Risk Assessment for CO_2 Sequestration- Uncertainty Quantification based on Surrogate Models of Detailed Simulations

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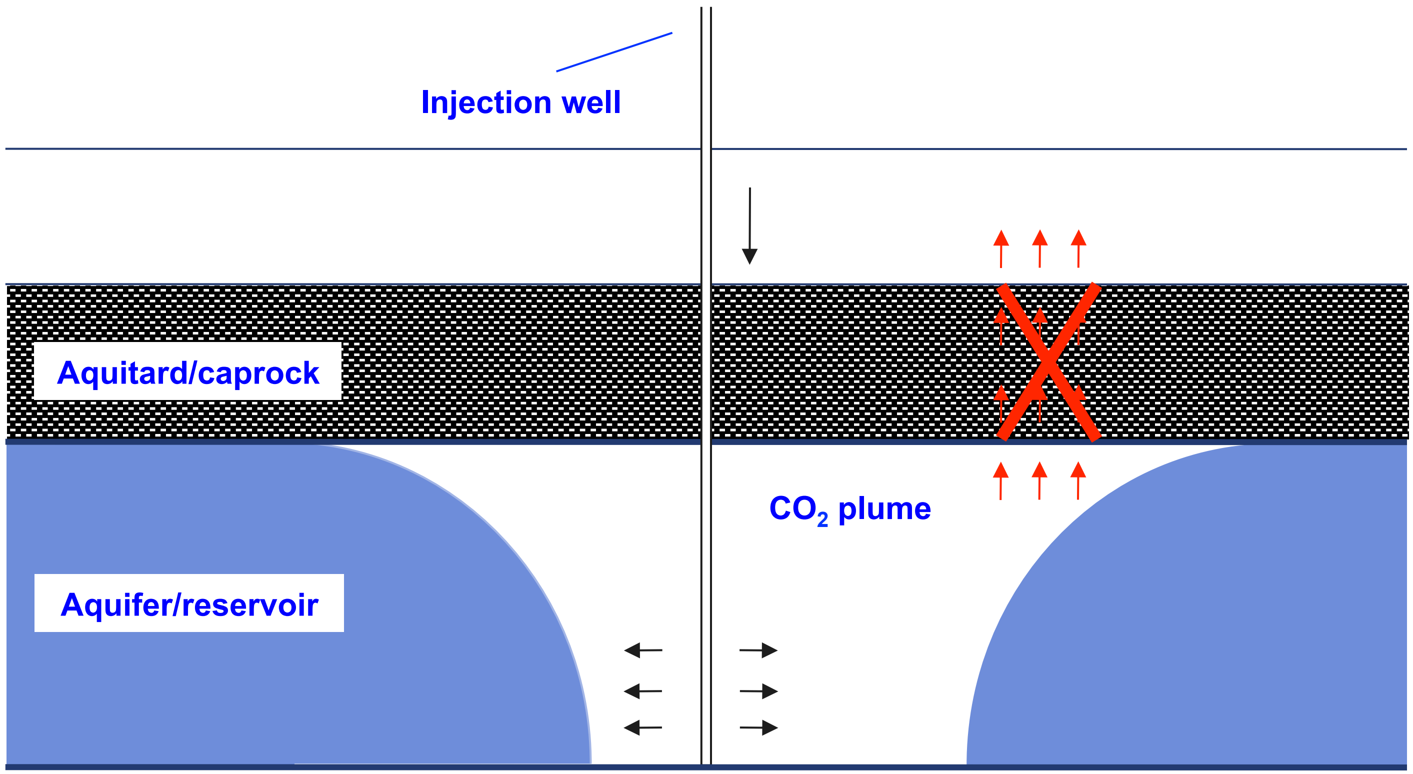
Modeling CO_2 Underground Plume



For $\alpha = \mathrm{CO_2}$, brine

$$\frac{\partial \boxed{\phi} \rho_\alpha S_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{v}_\alpha) = V_\alpha \rho_\alpha,$$

Mass balance

$$\mathbf{v}_\alpha = -\frac{K \boxed{k_\alpha}}{\mu_\alpha} (\nabla p_\alpha + \rho_\alpha g \nabla z)$$

Darcy's law

Uncertainty Analysis Options

- **Numerical model + Monte Carlo simulation**
- **Stochastic response surface methods**
  - **Surrogate model**
    - Approximate the output of the original model by polynomial functions of the uncertain parameters
  - **Monte Carlo simulation with surrogate model**

The primary goal of this work is to provide an assessment of surrogate-based uncertainty analysis for CO_2 injection into a saline aquifer

Polynomial Chaos Expansion (PCE)

- **A physical model**

$$\boldsymbol{Y} = M(\boldsymbol{x})$$

$\boldsymbol{x} = \{x_1, ..., x_M\}^T \in \mathbb{R}^M, M \geq 1$ porosity, permeability, etc

$\boldsymbol{Y} = \{y_1, ..., y_N\}^T \in \mathbb{R}^N, N \geq 1$ CO_2 mass, CO_2 plume dynamic, etc

- **Random $\boldsymbol{x}$ ➔ random model response y**
- **Assuming finite variance, chaos representation**

$$y = M(\boldsymbol{x}) = \alpha_0 + \alpha_1 B_1(\boldsymbol{x}) + \alpha_2 B_2(\boldsymbol{x}) + \alpha_3 B_3(\boldsymbol{x}) + ...$$

$\{B_1, B_2, B_3, ...\}$: orthogonal polynomial basis functions for $\boldsymbol{x}$

Orthogonal Polynomial Basis

- **Orthogonal polynomials for a <u>single</u> random x**

$$\varphi_d(x) = x^d + \text{lower-degree terms}, \quad d = 0, 1, 2, \ldots$$

$f(x)$: probability density function $\quad \int_\Omega \varphi_d(x)\varphi_c(x)f(x)dx = 0, d \neq c$

- **<u>Multivariate</u> polynomial basis for $\boldsymbol{x} = \{x_1, \ldots, x_M\}^T \in \mathbb{R}^M, M \geq 2$**

  - **Independent**

$$B_d(x_1, \ldots, x_M) = \prod_{i=1}^{M} \varphi_{d_i}(x_i), \quad \sum_{i=1}^{M} d_i = d$$

  - **Dependent: Nataf Transformation**

$\Phi(z_i) = F(x_i)$ correlated variables $\longrightarrow$ correlated standard normals

$\boldsymbol{z} = L\boldsymbol{\xi}$ correlated normals $\longrightarrow$ uncorrelated standard normals

$$y = M(\boldsymbol{\xi})$$

Coefficient Estimation

$$y = M_d(\boldsymbol{x}) = \alpha_0 + B_1\alpha_1 + \ldots + B_d\alpha_d$$

Regression

$\boldsymbol{X} = \{\boldsymbol{x}^{\mathbf{1}}, \ldots, \boldsymbol{x}^{\boldsymbol{N_p}}\}$: a set of N_p realizations of random input vectors

$\boldsymbol{y} = \{y^1, \ldots, y^{N_p}\}^T = \{y^i = M_d(\boldsymbol{x}^i), i = 1, \ldots, N_p\}^T$

$$\boldsymbol{B}\boldsymbol{\alpha} = \boldsymbol{y}$$

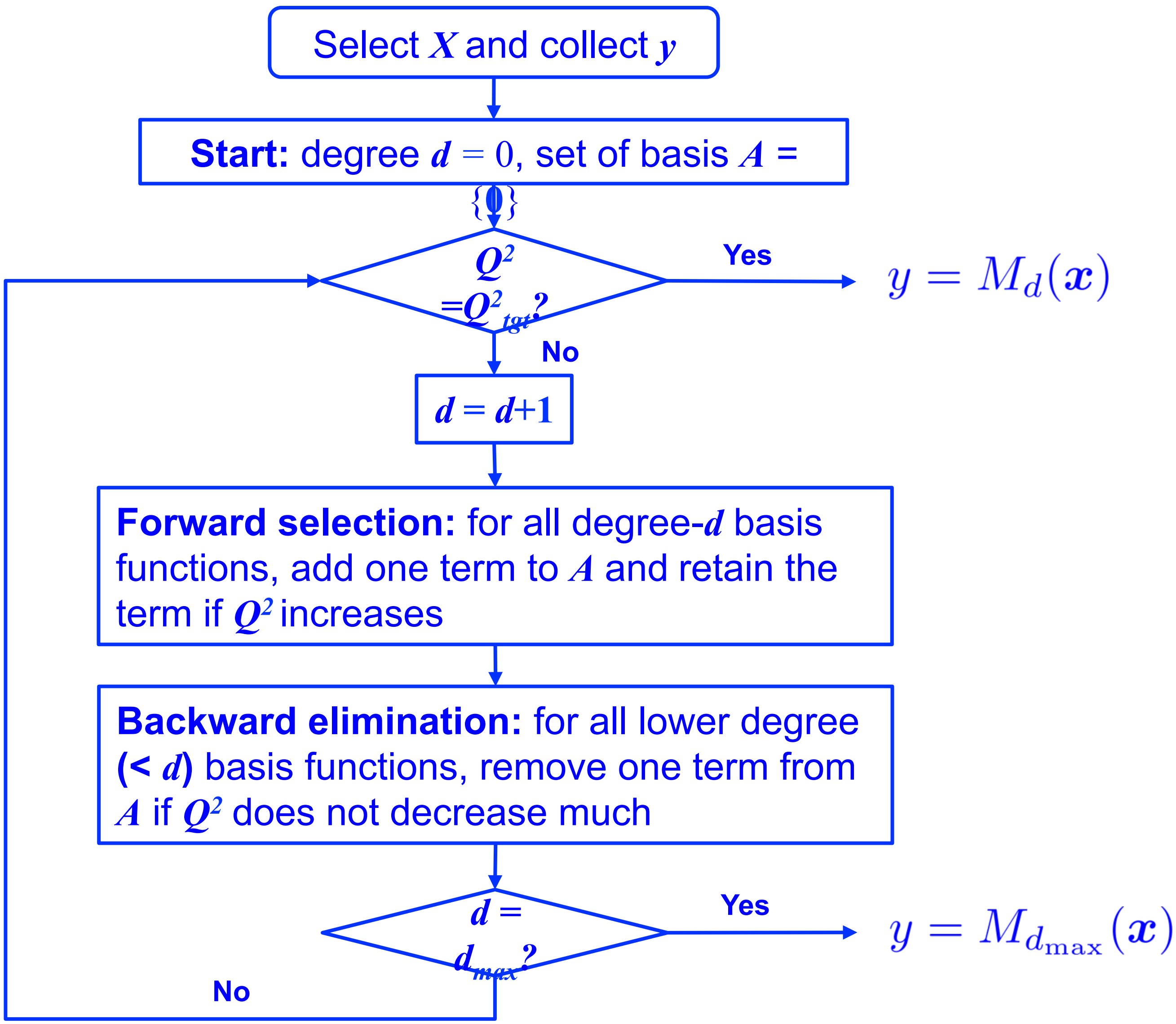
$$\boldsymbol{\alpha} = (\boldsymbol{B}^T\boldsymbol{B})^{-1}\boldsymbol{B}^T\boldsymbol{y}$$

