x) \approx h(t,x) = f_0 + \sum_{i=1}^{d} f_i\,(t,x_i) + \sum_{i}\sum_{j>i} f_{ij}\left(t,x_i,x_j\right)$$

x is a vector of independent input variables
f(t,x) is integrable

Decomposition using a complete basis set of orthonormal polynomials results in:

$$f_i(t,x_i) = \sum_{r=1}^{\infty} \alpha_r^i(t)\varphi_r\,(t,x_i)$$

$$f_{ij}\left(x_i,x_j\right) = \sum_{p=1}^{\infty}\sum_{q=1}^{\infty} \beta_{pq}^{ij}(t)\varphi_{pq}\left(t,x_i,x_j\right)$$

$\varphi_r(t,x_i), \varphi_{pq}(t,x_i,x_j)$:
Sets of 1D/2D basis functions

$\alpha_r^i(t), \beta_{pq}^{ij}(t)$:
Coefficients of decomposition

From the orthogonality of the basis functions it follows that

$$\alpha_r^i(t) = \int_0^1 f_i(t,x_i)\varphi_r(t,x_i)dx_i \qquad r = 1, \dots, k$$

$$\beta_{pq}^{ij}(t) = \int_0^1\int_0^1 f_i(t,x_i)\varphi_p(t,x_i)\varphi_q(t,x_j)dx_i dx_j \qquad p = 1, \dots, l, q = 1, \dots, l'$$

Random Sampling - High Dimensional Model Representation (RS-HDMR)

For practical purposes the summation in

$$f_i(t, x_i) = \sum_{r=1}^{\infty} \alpha_r^i(t)\varphi_r(t, x_i)$$

$$f_{ij}(x_i, x_j) = \sum_{p=1}^{\infty}\sum_{q=1}^{\infty} \beta_{pq}^{ij}(t)\varphi_{pq}(t, x_i, x_j)$$

limited to some maximum orders *k, l, l'*

$$f_i(t, x_i) \approx \sum_{r=1}^{k} \alpha_r^i(t)\varphi_r(t, x_i)$$

$$f_{ij}(t, x_i, x_j) \approx \sum_{p=1}^{l}\sum_{q=1}^{l'} \beta_{pq}^{ij}(t)\varphi_p(t, x_i)\varphi_q(t, x_j)$$

Coefficients of the decomposition can be used to evaluate Sobol' sensitivity indices as:

$$SI1 = \hat{S}_i(t) \approx \frac{\int_0^t V_i(t')\,dt'}{\int_0^t V(t')\,dt'} \approx \frac{\int_0^t \sum_{r=1}^{k}(\alpha_r^i(t'))^2 dt'}{\int_0^t V(t')\,dt'}$$

First

$$SI2 = \hat{S}_{ij}(t) \approx \frac{\int_0^t (\sum_{p=1}^{l}\sum_{q=1}^{l'}(\beta_{pq}^{ij}(t'))^2)dt'}{\int_0^t V(t')\,dt'}$$

Second

SIT = $\hat{S}_i^T(t) \sim \hat{S}_i(t) + \sum_{j\neq i}\hat{S}_{ij}(t)$

Total

Bayesian Sparse Polynomial Chaos Expansion Method (BSPCE)

↓ More efficient?!?

