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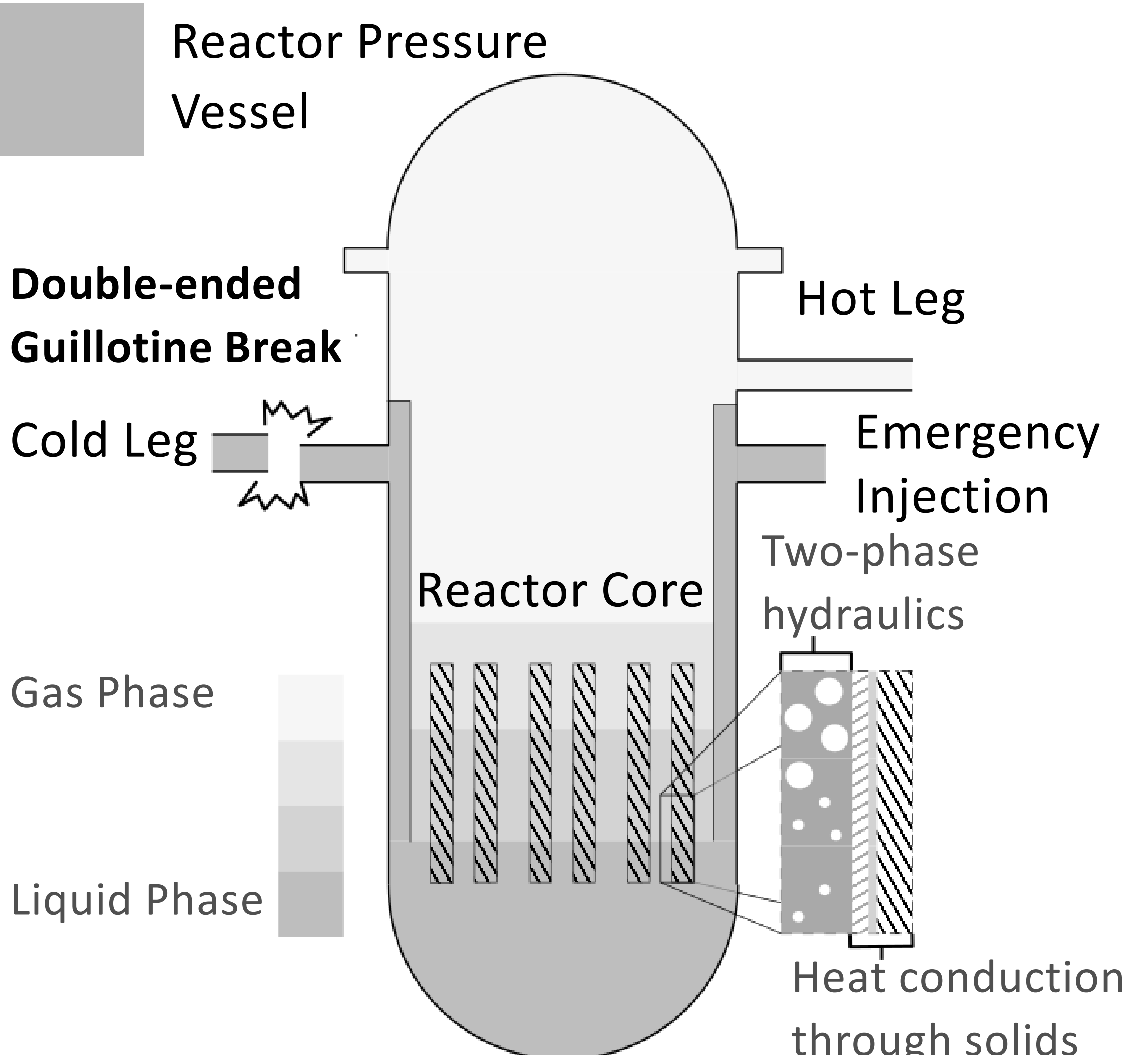
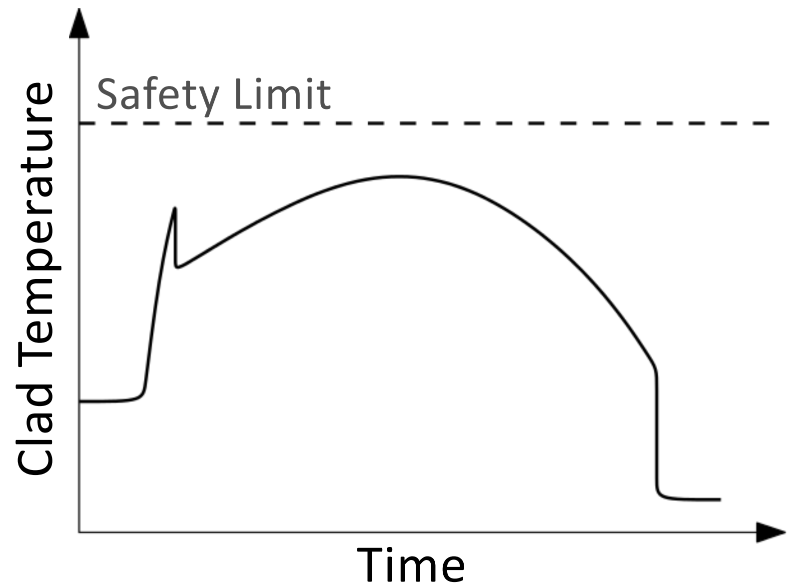
Bayesian Uncertainty Quantification of Physical Models in Thermal-Hydraulics System Codes

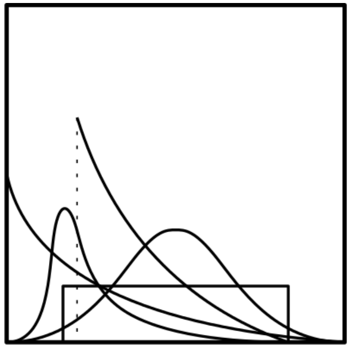
PhD Defense, EPF Lausanne, 19.01.2018

Safety Analysis of LWR under LBLOCA: Show max. clad temperature < safety limit





Forward Uncertainty Quantification: Uncertain Inputs ⇒ Uncertain Outputs

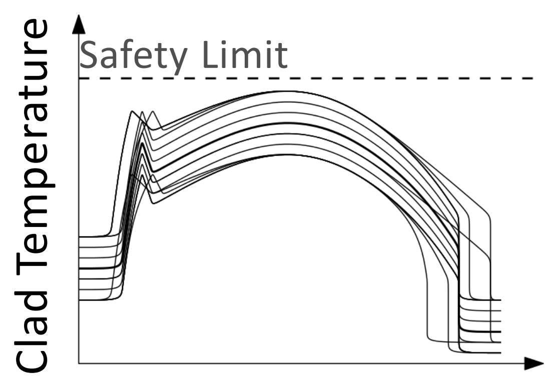


Uncertain Inputs
(random variables)

- Material properties
- Initial conditions
- Boundary conditions
- Physical model parameters

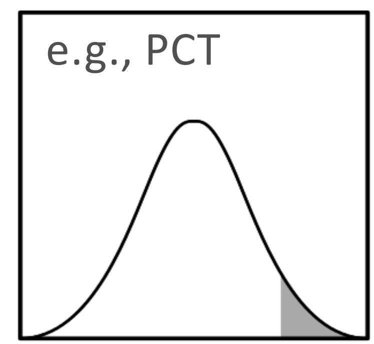
Forward Model (Code)
$\mathbf{f}: \boldsymbol{x} \mapsto y$

Monte Carlo simulation
(multiple code runs)



Uncertain Outputs

Statistical Analysis
of ``Quantities of Interest''



Decision Making

Safe/Fail, Accept/Reject, etc.

Physical Model Parameters: post-Critical Heat Flux (CHF) Flow Regimes

Closure Laws

Parametric models

Mass

$$\frac{\partial\langle\alpha_i\rho_i\rangle}{\partial t} + \langle\nabla\cdot\alpha_i\rho_i\,\vec{v}_i\rangle = \langle\Gamma_{\mathrm{int}}\rangle$$

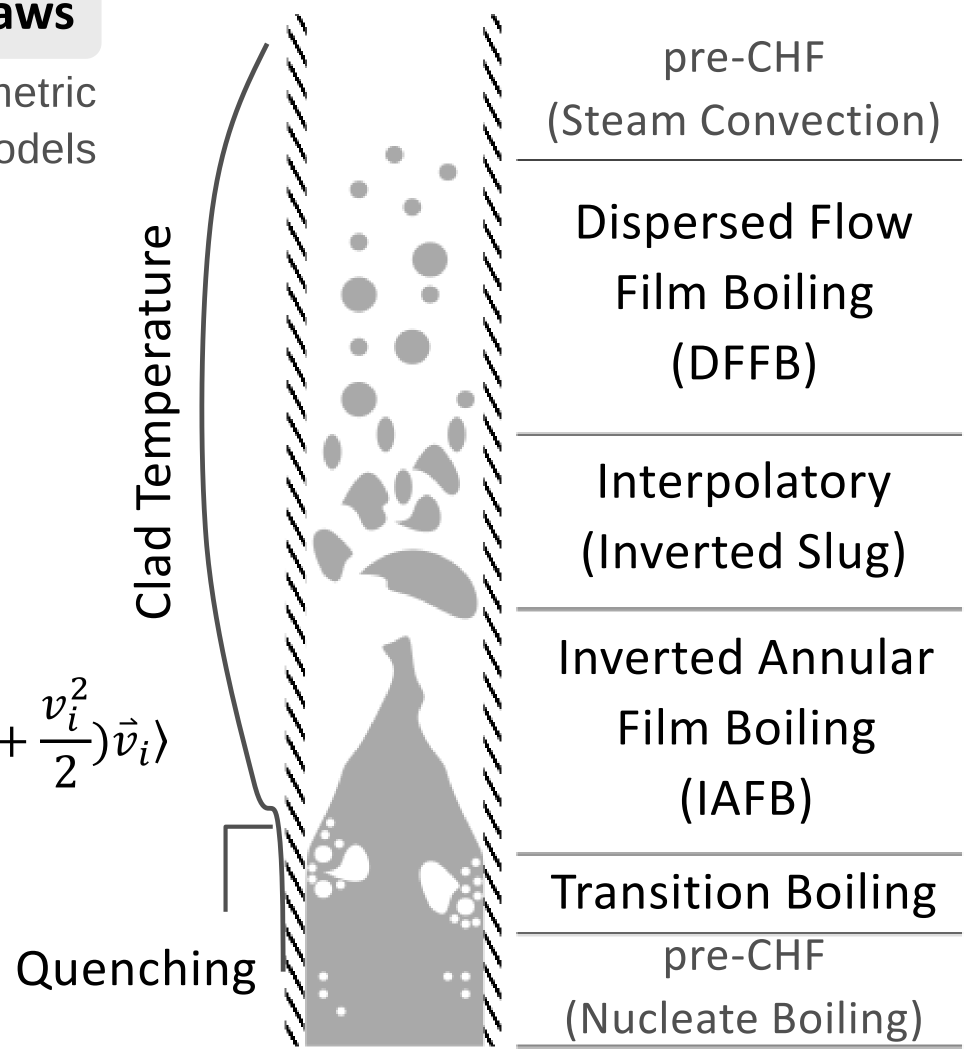
Momentum

$$\frac{\partial\langle\alpha_i\rho_i\vec{v}_i\rangle}{\partial t} + \langle\nabla\cdot\alpha\rho_i\,\vec{v}_i\vec{v}_i\rangle + \langle\alpha\nabla P\rangle$$
$$= -\langle\vec{\mathrm{f}}_{\mathrm{int}}\rangle + \langle\vec{\mathrm{f}}_{\mathrm{w}_i}\rangle + \langle\alpha\rho_i\vec{g}\rangle + \langle\Gamma_{\mathrm{int}}\vec{v}_i\rangle$$