- **Number of points to choose:**

$N_t = \frac{(M+d)!}{M!d!}$ $\quad$ d: degree of expansion, M: inputs

M	$d = 1$	$d = 2$	…	$d = 6$
1	1	3		7
5	6	21		462
10	11	66		8008

Stepwise PCE Approximation



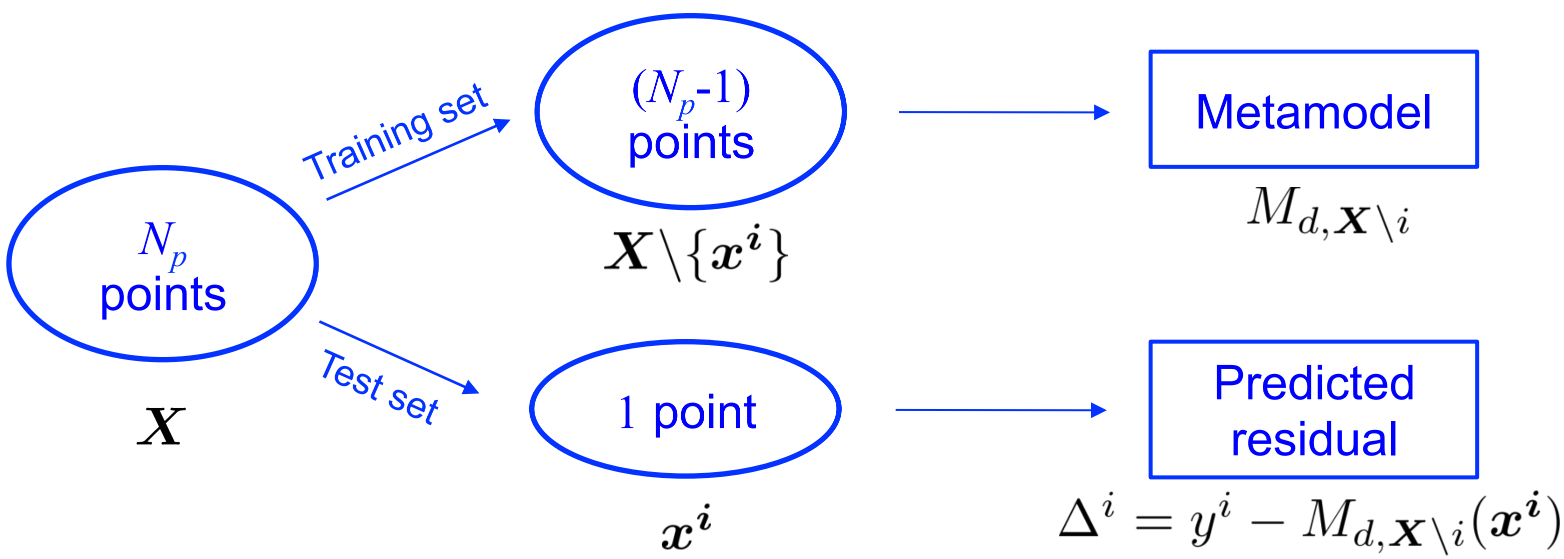
Assessment of PCE approximation

- **Empirical error**

$$R^2 = 1 - \frac{\frac{1}{N_p}\sum_{i=1}^{N_p}(y^i - M_d(\boldsymbol{x^i}))^2}{\sigma^2(\boldsymbol{y})}$$

$R^2 \rightarrow 1$ as N_t increases ➔ overfitting

- **Leave-one-out cross validation**



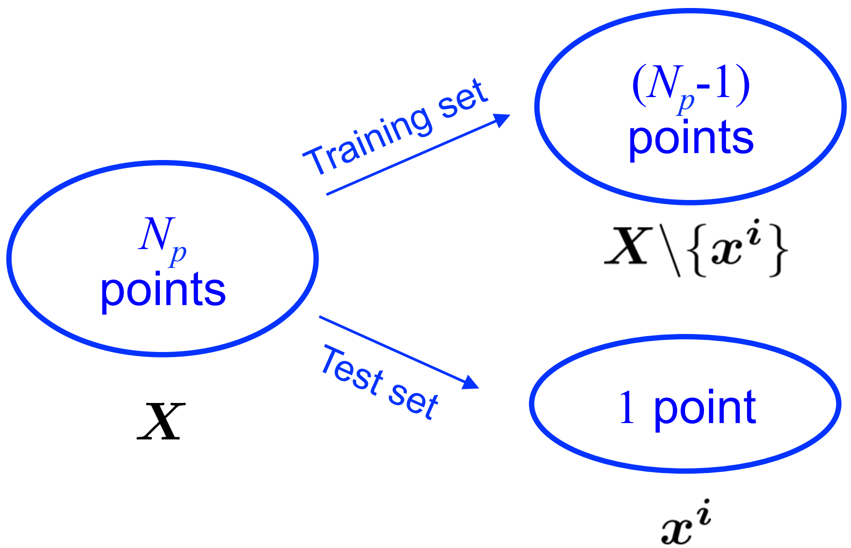
Assessment of PCE approximation

Empirical error

$$R^2 = 1 - \frac{\frac{1}{N_p}\sum_{i=1}^{N_p}\left(y^i - M_d(\boldsymbol{x}^{\boldsymbol{i}})\right)^2}{\sigma^2(\boldsymbol{y})}$$

$R^2 \rightarrow 1$ as N_t increases ➔ overfitting

Leave-one-out cross validation



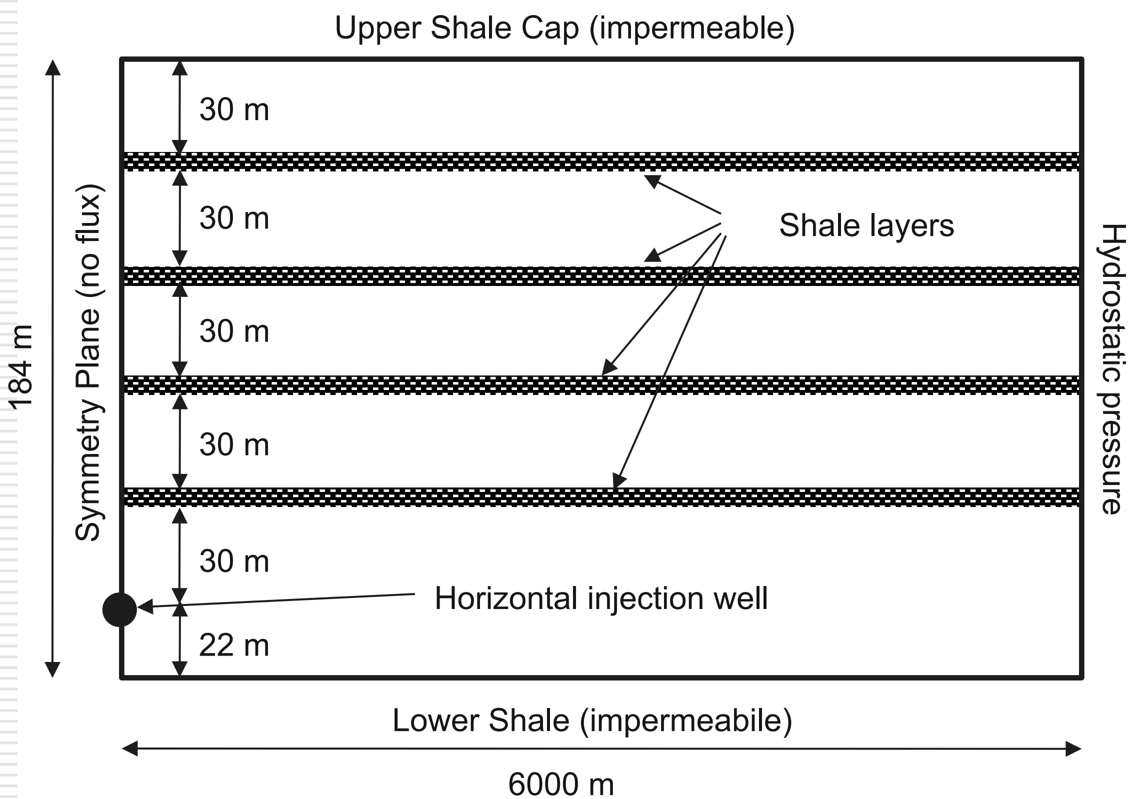
$$Q^2 = 1 - \frac{\frac{1}{N_p}\sum_{i=1}^{N_p}\left(\Delta^i\right)^2}{\sigma^2(\boldsymbol{y})}$$