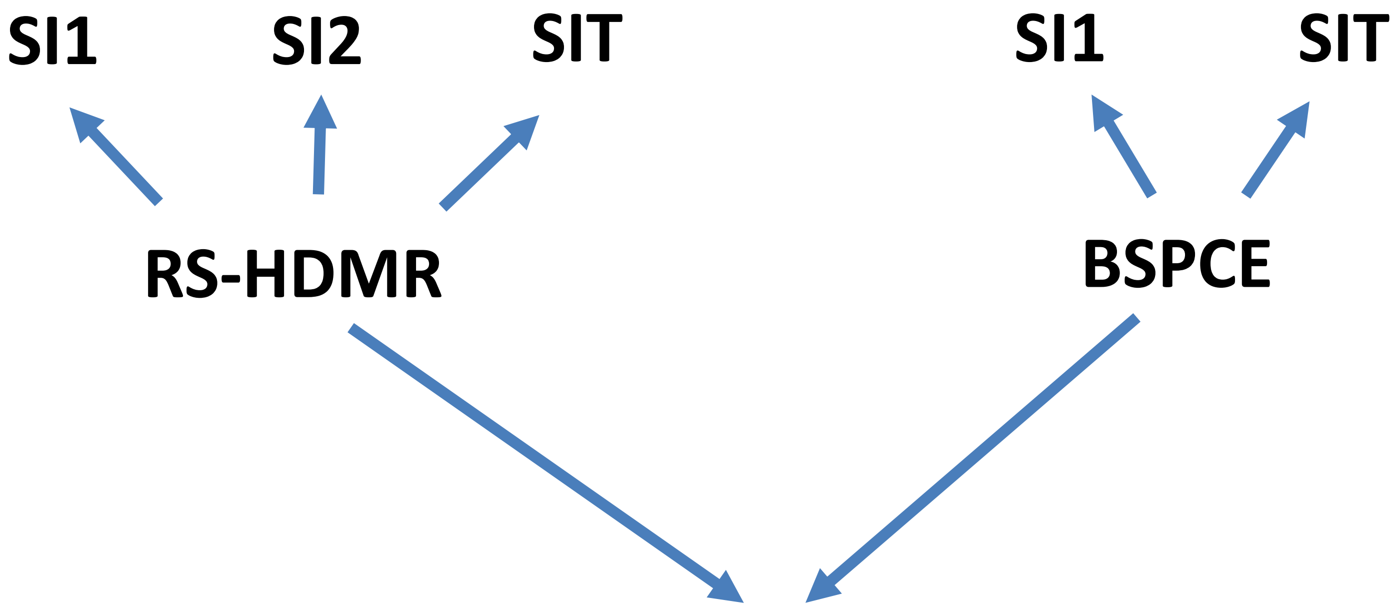
Usually only a few terms are relevant in the PCE structure

↓

The Bayesian Sparse PCE method (BSPCE) makes use of sparse PCE

Selection of the proposed PCE structure is based on a Bayesian approach using the Kashyap information criterion for model selection