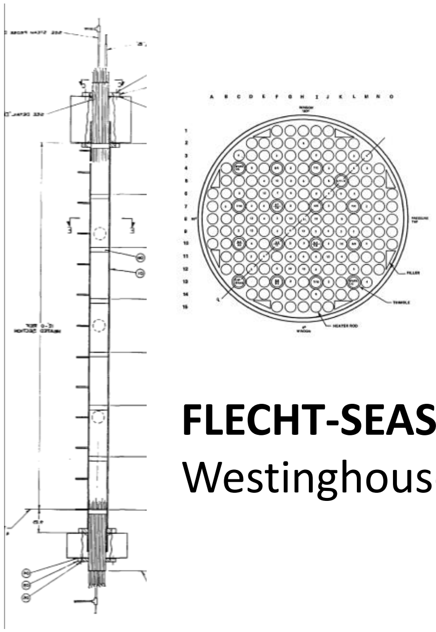
Energy

$$\frac{\partial\left\langle\alpha_i\rho_i\left(e_i+\frac{v_i^2}{2}\right)\right\rangle}{\partial t} + \left\langle\nabla\cdot\alpha_i\rho_i\left(e_i+\frac{P}{\rho_i}+\frac{v_i^2}{2}\right)\vec{v}_i\right\rangle$$
$$= \langle q_{\mathrm{int}_i}\rangle + \langle q_{\mathrm{w}_i}\rangle + \langle q_{d_i}\rangle + \langle\alpha_i\rho_i\vec{g}\cdot\vec{v}_i\rangle$$
$$- \langle\Gamma_{\mathrm{int}}h_i'\rangle + \langle(-\vec{\mathrm{f}}_{\mathrm{int}}+\vec{\mathrm{f}}_{\mathrm{w}_i})\cdot\vec{v}_i\rangle$$

$i = G$ (Gas), L (Liquid)



Origin of Uncertainty in Physical Model Parameters



FLECHT-SEASET
Westinghouse, USA

Excerpt from the TRACE Code Theory Manual:

- "…the **approximate value of the coefficient** in Eq. (4-119) **was determined from data comparisons with FLECHT-SEASET** high flooding rate reflood data…" (pp. 164)
- "In TRACE, the above interfacial drag coefficient **has been reduced by a factor of ¾ to better match FLECHT-SEASET** high flooding rate reflood data, so…" (pp. 166)

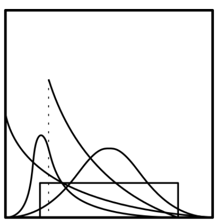
No statement of uncertainty on these parameters

Research Objectives

Given experimental data from a Separate Effect Test Facility (SETF), develop a methodology to:

quantify the uncertainty of physical model parameters in a TH System Code

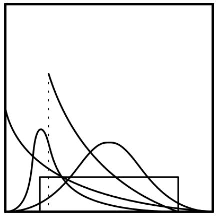
to be propagated within statistical uncertainty analysis framework.



Pre-calibration uncertainties

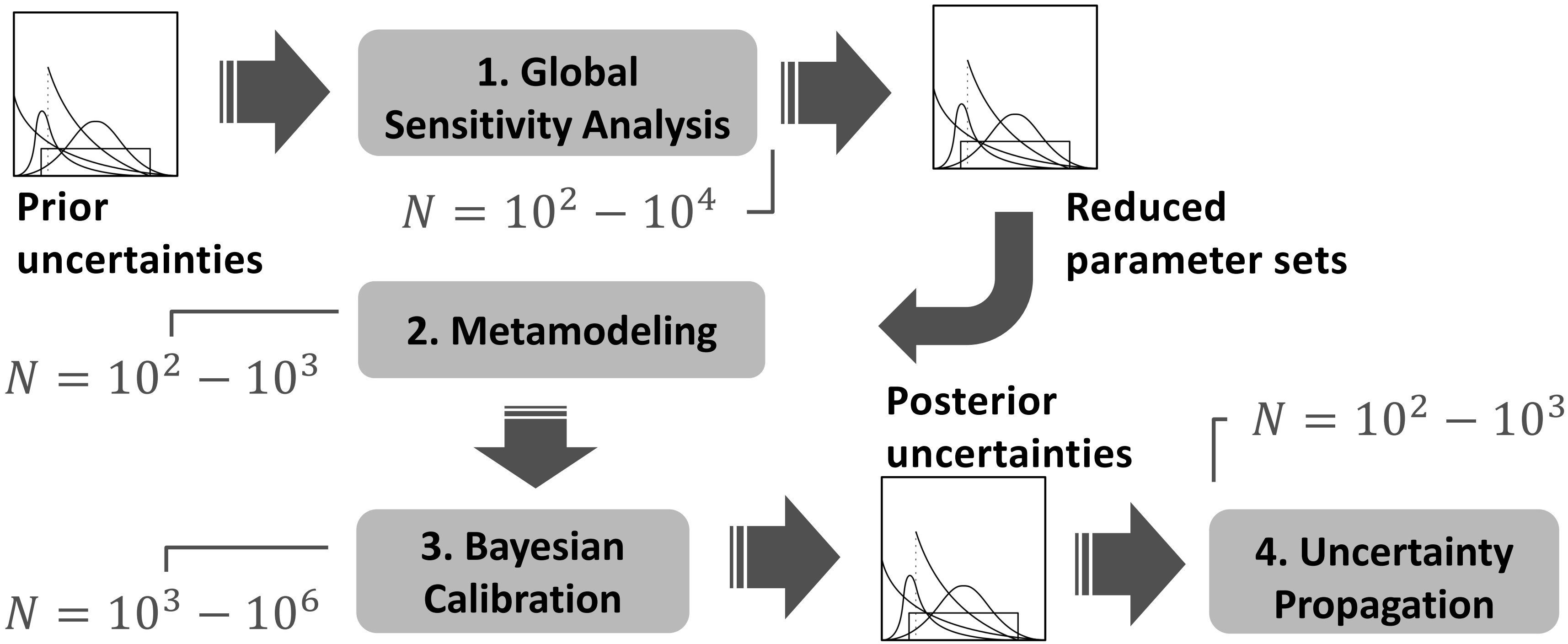
Calibration

Experimental Data from SETF



Post-calibration uncertainties

Scope of Research (1/2): Statistical Framework

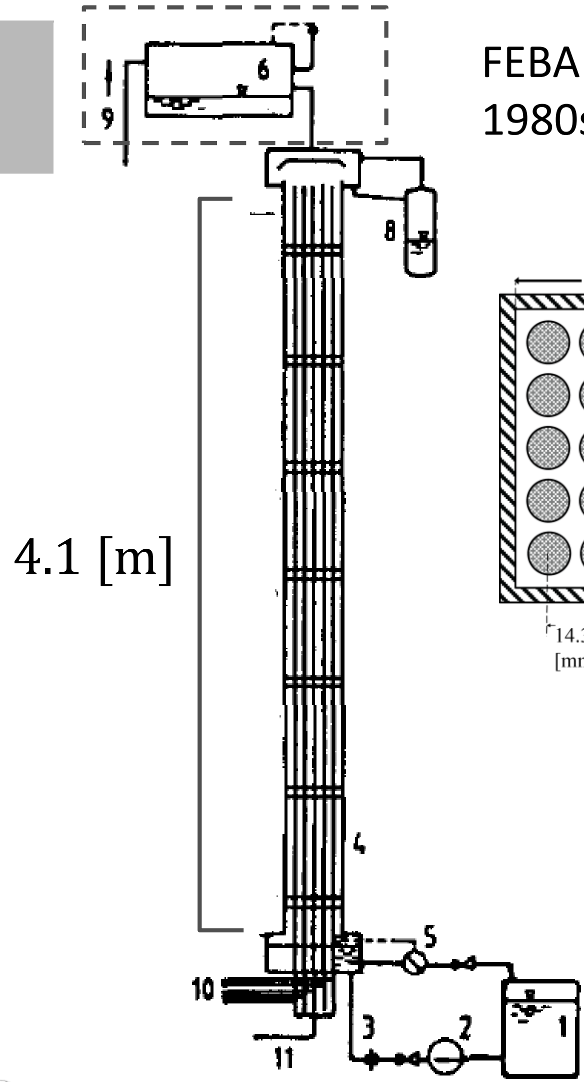


- Methods are non-intrusive
- Methods require less assumptions about the underlying model
- Results conform with probabilistic framework for UQ

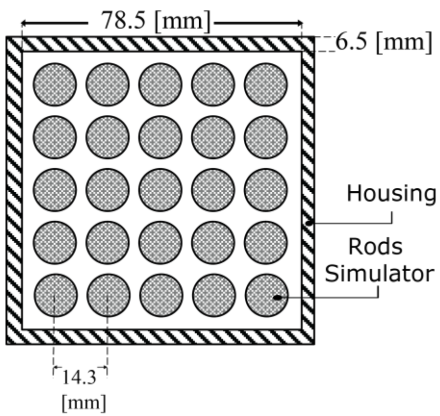
- Methods tend to be expensive

(require numerous code runs)

Scope of Research (2/2): FEBA Separate Effect Test Facility (SETF)



FEBA Reflood Tests were conducted at Kfz Karlsruhe (KIT) during 1980s for investigating bottom reflood using rod simulators (NiCr)



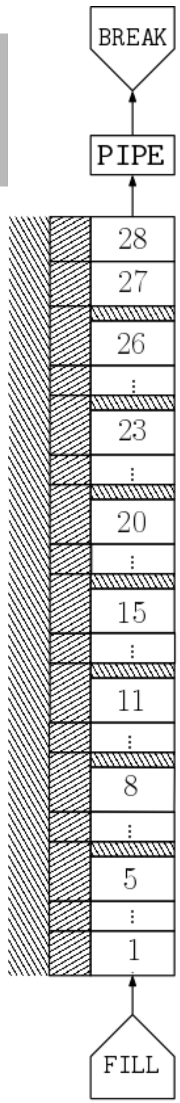
Main analyses are based on Test No. 216:

- $V_{\text{inlet}} = 3.8\ [\text{cm.s}^{-1}]$
- $P_{\text{sys}} = 4.1\ [\text{bar}]$
- $T_{\text{inlet}} = 312\ [\text{K}]$
- Power = 120% ANS Decay Curve

Three types of measurements were taken:

- Clad temperature (8 axial locations)
- Pressure drop (4 axial segments)
- Liquid carryover

Scope of Research (2/2): TRACE Model of FEBA SETF



Backpressure

Upper plenum

Inlet flow

27 Parameters are required to specify the model:

Controllable inputs $\boldsymbol{x}_c$

- **(4)** Experimental boundary conditions (P_{sys}, V_{inlet}, etc.)
- **(9)** Material properties (k, C_p, etc.)