$$\Delta^i = y^i - M_{d,\boldsymbol{X}\backslash i}(\boldsymbol{x}^{\boldsymbol{i}})$$

Case Study

- CO_2 injection into a deep saline aquifer
- Simulated using TOUGH2 developed by LBNL since 1980

$$\text{output} = M\ (\text{porosity, permeability})$$



Pressure at well	110 bar
Temperature	37 ℃
Salinity	3.2 wt.-% NaCl
Injection rate	0.1585 kg/s

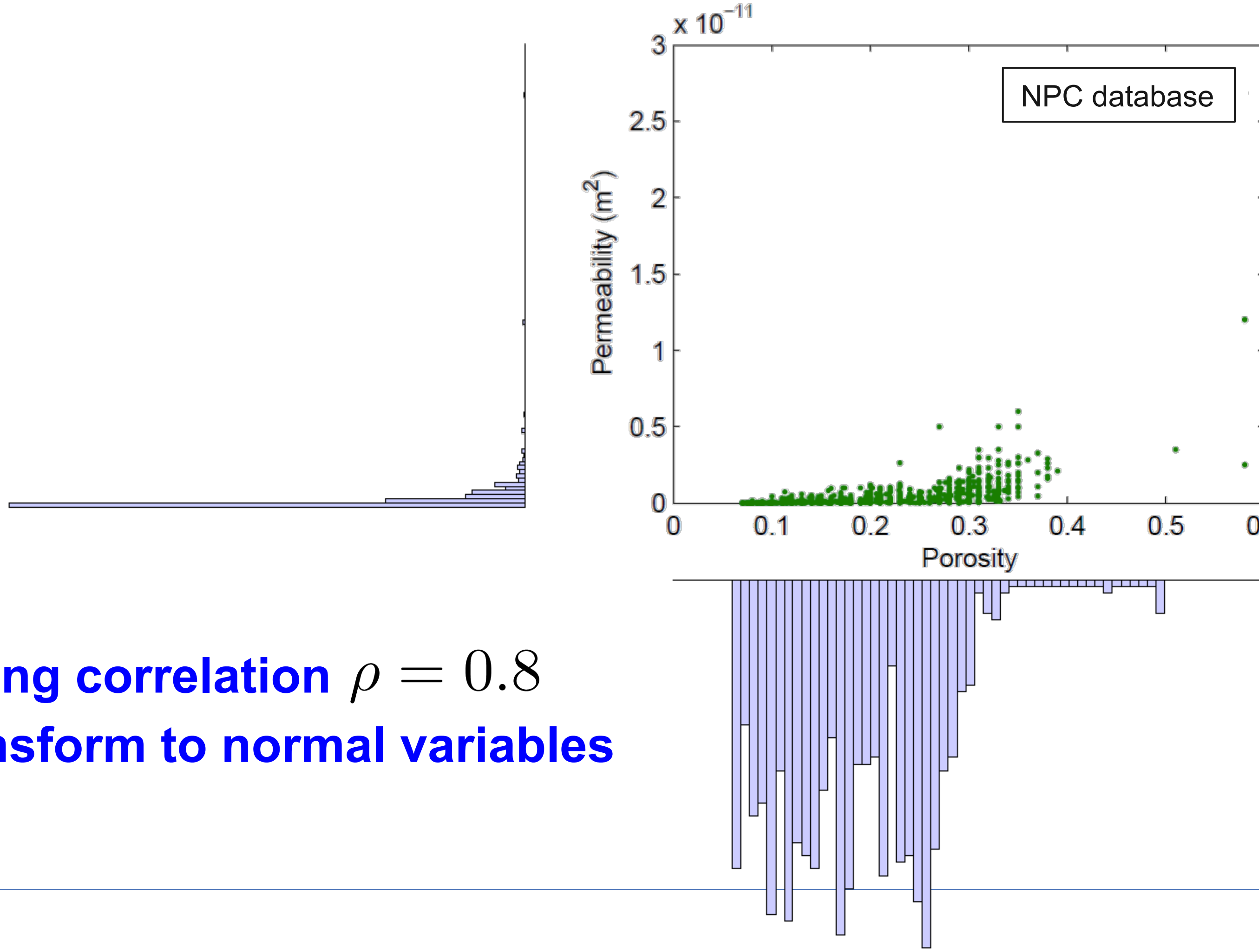
Output:

Gas saturation (space, time)
Pressure (space, time)
CO_2 mass distribution
…

ECO2N manual, 2005

Specify Input Random Variables

- National Petroleum Council Public Database
- Non-standard marginal distributions



- Strong correlation $\rho = 0.8$
- Transform to normal variables

Derive Orthogonal Polynomial Basis

- **Hermite polynomials for a standard normal random variable**

$$\begin{aligned}
\varphi_0(\xi) &= 1 \\
\varphi_1(\xi) &= \xi \\
\varphi_2(\xi) &= \xi^2 - 1 \\
\varphi_3(\xi) &= \xi^3 - 3\xi \\
&\ldots
\end{aligned}$$

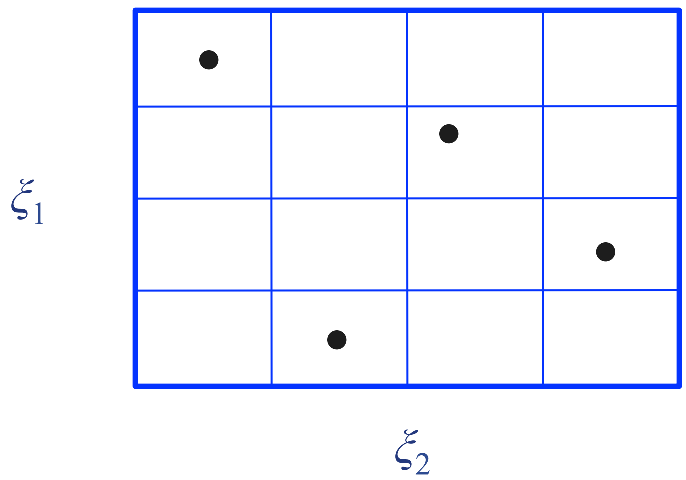
$$\varphi_{d+1} = \xi\varphi_d - d\varphi_{d-1}$$

- **Basis for the two-dimensional independent input vector** (ξ_1, ξ_2)

$$\begin{aligned}
B_0(\boldsymbol{\xi}) &= \varphi_0(\xi_1)\varphi_0(\xi_2) = 1 \\
B_1(\boldsymbol{\xi}) &= \varphi_1(\xi_1)\varphi_0(\xi_2) = \xi_1 \\
B_1(\boldsymbol{\xi}) &= \varphi_0(\xi_1)\varphi_1(\xi_2) = \xi_2 \\
B_2(\boldsymbol{\xi}) &= \varphi_2(\xi_1)\varphi_0(\xi_2) = \xi_1^2 - 1 \\
B_2(\boldsymbol{\xi}) &= \varphi_1(\xi_1)\varphi_1(\xi_2) = \xi_1\xi_2 \\
B_2(\boldsymbol{\xi}) &= \varphi_0(\xi_1)\varphi_2(\xi_2) = \xi_2^2 - 1 \\
&\ldots
\end{aligned}$$

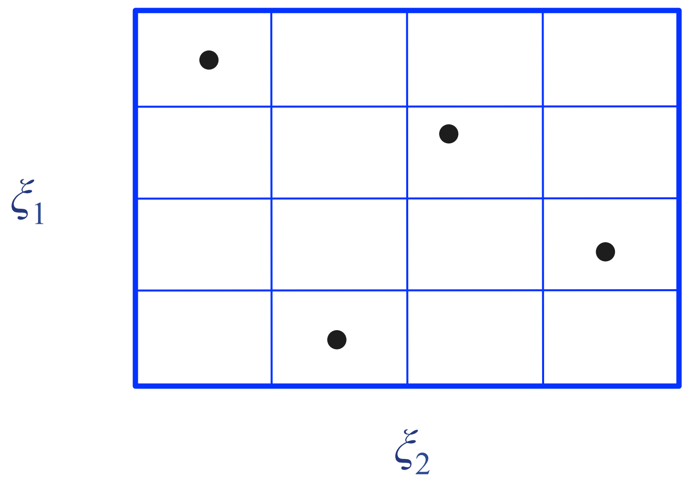
Build PCE Model

- **Select an experimental design** ξ (Latin Hypercube Sampling)