RS-HDMR and BSPCE



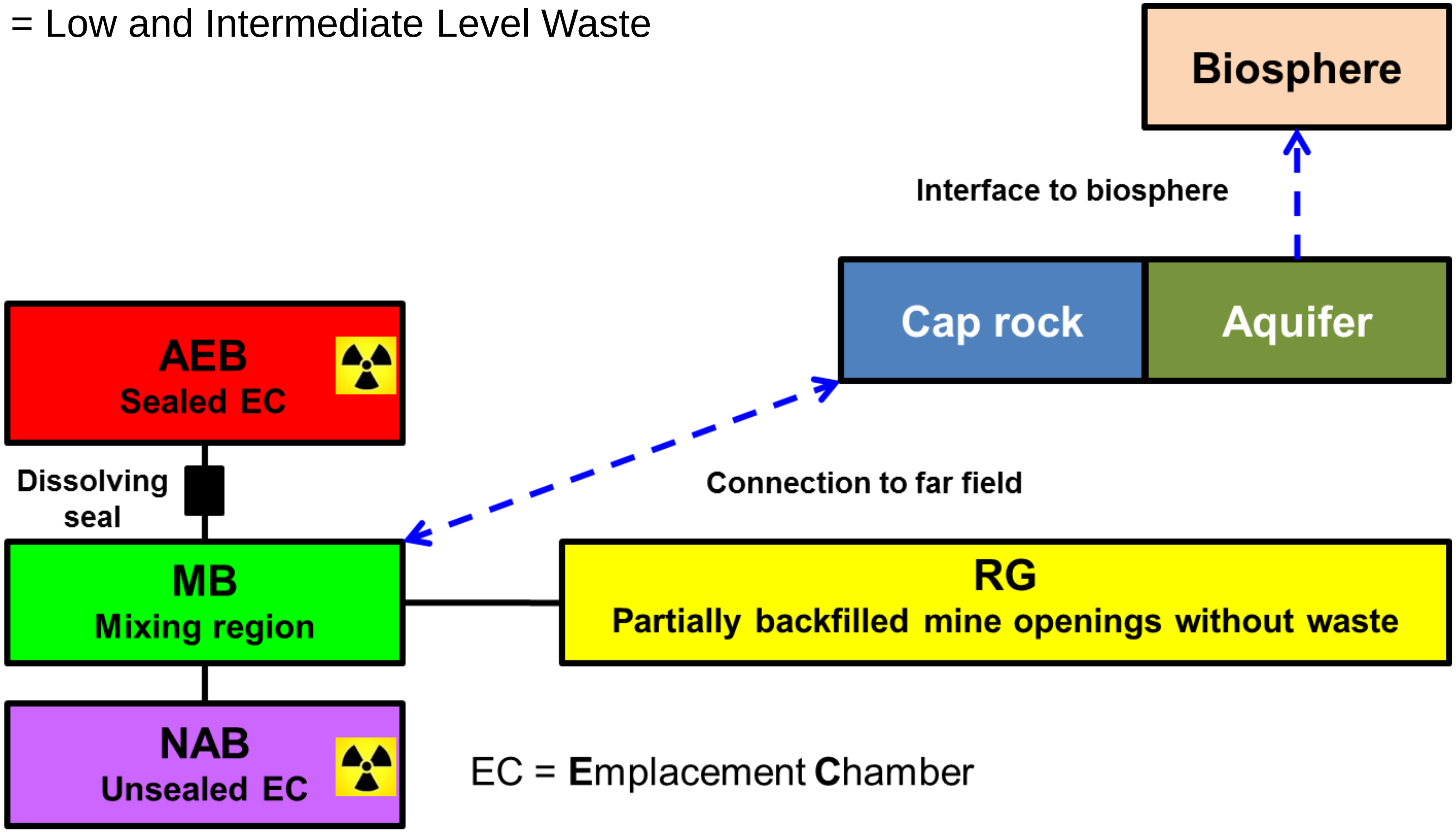
SobolGSA software package

http://www.imperial.ac.uk/process-systems-engineering/research/free-software/sobolgsa-software/

Generic PA Testmodel

Based upon real LILW repository in an abandoned salt mine
Near field model: substantially simplified structure

LILW = Low and Intermediate Level Waste



EC = **E**mplacement **C**hamber

Model Parameters

LILW6 Model

Parameter	Unit	Description	Distribution Type	Minimum μ(1) Peak(3)	Maximum σ(2)
IniPermSeal	$[m^2]$	Initial permeability of dissolving seal	Normal	$3.23 \cdot 10^{-21}$ 41.0605(1)	$6.7 \cdot 10^{-16}$ 1.9809(2)
AEBConv	[-]	Factor of local convergence variation in the sealed emplacement chamber	Log uniform	0.05	5
GasEntryP	[MPa]	Gas entry pressure	Uniform	0	2.5
GasCorrPE	[1/yr]	Corrosion rate of organics	Log normal	10^{-7} -12.6642(1)	10^{-4} 1.1177(2)
RefConv	[1/yr]	Reference convergence rate	Log uniform	10^{-5}	10^{-4}
TBrine	[yr]	Brine intrusion time	Log normal	848.4 8.8857(1)	61573 0.6933(2)