Model parameters $\boldsymbol{x}_m$

- **(2)** Spacer grid model ($\mathrm{HTC}_{\mathrm{enh.}}, \Delta P$)
- **(10)** Post-CHF closure relations (IAFB wall HTC, DFFB interfacial drag, etc.)
- **(1)** Quench temperature
- **(1)** Transition boiling HTC

Powered Heater Rods

Housing/Enclosure

Spacer grid

With flat independent uncertainties, either in linear or log scales

Statistical Framework (1/4): Global Sensitivity Analysis

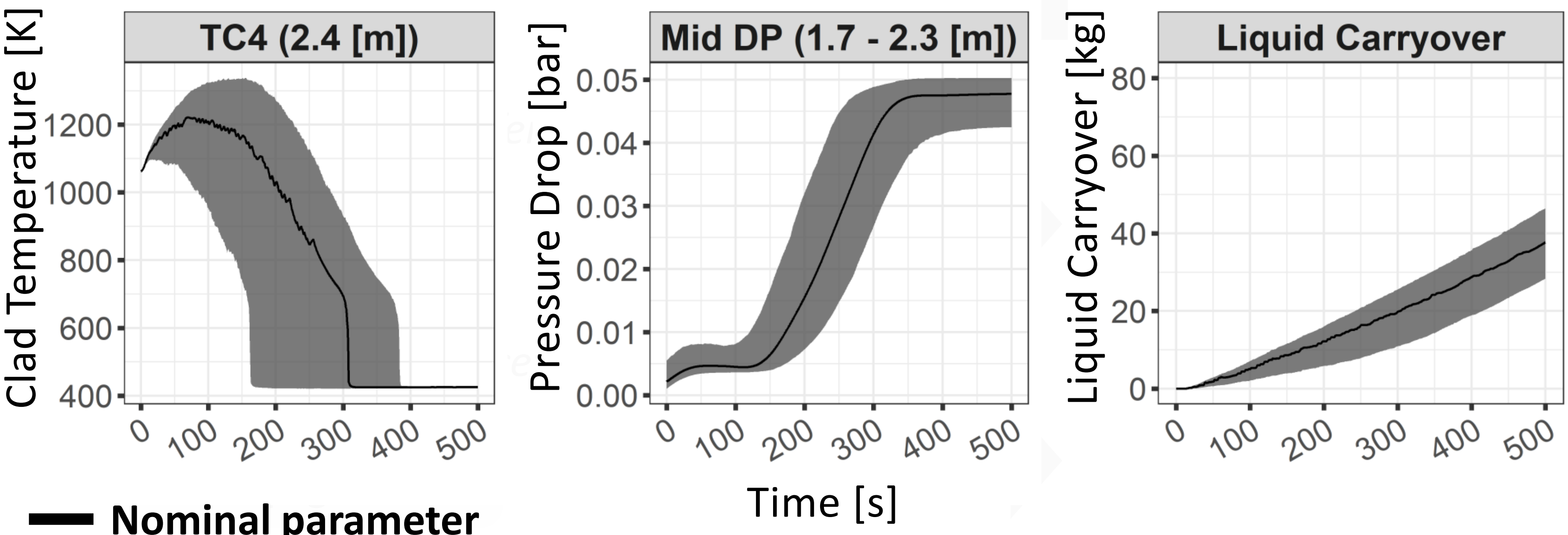
How to select the important parameters?

1. Global Sensitivity Analysis

27 initial parameters

Identify the least influential parameters, and exclude them

Propagation based on 1’000 samples



Global Sensitivity Analysis for Screening: The Morris Screening and Sobol' Total-Effect

Elementary effect EE_d:

Perturbation of one parameter at a time

$$EE_d \equiv \frac{f(\boldsymbol{x} + \Delta \cdot \boldsymbol{e}_d) - f(\boldsymbol{x})}{\Delta}$$

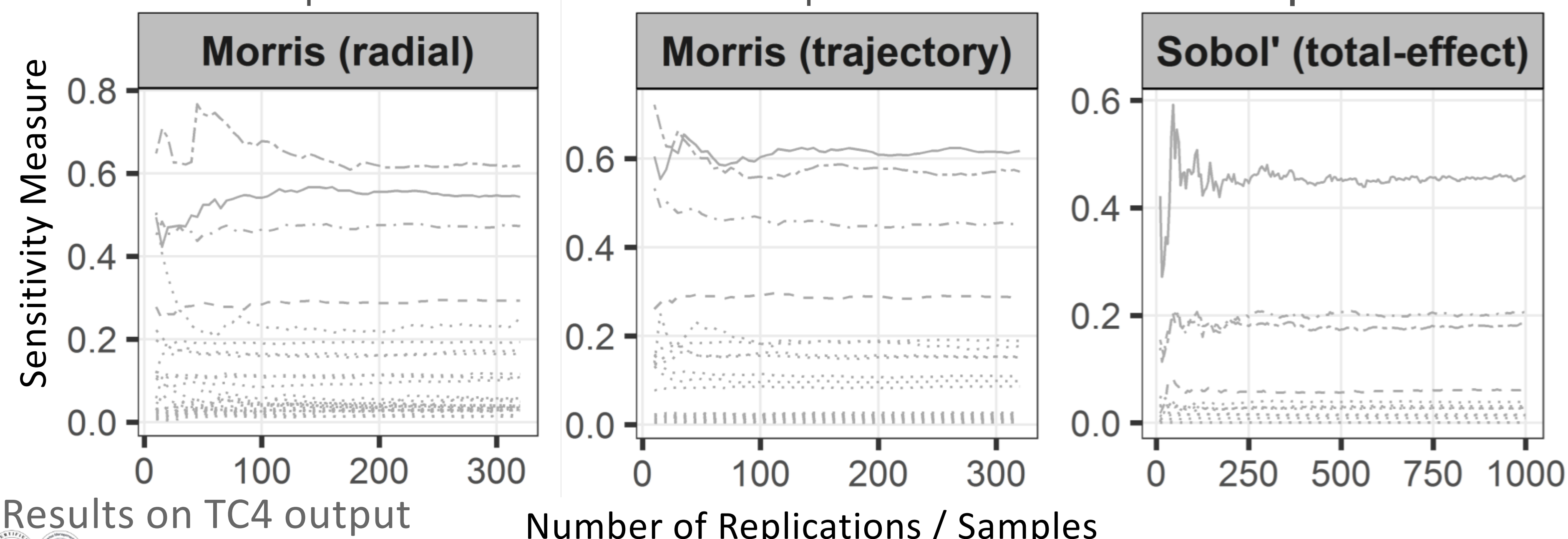
Grid size

Sobol' total-effect index for x_d:

$$ST_d \equiv \frac{\mathbb{E}_{\sim d}\left[\mathbb{V}_d[Y|\boldsymbol{X}_{\sim d}]\right]}{\mathbb{V}[Y]}$$

320 replications ⇒ $8'960$ code runs

10^3 samples ⇒ $29'000$ code runs



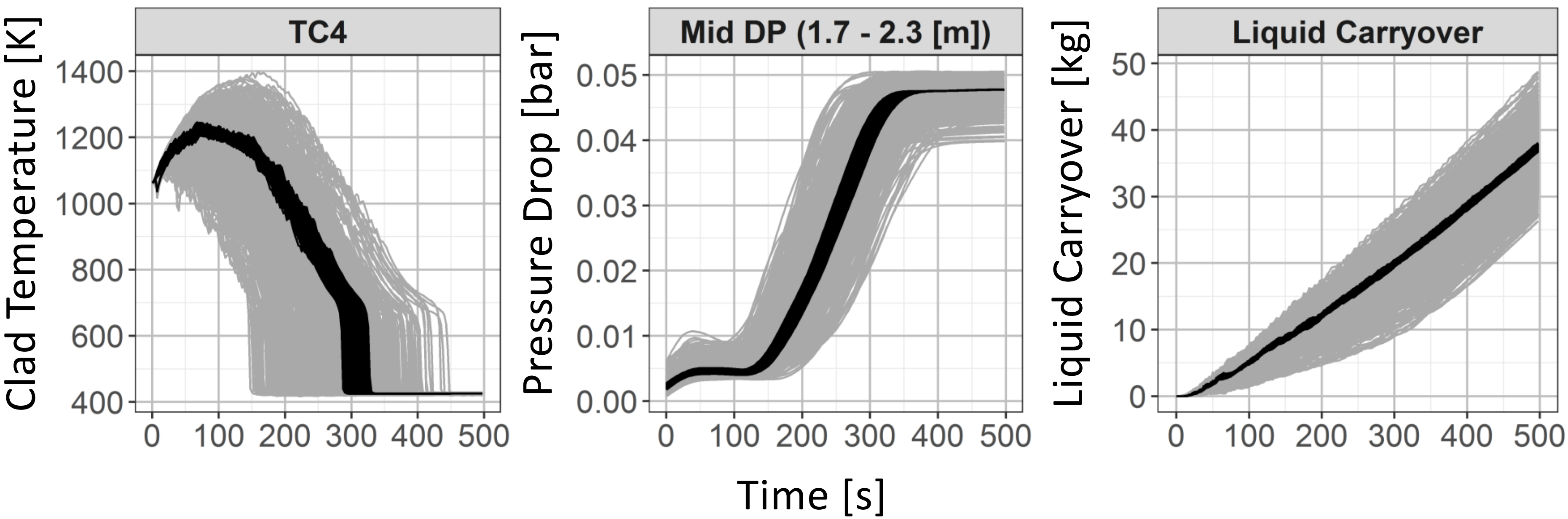
Results on TC4 output

Uncertainty Propagation using Influential vs. Non-Influential Parameters

12 parameters are influential: **(4)** x_c **Boundary conditions**
(8) x_m **Closure laws** and **spacer grid**

Uncertainty propagation using 2 parameter subsets
and 500 Monte Carlo samples

Parameter subsets — **12** Influential; **15** Non-influential



Statistical Framework (2/4): Metamodeling

How to select the important parameters?