Build PCE Model

- **Select an experimental design** ξ (Latin Hypercube Sampling)

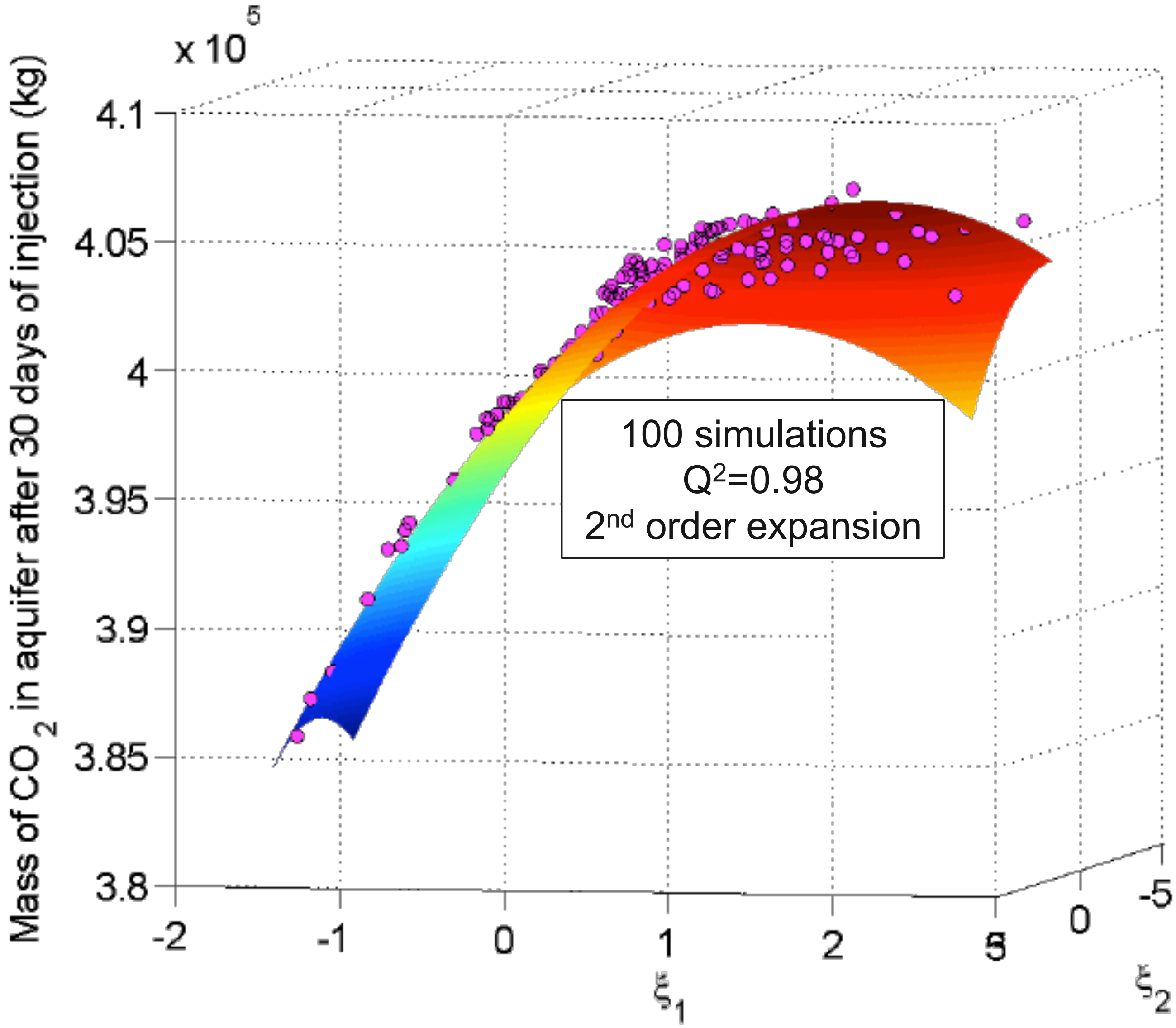


- **Reverse of Nataf transformation**

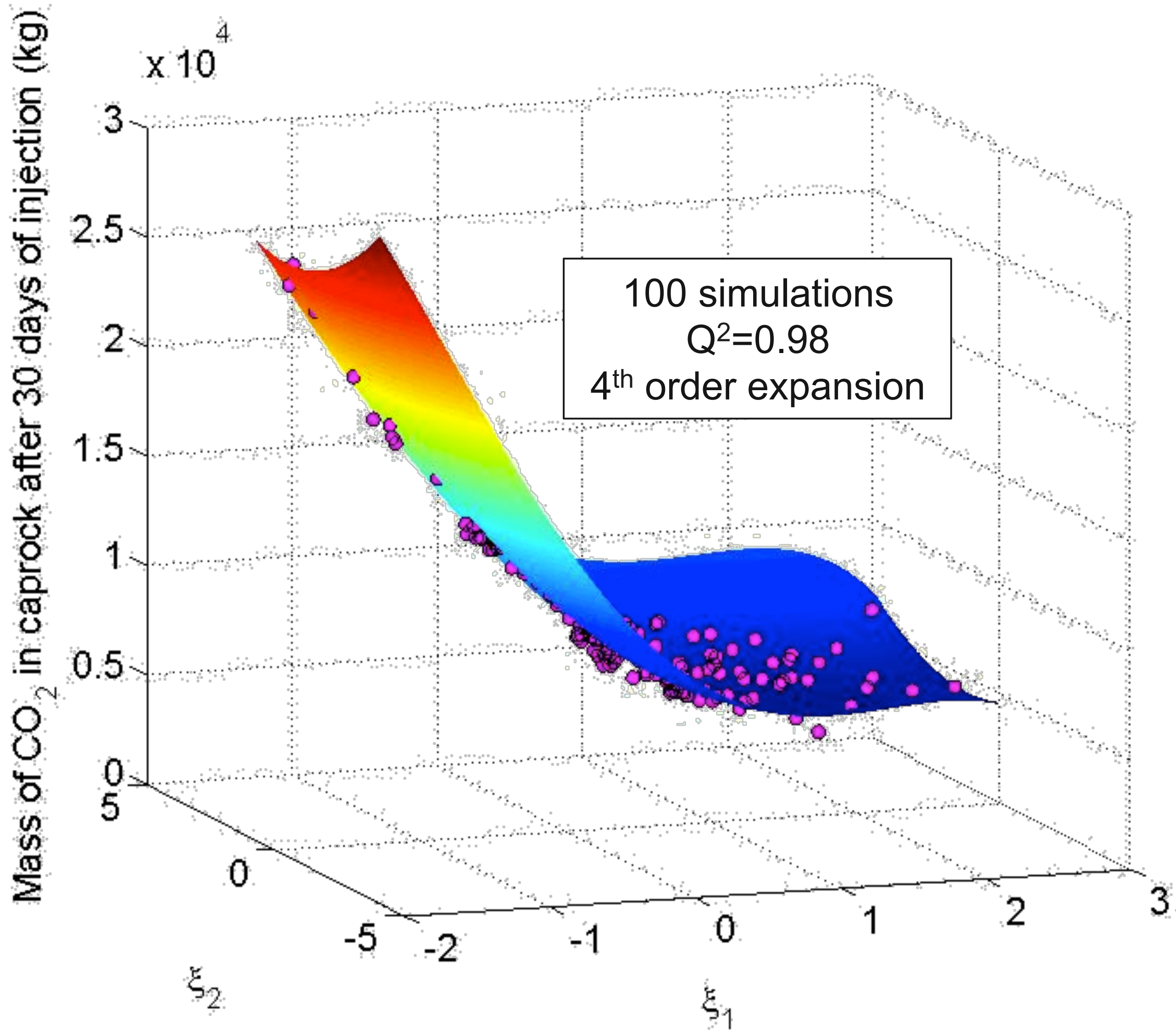
$$\boldsymbol{z} = L\boldsymbol{\xi} \qquad\qquad x_i = F^{-1}(\Phi(z_i))$$

- **Model output evaluations**
- **Stepwise regression for coefficients and degree**