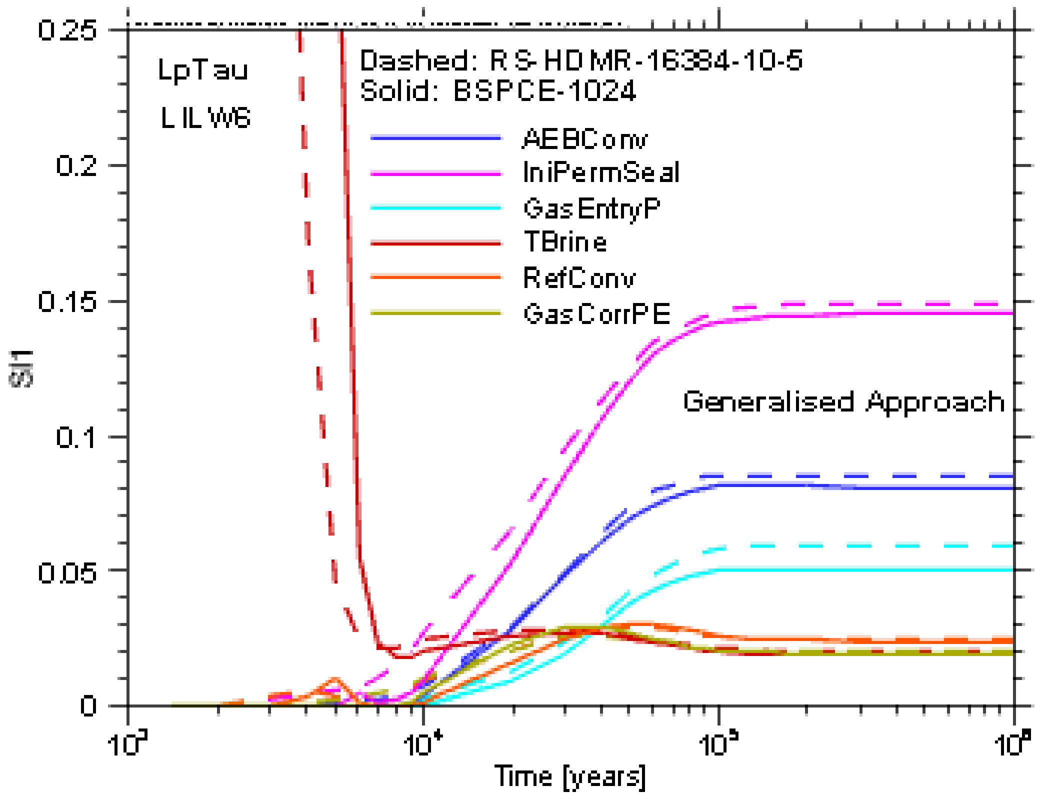
(1) μ value(*)
(2) σ value with quantiles of 0.001 and 0.999(*)
(*) μ and σ values describe mean value and standard deviation of a normal or lognormal distribution

LILW11 and LILW20 Models

LILW11 model = LILW6 model + 5 additional parameters
LILW20 model = LILW11 model + 9 additional parameters

SI1 Results – LILW6 Model

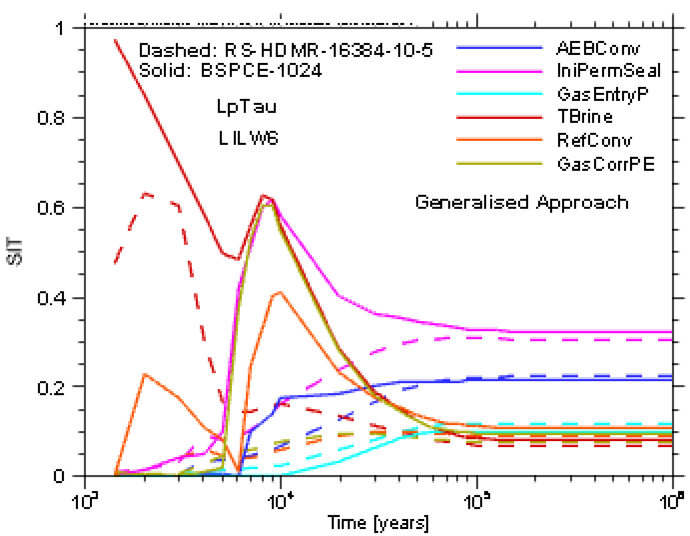
Good agreement of the SI1 results obtained from the BSPCE approach with the ones from the RS-HDMR approach with optimal choice of polynomial coefficients and 16384 runs can already be obtained with 1024 runs