1. Global Sensitivity Analysis

27 initial parameters → **12 influential** parameters

How to approximate the input/output of a computer model?

2. Metamodeling

- $\sim$ [min]/run
- $\sim 10^2$ [MB]/run

Construct a metamodel for fast and efficient approximation

Metamodel: “a model of a model”

Gaussian Process (GP) Metamodel

Gaussian process is a **Gaussian with continuous variates**: $Y(\boldsymbol{x}) \in \mathbb{R}; \boldsymbol{x} \in \mathbb{R}^{D}$

Gaussian Process

process variance

$$Y(\boldsymbol{x}) \sim GP\left(m(\boldsymbol{x}), \sigma^2 k(\boldsymbol{x}, \boldsymbol{x}^*)\right)$$

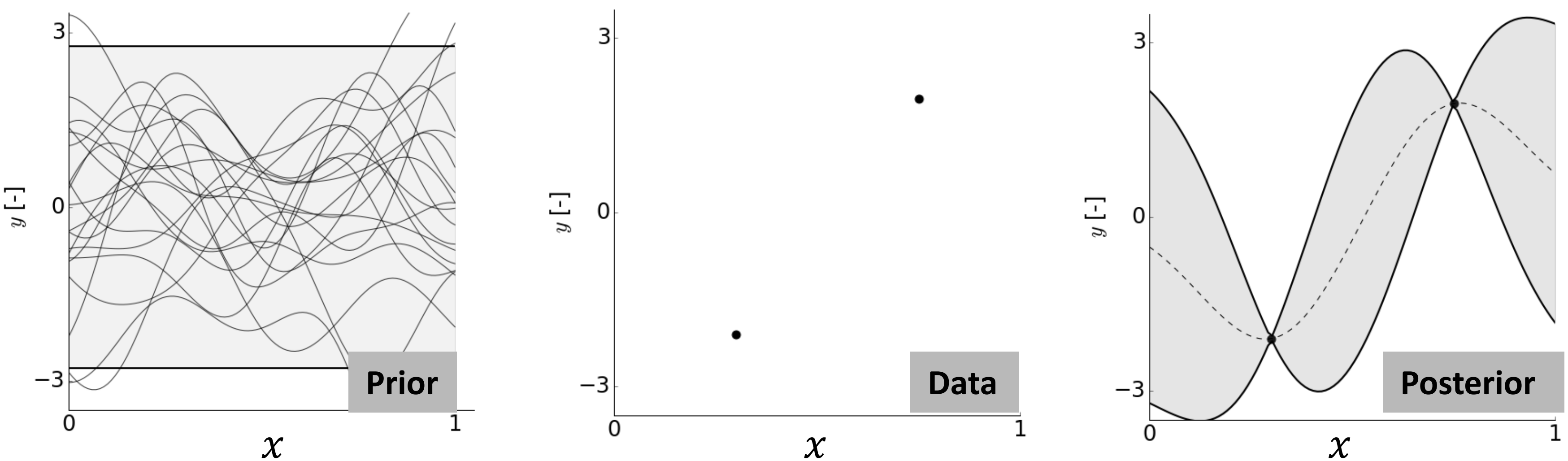
Probability distribution of functions

mean function

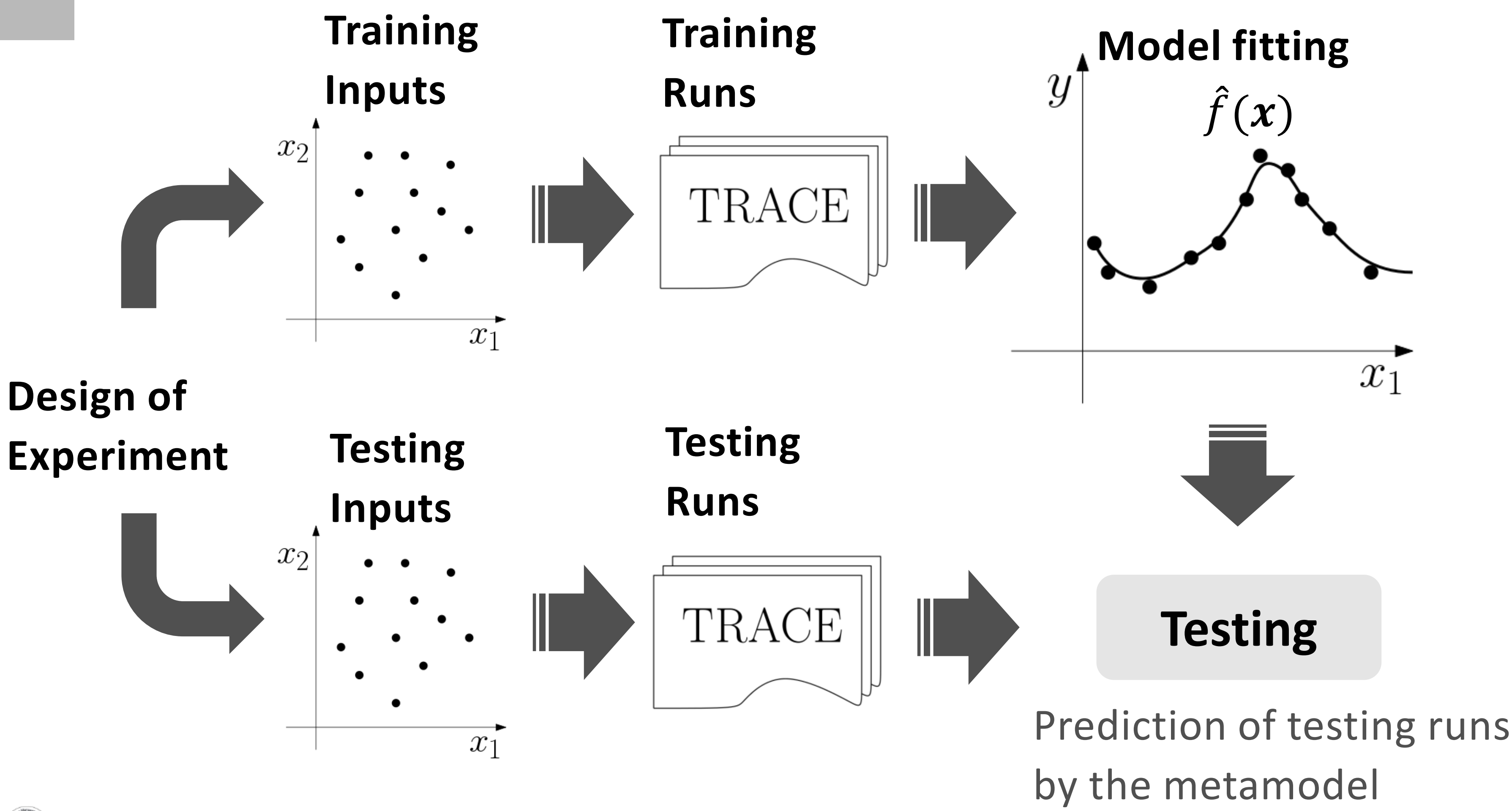
correlation (kernel) function

$$k(\boldsymbol{x}, \boldsymbol{x}^*) \equiv \mathrm{Cov}[Y(\boldsymbol{x}), Y(\boldsymbol{x}^*)]$$