PCE Model Example 1



PCE Model Example 2

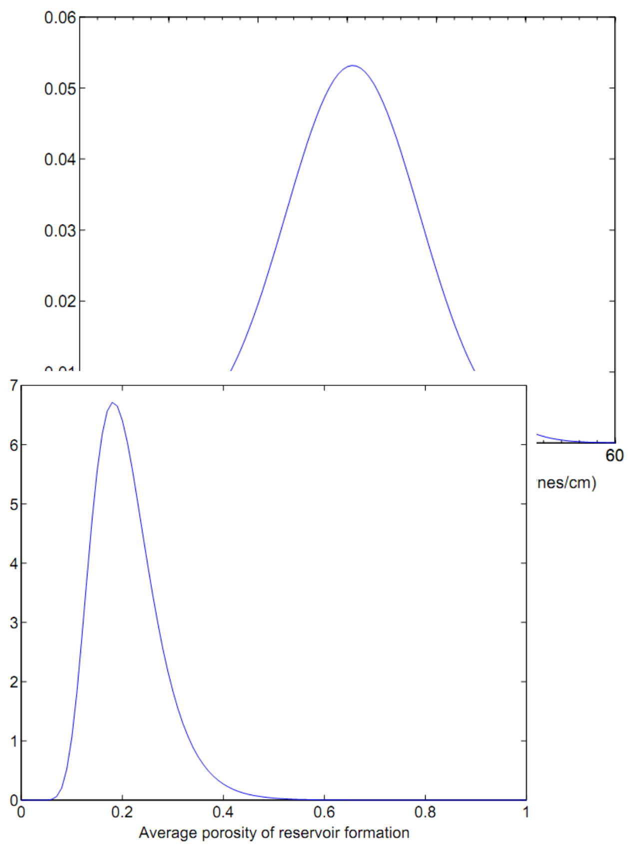


Use PCEs for Uncertainty Analysis

Input:
Randomly sampled from probability distribution function of independent parameters

Monte Carlo simulation →

Output:
Statistical analysis

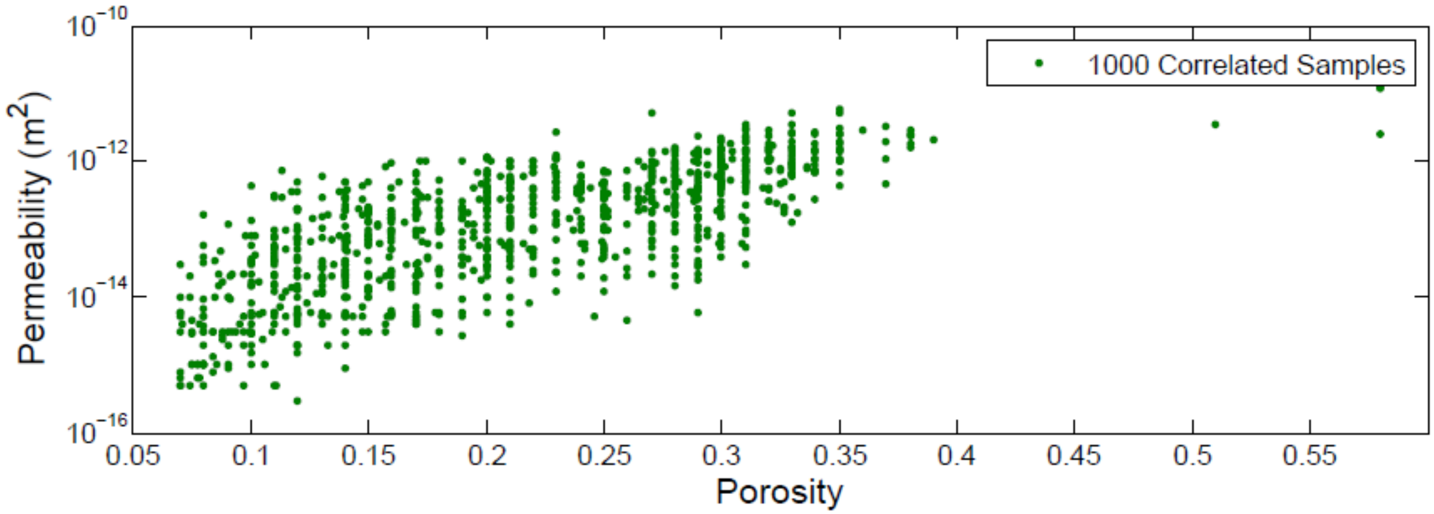


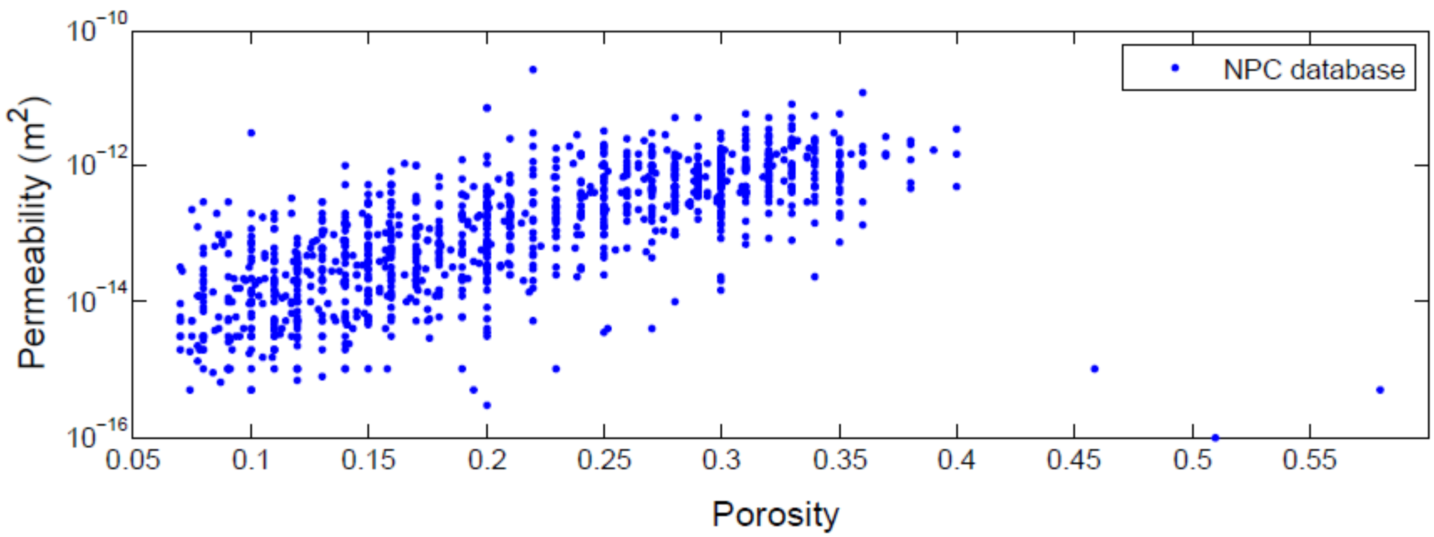
Surrogate Model

Generated random samples				
Sample #	x_1	x_2	…	x_n
	Permeability	**Porosity**	…	
1				
2				
…				
4000				

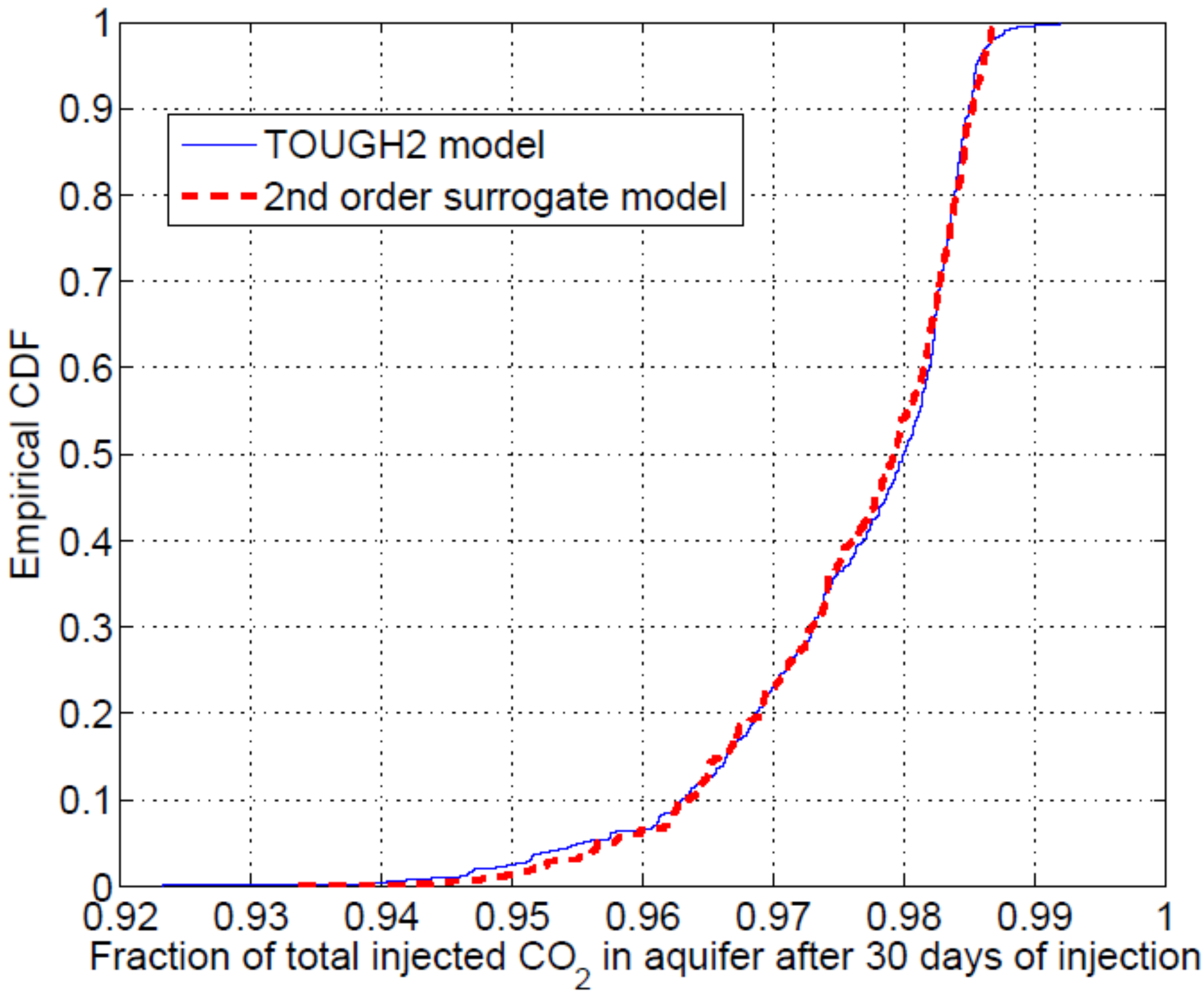
Outputs evaluated using PCEs			
y_1	y_2	…	y_m
Mass	**Pressure**		