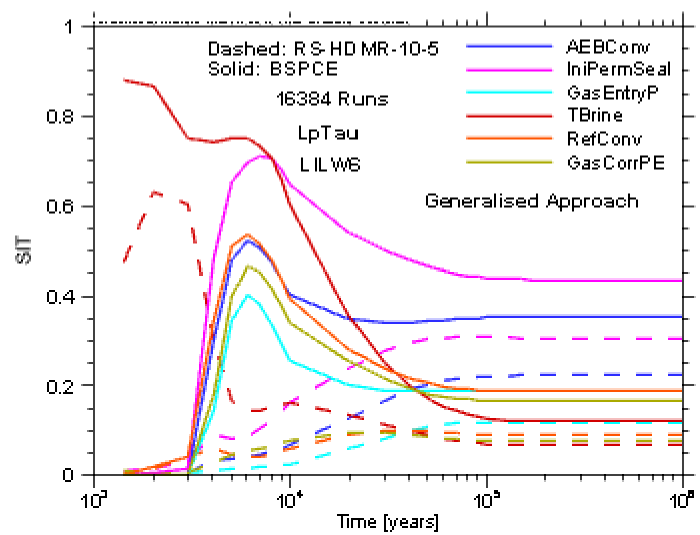
SIT Results – LILW6 Model

While SI1 indices for both approaches agree well starting from 1024 runs, there are increasing differences in the SIT indices obtained from the BSPCE approach for sets with more than 1024 runs

➔ Interaction effects higher than second order in the systems ?!?