Application in **Regression**

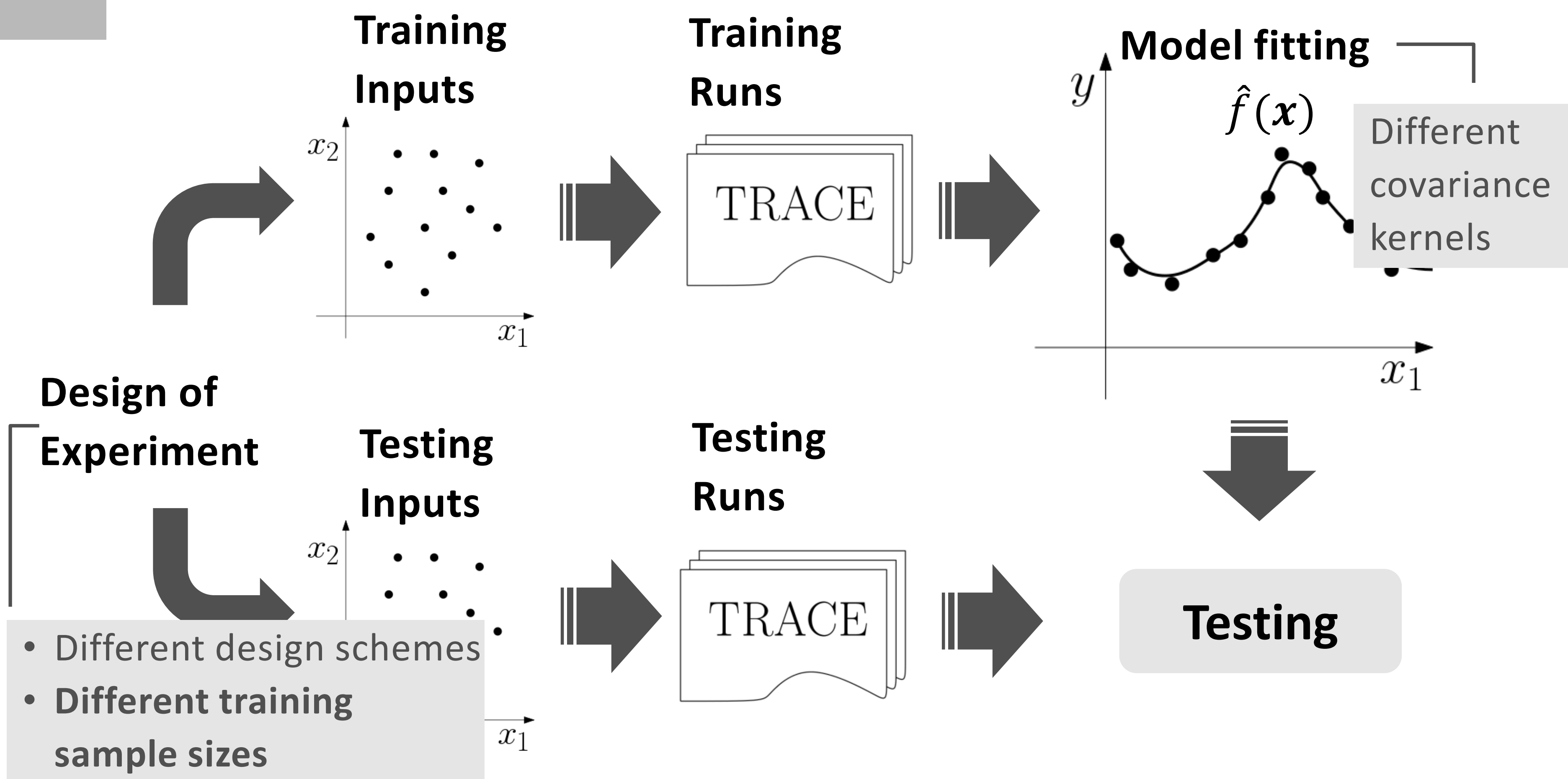


Constructing GP Metamodel: Training and Testing



Constructing GP Metamodel: Training and Testing

Different factors involved in the construction of GP Metamodel



Dealing with Multivariate Output: Principal Component Analysis

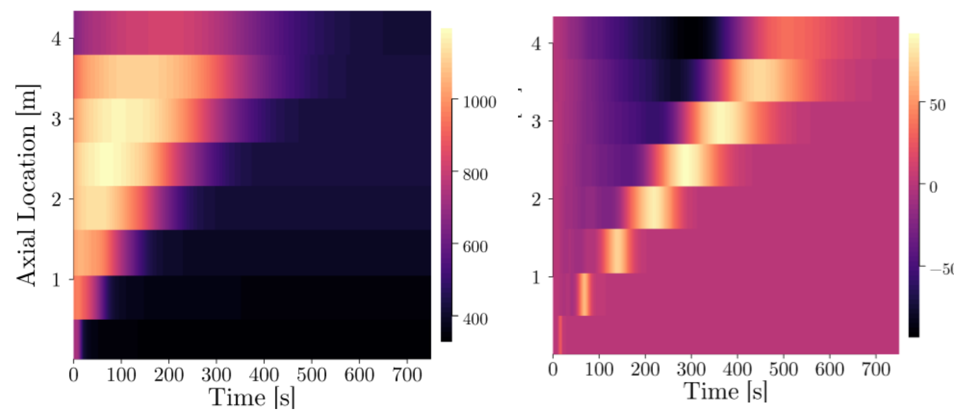
Output of the TRACE model of FEBA is highly **multivariate**.

Output Type	# of outputs $\mathrm{P} = \Delta z \times \Delta t$
Clad Temperature	$8 \times 10'000 = 80'000$
Pressure Drop	$4 \times 10'000 = 40'000$
Liquid Carryover	$1 \times 10'000 = 10'000$

Dimension reduction by **Principal Component Analysis** (PCA)

$$Y' = \overbrace{U \cdot S \cdot V^T}^{\textbf{SVD}} = W \cdot V^T$$

- Y': Concatenate and centered outputs
- V^T: Eigenvectors (**principal components**)
- W: PC scores



Mean and 1st PC of clad temperature output

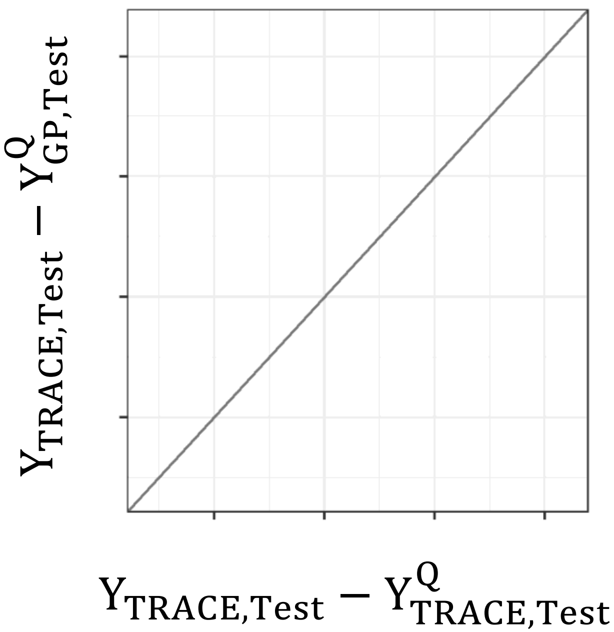
$$y^{\mathrm{model}}(\boldsymbol{x}; z, t) = \bar{y}^{\mathrm{model}}(z, t) + \sum_{i=1}^{Q} v_i(z, t) \cdot w_i(\boldsymbol{x})$$

- $y^{\mathrm{model}}(\boldsymbol{x}; z, t)$: Prediction of multivariate output
- $\bar{y}^{\mathrm{model}}(z, t)$: the mean of output
- $w_i(\boldsymbol{x})$: **PC scores, predicted by GP metamodel**

$\boldsymbol{Q_{TC} = 7}$
$\boldsymbol{Q_{DP} = 10}$
$\boldsymbol{Q_{CO} = 5}$

Testing the Metamodel against Testing Samples

Metamodel predictive performance is assessed by comparison against large independent test data (i.e. actual TRACE runs)



X-axis: $Y_{\mathrm{TRACE,Test}} - Y^{Q}_{\mathrm{TRACE,Test}}$

- Dimension reduction error
- Due to **smaller *Q*** to reconstruct the full output space

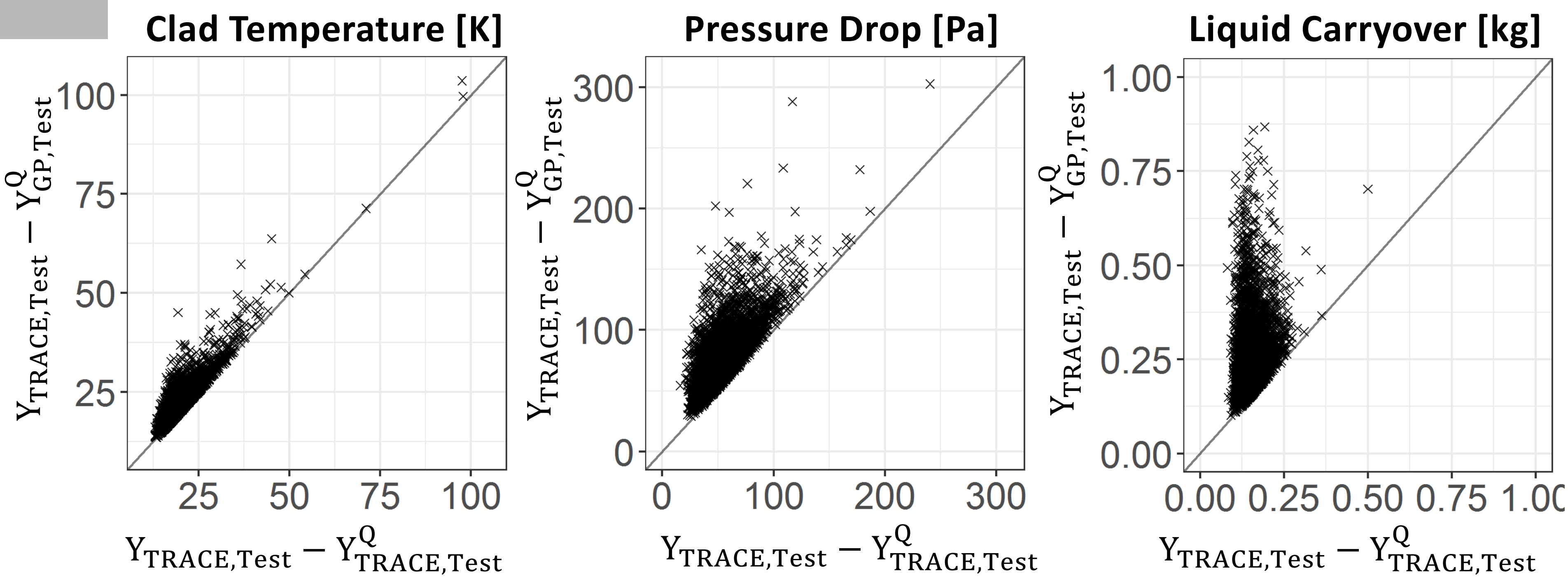
Y-axis: $Y_{\mathrm{TRACE,Test}} - Y^{Q}_{\mathrm{GP,Test}}$

- Dimension reduction error **and** GP error
- Due to (also) **miss-prediction of PC scores**

Both are in terms of RMSE

Testing the Metamodel against Testing Samples ($N_{test} = 5'000$)

Metamodel predictive performance is acceptable for each output ($N_{train} = 1'920$)



	Clad Temperature	Pressure Drop	Liquid Carryover
GP PC RMSE	22.4 [K]	77.95 [Pa]	0.27 [kg]
Testing Samples σ	254. [K]	9'200 [Pa]	30.4 [kg]
	$(< \mathbf{9}\%)$	$(< \mathbf{0.9}\%)$	$(< \mathbf{0.9}\%)$

Statistical Framework (3/4): Bayesian Calibration

How to select the important parameters?

1. Global Sensitivity Analysis

27 initial parameters → **12 influential** parameters

How to approximate the input/output of a computer model?

2. Metamodeling

- $\sim$ [min]/run
- $\sim 10^2$ [MB]/run

→

- $\sim$ [s]/run
- $\sim 10^2$ [MB]

How to make the uncertainty quantification?