Correlated Sampling Using Copulas

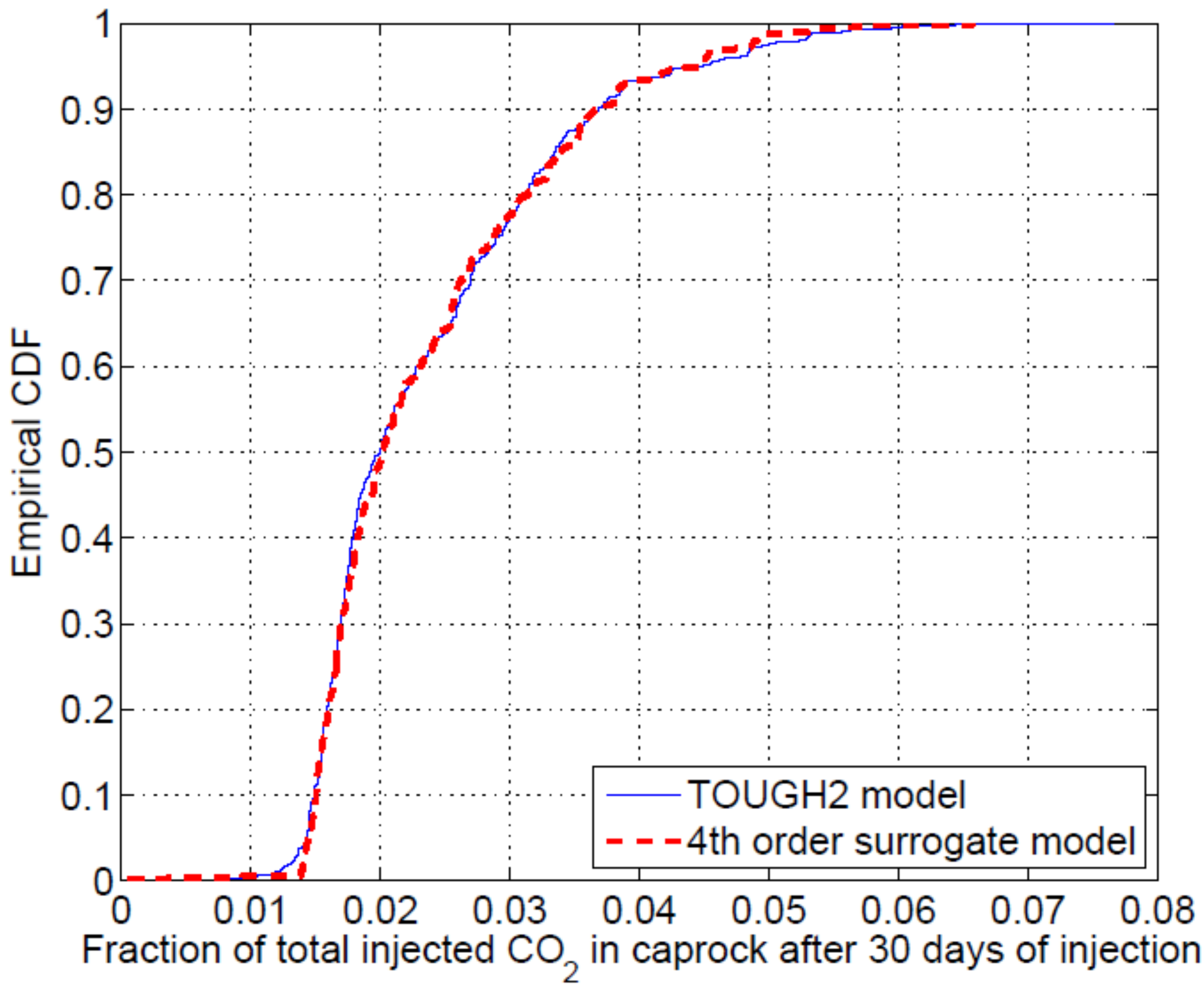




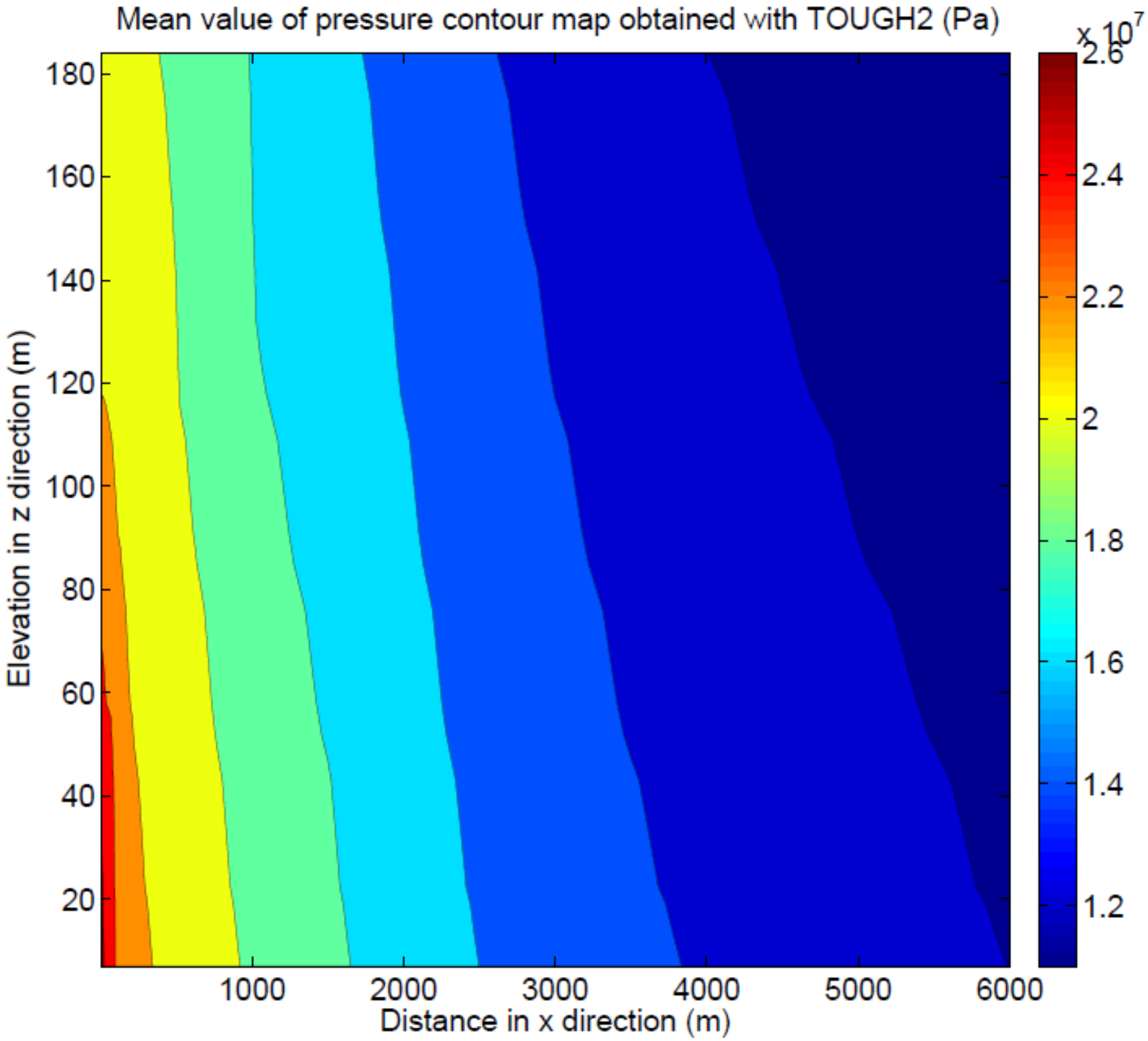
MC Simulation Result 1



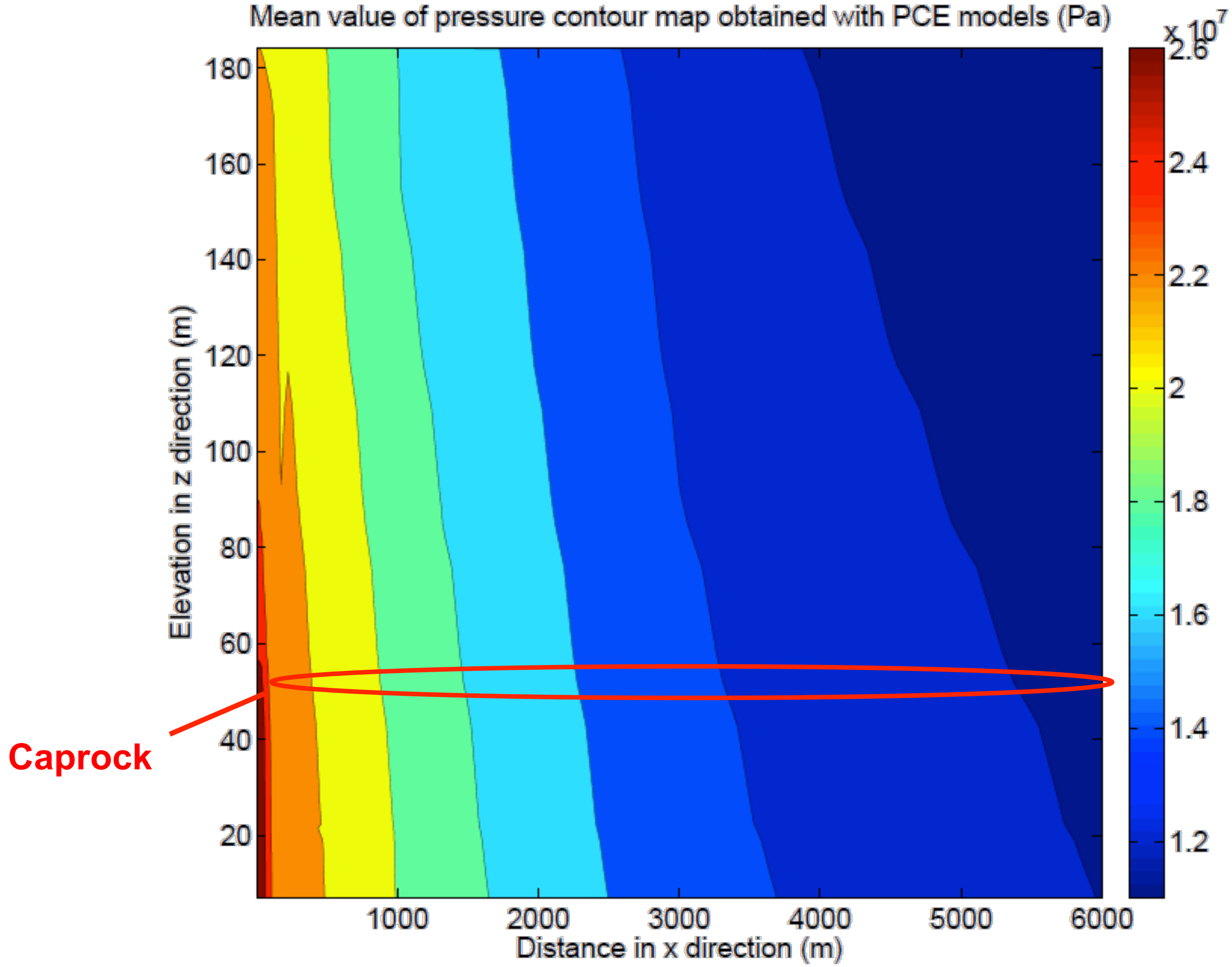
MC Simulation Result 2



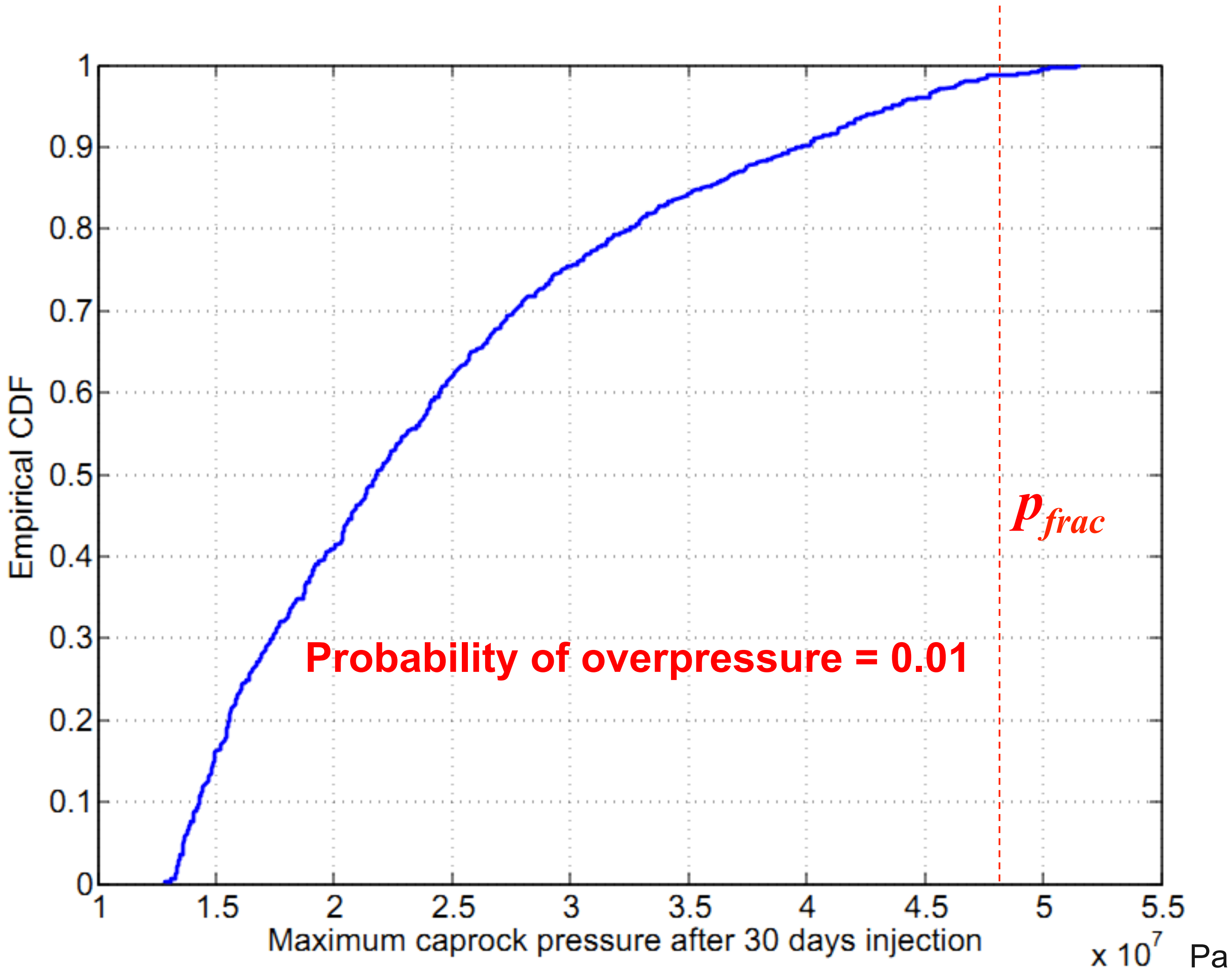
Pressure Map with TOUGH2



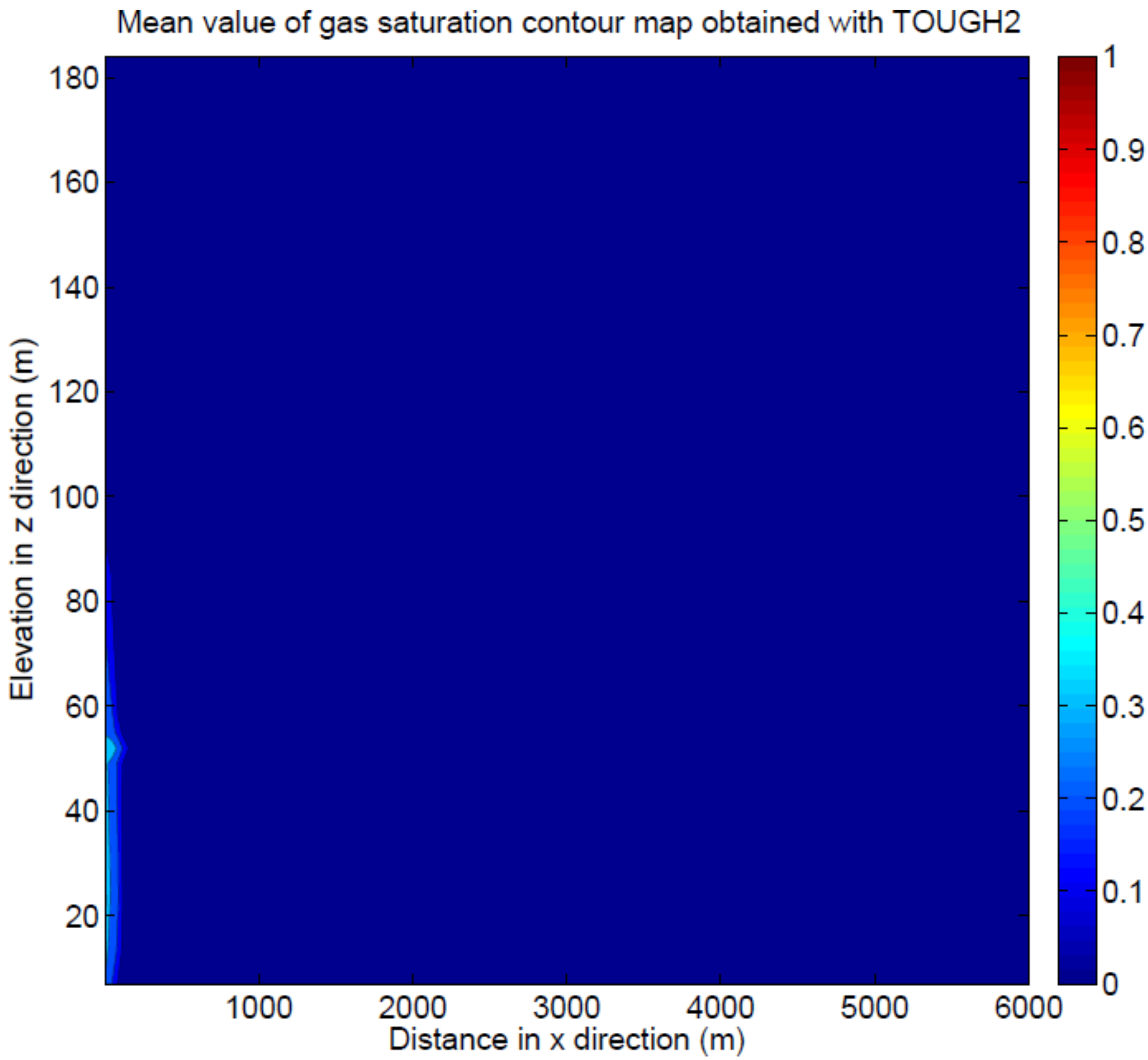
Pressure Map with PCE Model



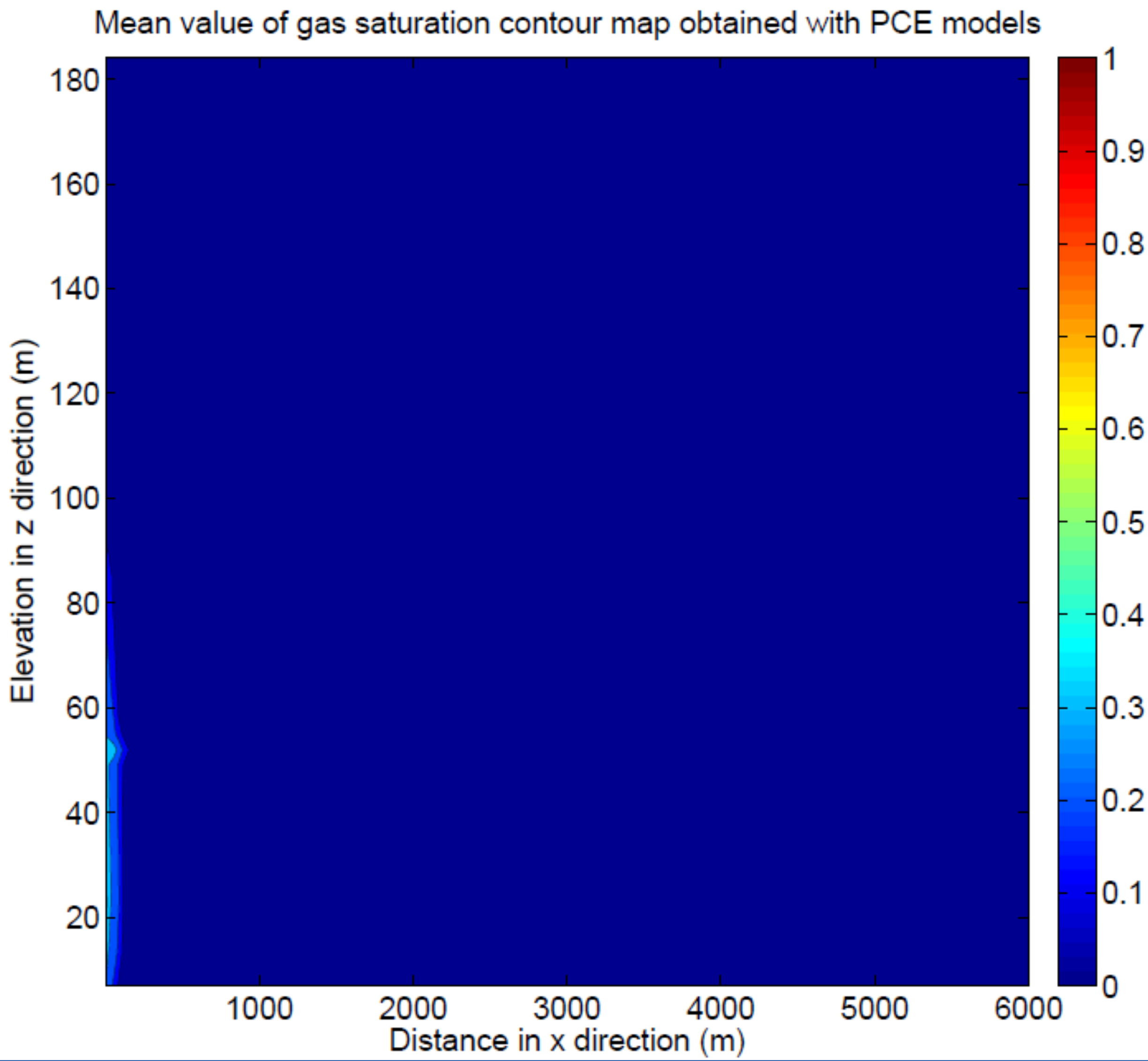
Maximum Caprock Pressure