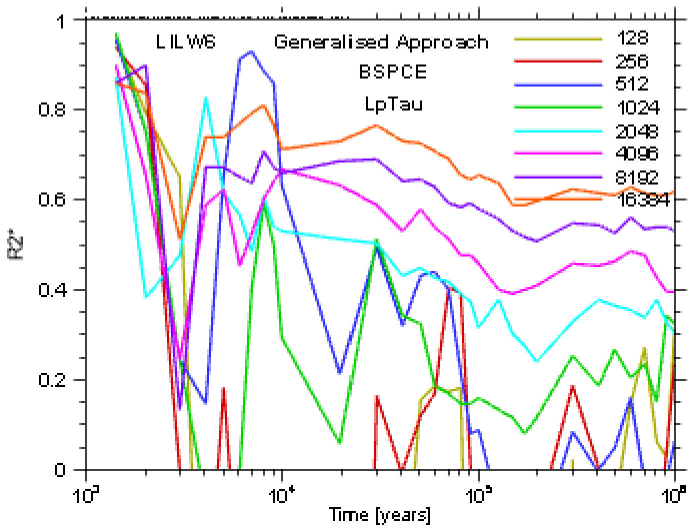
1024 runs



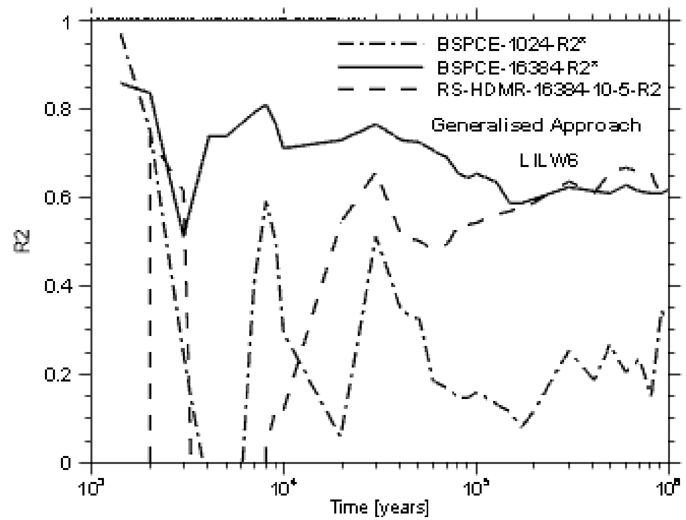
16384 runs

Results – Metamodel Error (R^2) - LILW6 Model

R^2 obtained from the BSPCE approach increases with increasing number of runs



Different sets of runs

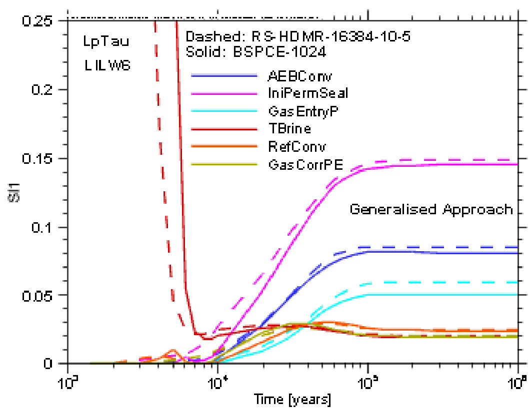


1024 versus 16384 runs

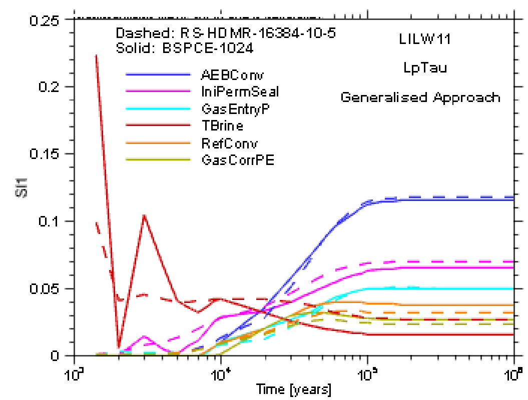
SI1 Results – LILW11 and LILW20 Models

As for the LIW6 model, good agreement of the SI1 results obtained from the BSPCE approach with the RS-HDMR approach with optimal choice of polynomial coefficients and 16384 runs can already be obtained with 1024 runs for the LILW11 and LILW20 models as well

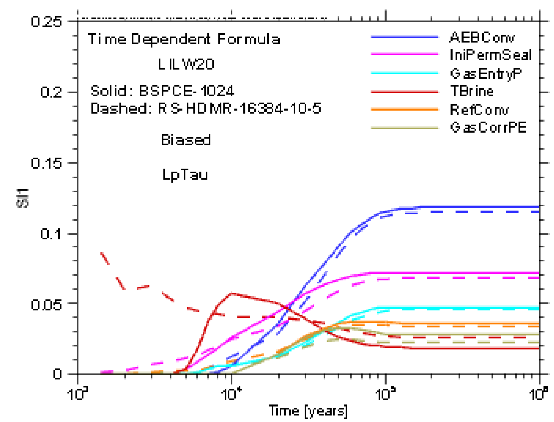
BSPCE: 1024 runs



LILW6



LILW11

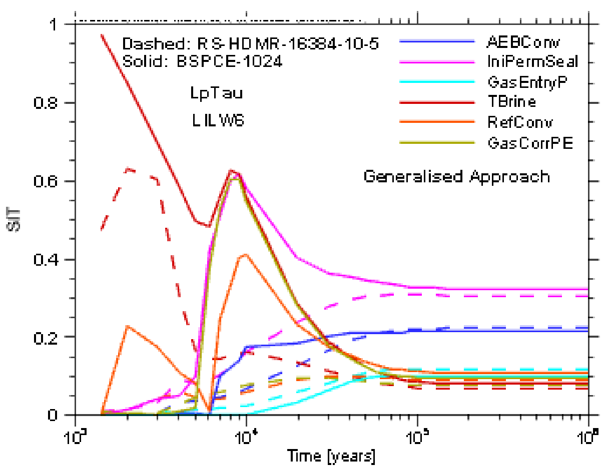


LILW20

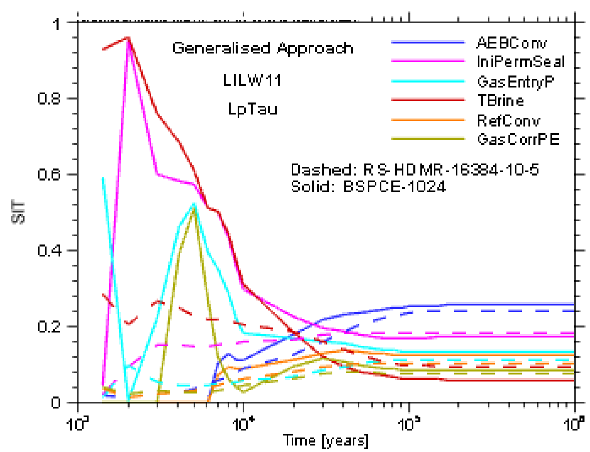
SIT Results – LILW11 and LILW20 Models

As for the LIW6 model, good agreeing SIT results of the BSPCE approach with the RS-HDMR approach with optimal choice of polynomial coefficients and 16384 runs can already be obtained with 1024 runs