3. Bayesian Calibration

Wide, independent prior uncertainties

Use experimental data to constrain the prior

Bayesian Calibration, Inverse Quantification:
Uncertain (Inputs + Data) ⇒ Uncertain Inputs Updated

Experimental Data from SETF $\boldsymbol{D}$

Probability of observing data given parameters

Controllable inputs (w.r.t experiment) $\boldsymbol{x}_c$

Uncertain model parameters (prior) $\boldsymbol{X}_m$

Forward Model
$\boldsymbol{M}: (\boldsymbol{x}_c, \boldsymbol{x}_m) \mapsto \boldsymbol{Y}$

Likelihood
$p(\boldsymbol{D}|\boldsymbol{x}_m, \boldsymbol{x}_c)$

Additional sources of uncertainty

$\boldsymbol{X}_m|\boldsymbol{D}, \boldsymbol{x}_c$

Uncertain model parameters (posterior)

Bayes' Theorem

Normal Likelihood

Experimental Data | Model prediction | Model bias | Measurement error

$$y^{\exp}(z,t) = y^{\mathrm{M}}(\boldsymbol{x}_m; z,t) + \delta(z,t) + \epsilon$$

given | GP | unknown | GP | Gaussian

Likelihood

Multiple sources of variance

$$p(y^{\exp}|\boldsymbol{x}_m) \sim N\Big(\tilde{y}^M + m_b, \underbrace{\boldsymbol{V}\Sigma_w\boldsymbol{V}^{\boldsymbol{T}}}_{\text{GP metamodel}} + \underbrace{\boldsymbol{V}_{>\boldsymbol{P_{tr}}} S_{>P_{tr}} \boldsymbol{V}^{\boldsymbol{T}}_{>\boldsymbol{P_{tr}}}}_{\text{Principal Comp. truncation}} + \underbrace{\Sigma_b}_{\text{Model bias}} + \underbrace{\sigma^2_{\exp}\boldsymbol{I}}_{\text{measurement}}\Big)$$

6 calibration schemes were investigated:

- Considering different types of data
- With or without model bias term
- Excluding a model parameter

Posterior Formulation and Computation

Uncertainty on $\boldsymbol{x}_m$ is fully specified by $p\left(\boldsymbol{x}_m \middle| \{y^{\text{exp}}\}\right)$, the posterior pdf.

Bayes' Theorem

Posterior, Likelihood, Prior

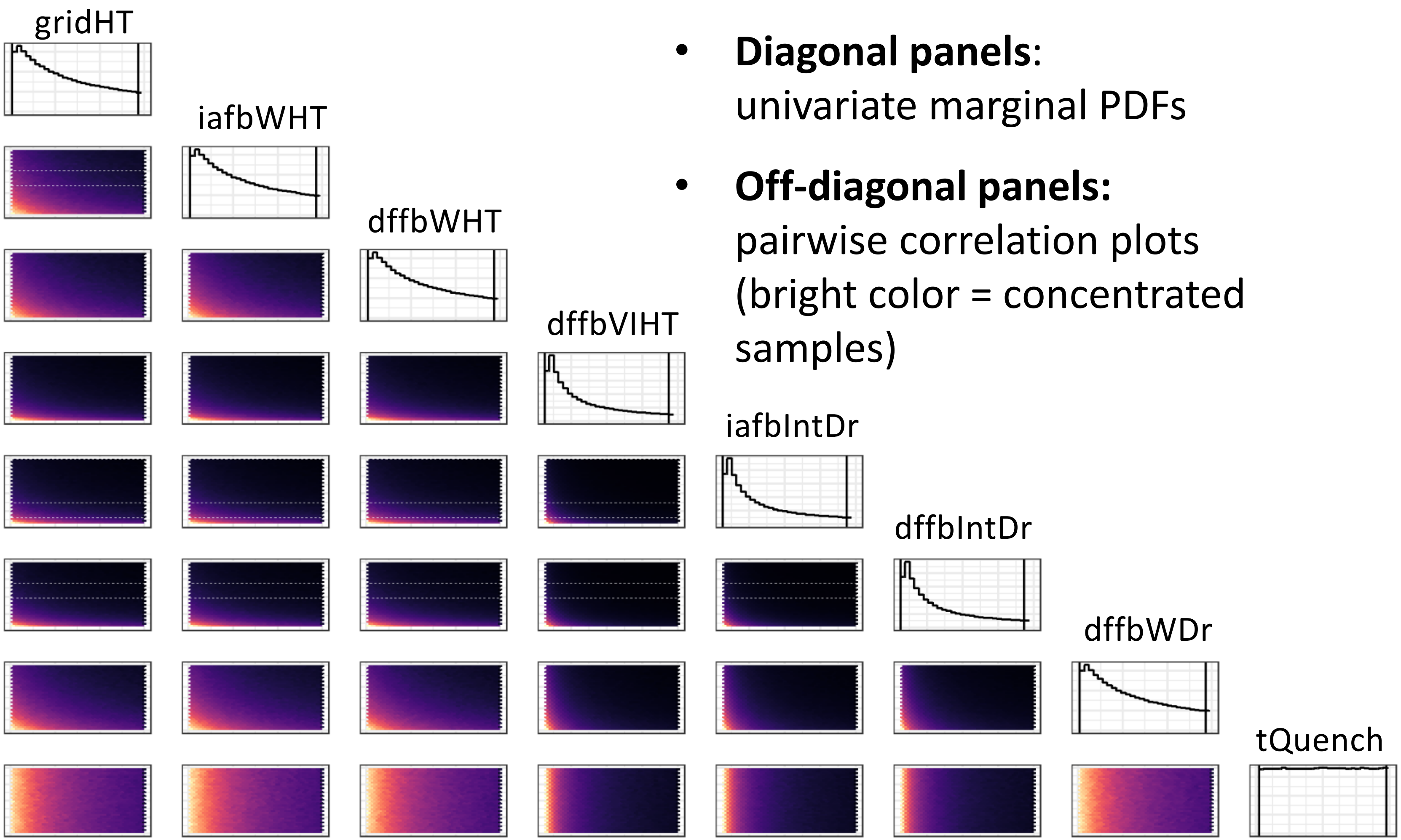
$$\underbrace{p\left(\boldsymbol{x}_m \middle| \{y^{\text{exp}}\}\right)}_{\text{Posterior}} = \frac{\underbrace{p(\{y^{\text{exp}}\}|\boldsymbol{x}_m)}_{\text{Likelihood}} \times \underbrace{p(\boldsymbol{x}_m)}_{\text{Prior}}}{\int_{\boldsymbol{x}_m} p(\{y^{\text{exp}}\}|\boldsymbol{x}_m) \times p(\boldsymbol{x}_m)\, d\boldsymbol{x}_m}$$

How $p\left(\boldsymbol{x}_m \middle| \{y^{\text{exp}}\}\right)$ is used:

- Uncertainty propagation in an application setting (**integration of a function under the posterior pdf**)
- Characterization of parameter uncertainty, e.g., moments (**integration of the pdf over the parameter space**)

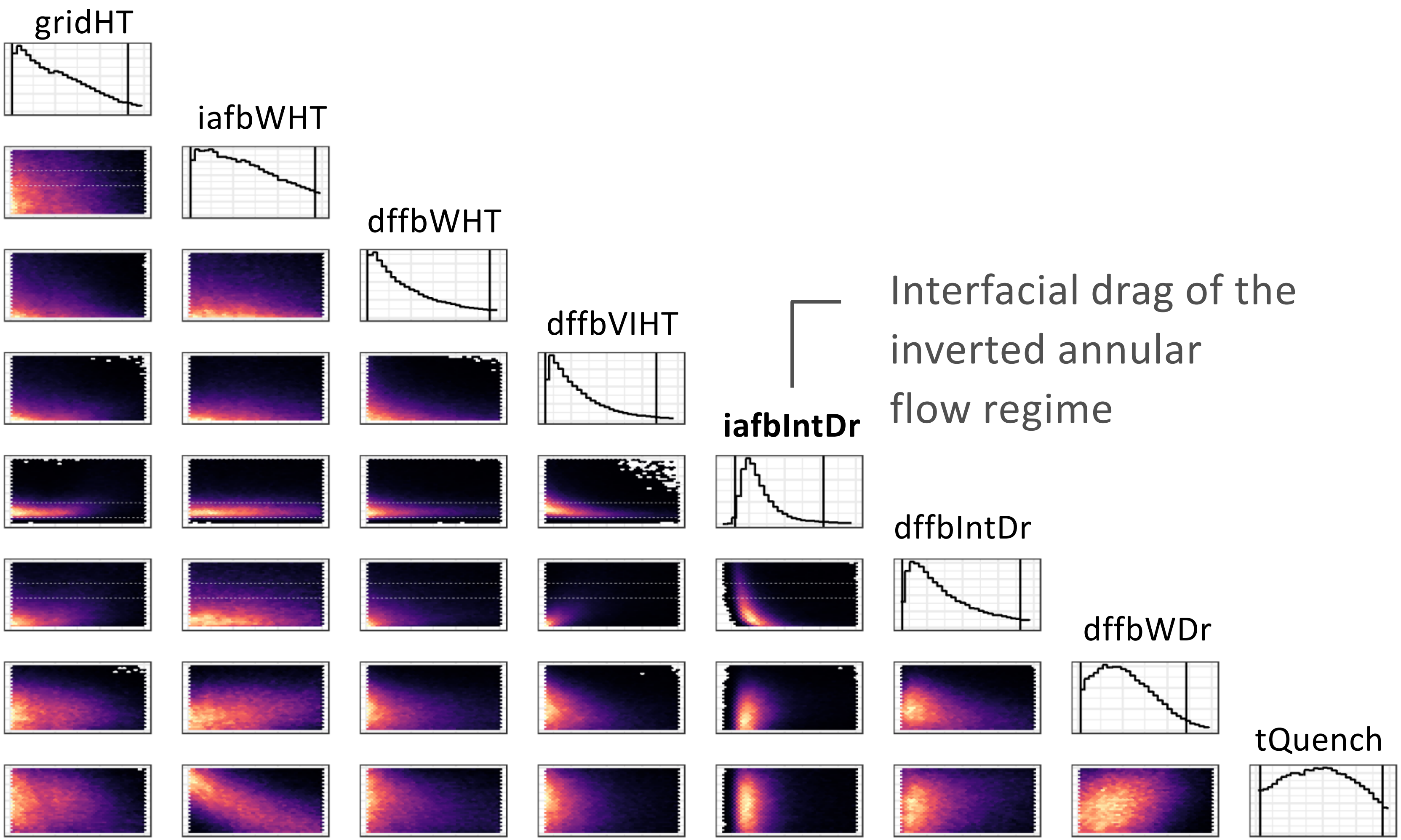
Markov Chain Monte Carlo (MCMC) Simulation