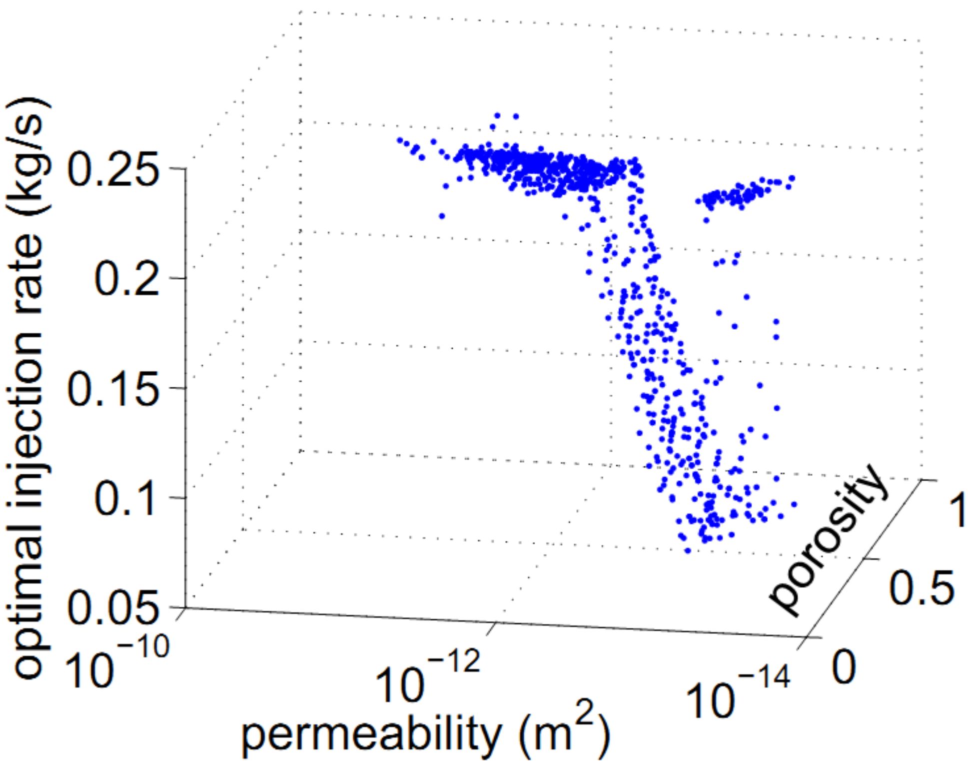
Gas Saturation Map with TOUGH2



Gas Saturation Map with PCE Model



Optimal Injection under Uncertainty



Optimal injection rates under various realizations of uncertain parameters

$$\max_{z} \quad \mathbb{E}_{\xi_1,\xi_2 \in \Omega}\left(\sum_{i=1}^{986} S_{g_i}(z,\xi_1,\xi_2)\right)$$

$$\text{s.t.} \quad p(z,\xi_1,\xi_2) \le p_{\text{limit}}$$

Nonconvex stochastic NLP solved with BARON using scenario-based approach

Conclusions

- **Polynomial chaos expansion model was iteratively built with stepwise regression for correlated uncertain parameters**
- **Results obtained with PCE-based surrogate model match well the results obtained with TOUGH2**
- **Developed a nonconvex stochastic NLP model for finding optimal injection rate under model uncertainty**

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