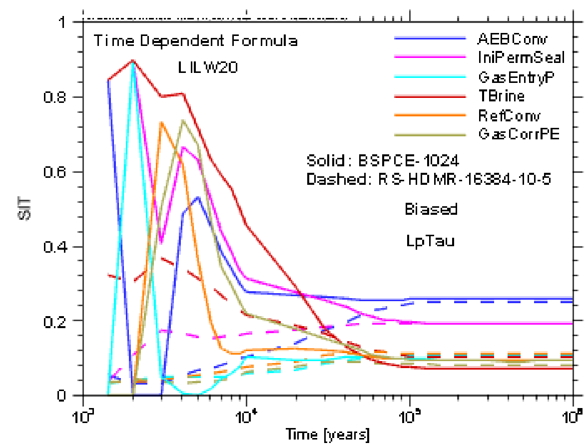
BSPCE: 1024 runs



LILW6



LILW11

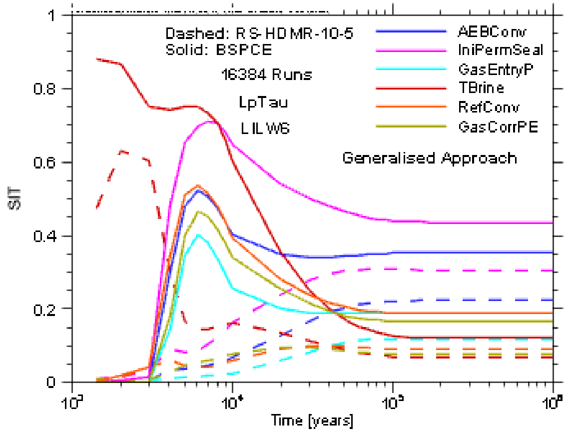


LILW20

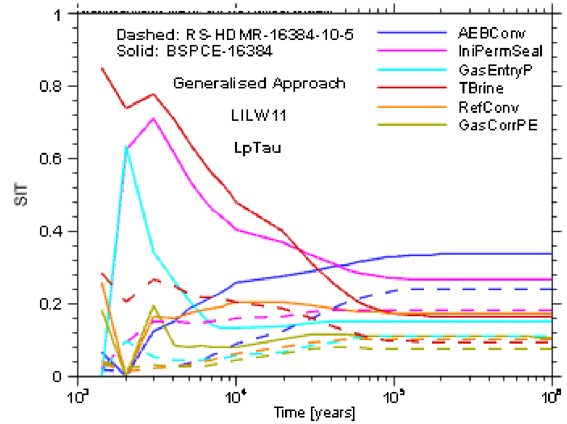
SIT Results – LILW11 and LILW20 Models

As for the LIW6 model, there are increasing differences in the SIT indices obtained from the BSPCE approach for the sets with more than 1024 runs for the LILW11 and LILW20 models as well