Prior uncertainty of the model parameters



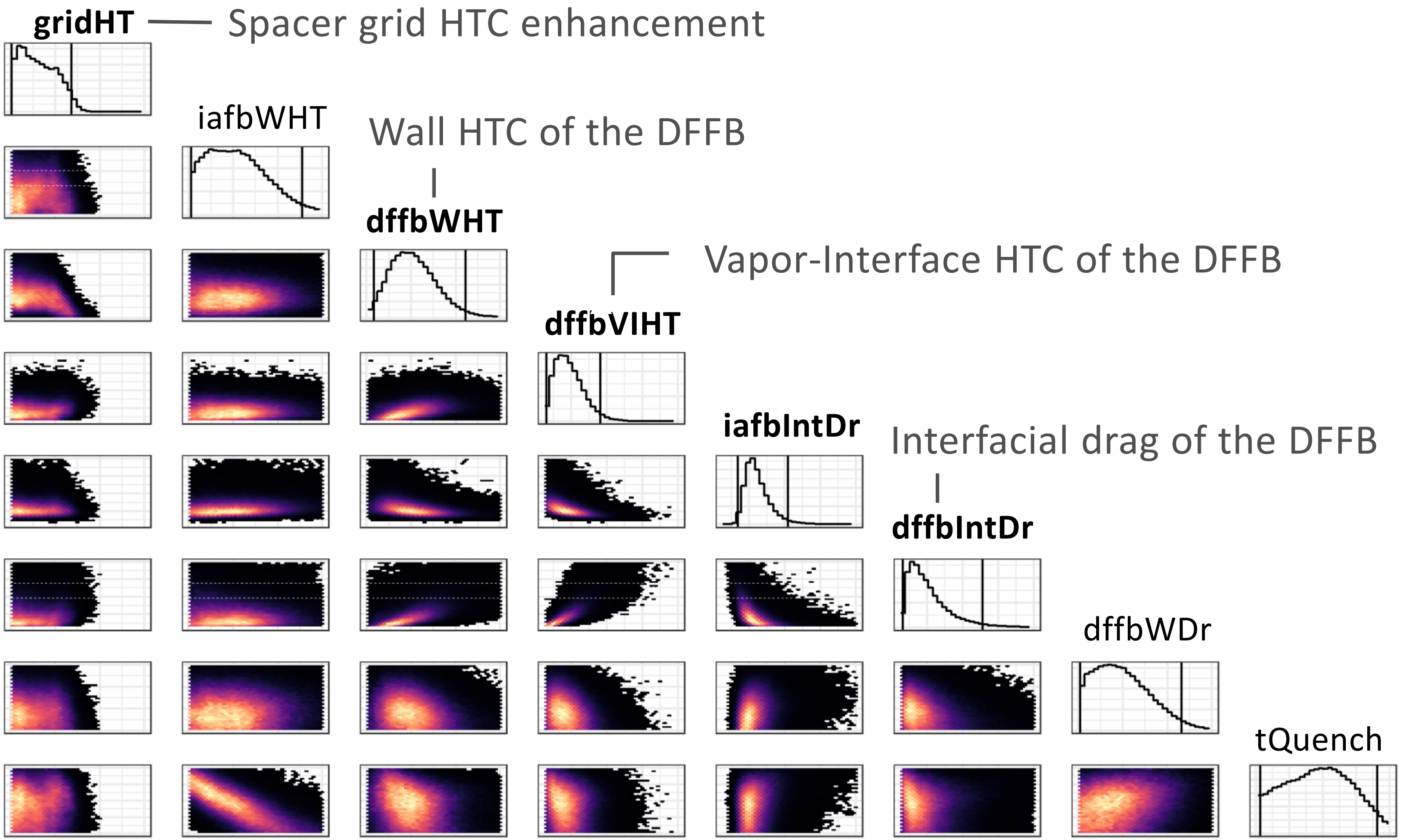
- **Diagonal panels**: univariate marginal PDFs
- **Off-diagonal panels:** pairwise correlation plots (bright color = concentrated samples)

The posterior uncertainty based on pressure drop data only ($\approx 10^6$ samples)

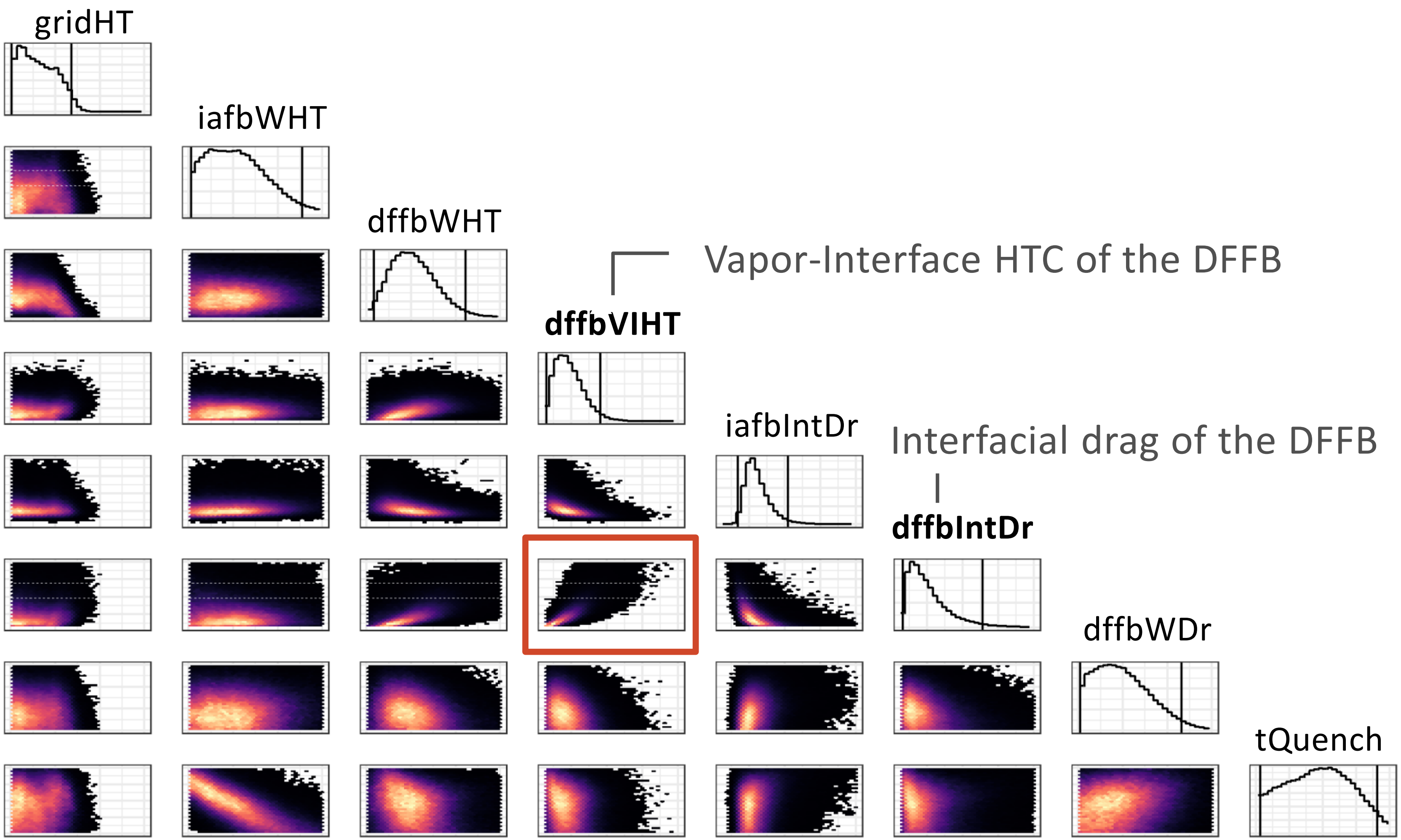


Interfacial drag of the inverted annular flow regime

Posterior on all types of data ($\approx \mathbf{10^6}$ samples)

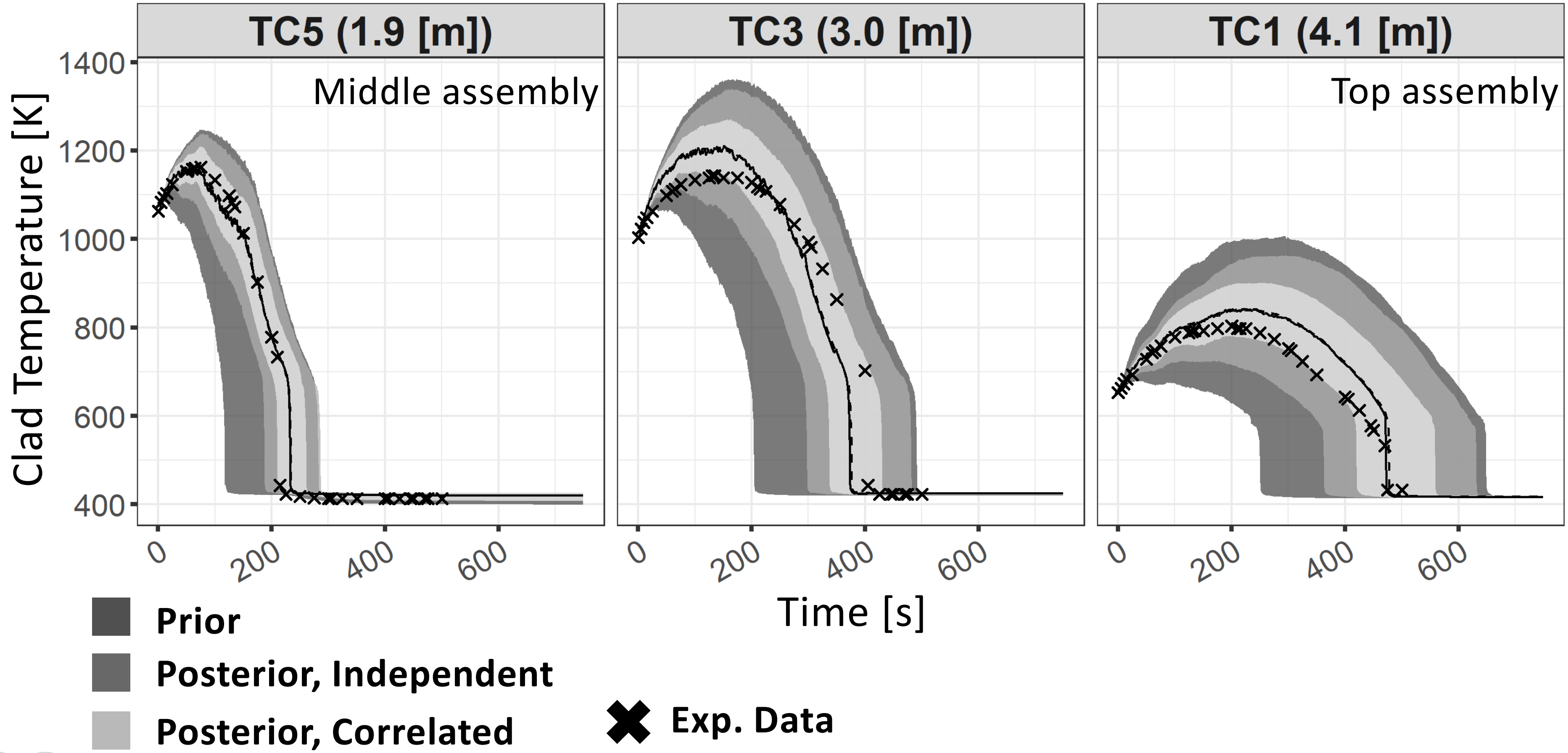


Posterior on all types of data ($\approx \mathbf{10^6}$ samples)



Posterior Samples are Correlated (i.e., a set of "collectively-fitted" values)

Uncertainty propagation on FEBA Test. No. 216 (the calibration data) based on 1'000 Monte Carlo samples.