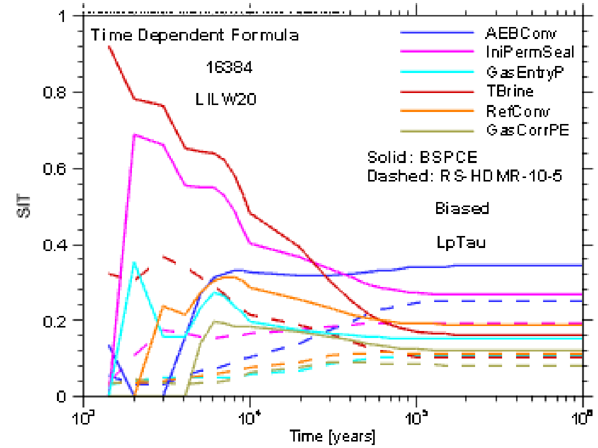
BSPCE: 16384 runs



LILW6



LILW11



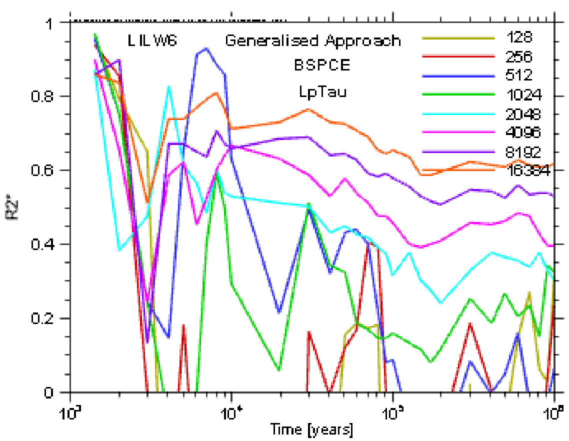
LILW20

Results – Metamodel Error (R^2) – LILW11 and LILW20 Models

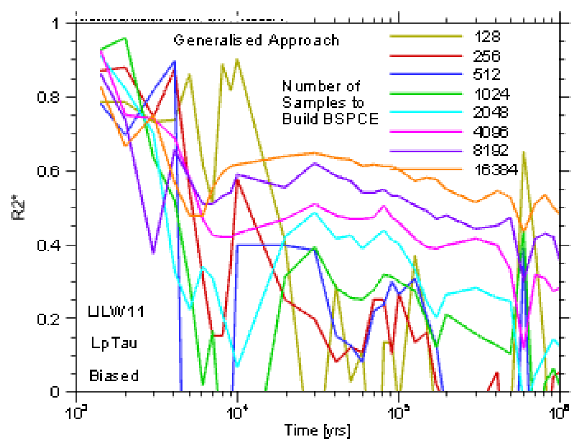
As for the LILW6 model, R^2 obtained from the BSPCE approach increases with increasing number of runs for the LILW11 and LILW20 models as well

BSPCE: Different sets of runs

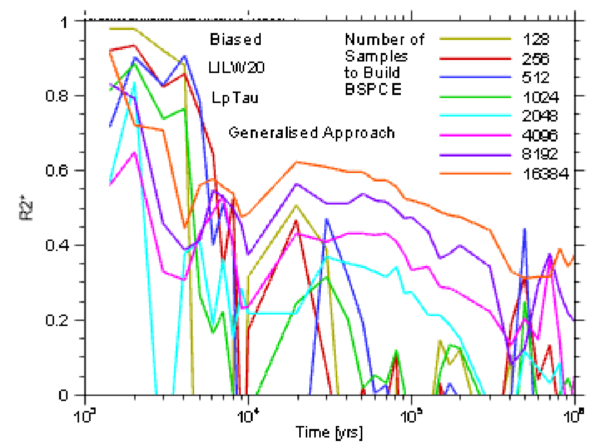
LILW6



LILW11



LILW20



R^2 decreases with number of parameters considered

Summary and Conclusions

- For all three repository models with different number of parameters (6, 11 and 20),
  - good agreement of the SI1 results obtained from the BSPCE approach in comparison with the ones from the RS-HDMR approach with optimal choice of polynomial coefficients and 16384 runs can already be obtained with 1024 runs
  - however, there are increasing differences in the SIT indices obtained from the BSPCE approach for the sets with more than 1024 runs => hint for the existence of third- or higher-order effects (BSPCE approach takes account of all orders of interaction while RS-HDMR only up to second order) ?
  - R^2 obtained from the BSPCE approach increases with increasing number of runs. Though, R^2 decreases with number of parameters considered
- Based upon the presented results, the question arises how many simulations do we need for building appropriate metamodels for the estimation of reliable indices higher order, especially for cases with many parameters or uncertainties?

THANK you for your Attention

Questions?

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