Statistical Framework (4/4): Posterior Uncertainty Propagation

How to select important parameters to be inferred?

1. Global Sensitivity Analysis	**27 initial** parameters	➡	**12 influential** parameters

How to approximate the input/output of a computer model?

2. Metamodeling	• $\sim$ [min]/run • $\sim 10^2$ [MB]/run	➡	• $\sim$ [s]/run • $\sim 10^2$ [MB]

How to make the uncertainty quantification?

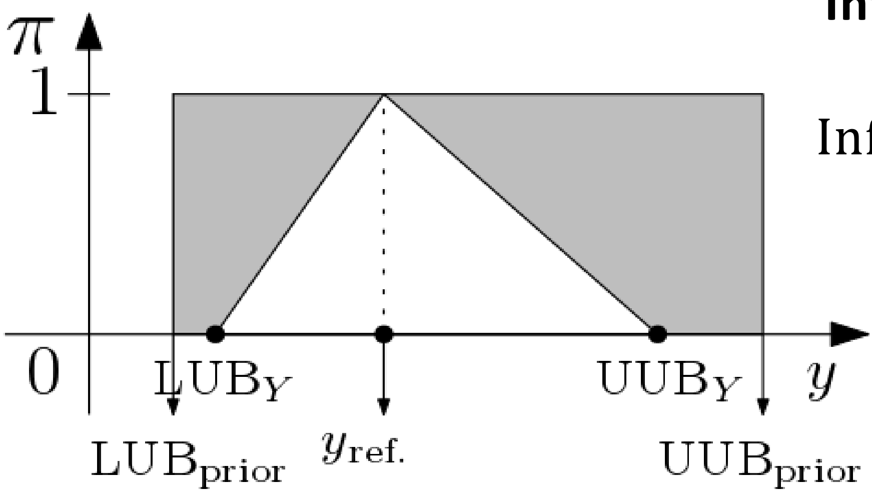
3. Bayesian Calibration	Wide, independent prior uncertainties	➡	Narrower, correlated posterior uncertainties

How good is the quantified uncertainty?

4. Uncertainty Propagation	Wide prior prediction uncertainties	**Propagate posterior uncertainties for different experimental conditions**

Comparing Different Calibration Results: Informativeness

Two scores to summarize and compare results of uncertainty propagation using different posterior samples w.r.t the prior



Informativeness for output y

$$\mathrm{Inf}_Y = 1 - \frac{1}{2}\frac{\mathrm{UUB}_{\mathrm{post.}} - \mathrm{LUB}_{\mathrm{post.}}}{\mathrm{UUB}_{\mathrm{prior}} - \mathrm{LUB}_{\mathrm{prior}}}$$

LUB: Lower Uncertainty Bound
(2.5$^{\mathrm{th}}$ prediction percentile)

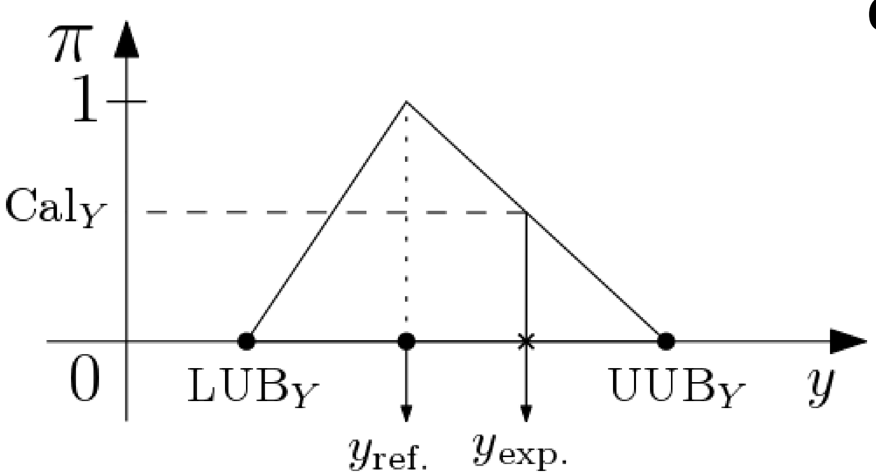
UUB: Upper Uncertainty Bound
(97.5$^{\mathrm{th}}$ prediction percentile)

$\mathrm{Inf}_Y = 0.5$ Posterior prediction uncertainty **is equal to** that of the prior

$\mathrm{Inf}_Y = 1.0$ No posterior prediction uncertainty

Comparing Different Calibration Results: Calibration Score

Two scores to summarize and compare results of uncertainty propagation using different posterior samples w.r.t the prior



Calibration Score for output y

$$\mathrm{Cal}_{\mathrm{Y}} = \pi_Y(\mathrm{y}_{\mathrm{exp}})$$

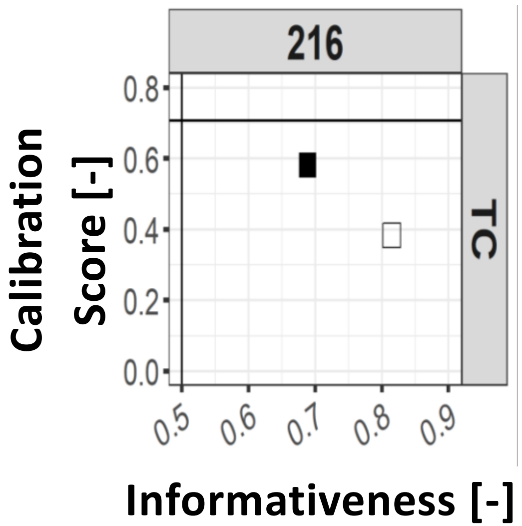
The height of the experimental data in the information triangle

$y_{\mathbf{ref}}$: Reference value
(50^{th} prediction percentile; median)

$\mathrm{Cal}_{\mathrm{Y}} = 0.0$ Experimental data **falls outside** the uncertainty band

$\mathrm{Cal}_{\mathrm{Y}} = 1.0$ Experimental data matches the reference value **exactly**

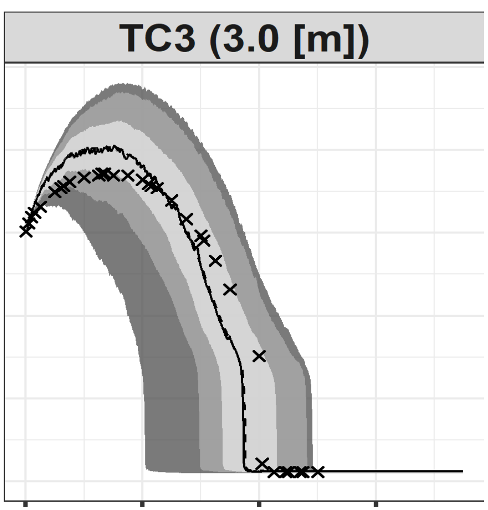
Posterior Prediction Uncertainty in Terms of Calibration Score and Informativeness



$P_{sys} = 4.1$ [bar]
$V_{inlet} = 3.8$ [cm. s^{-1}]

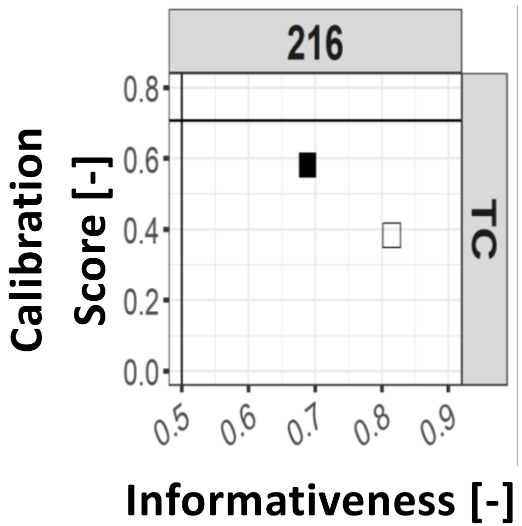
Calibration Scheme

- All Parameters, Correlated
- All Parameters, Independent



Prior
Posterior, Independent
Posterior, Correlated
Exp. Data

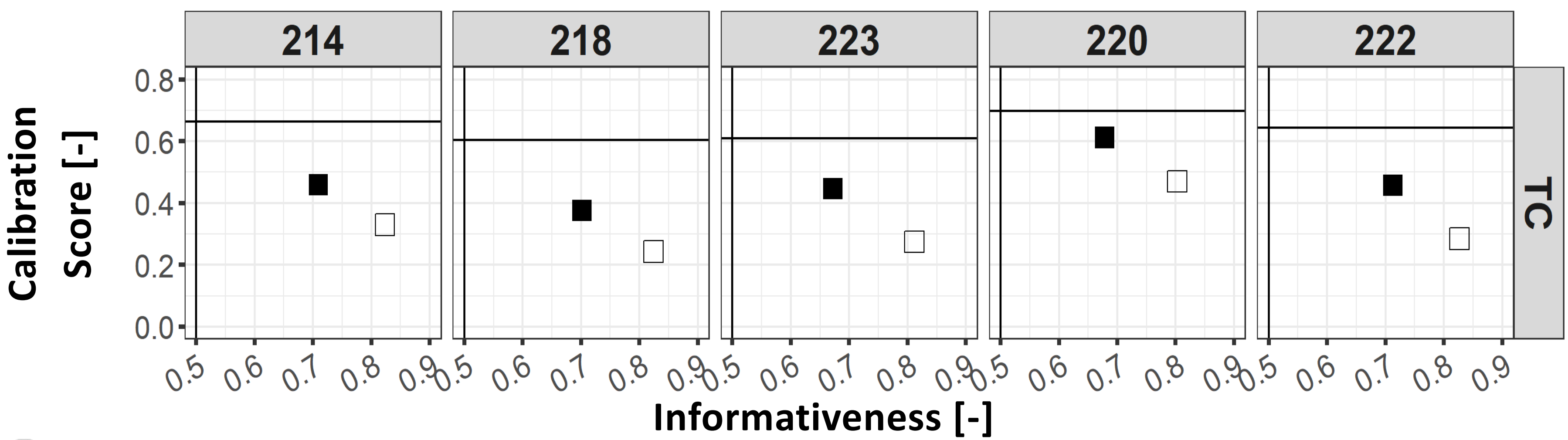
Effects of Experimental Conditions on Posterior Prediction Uncertainty



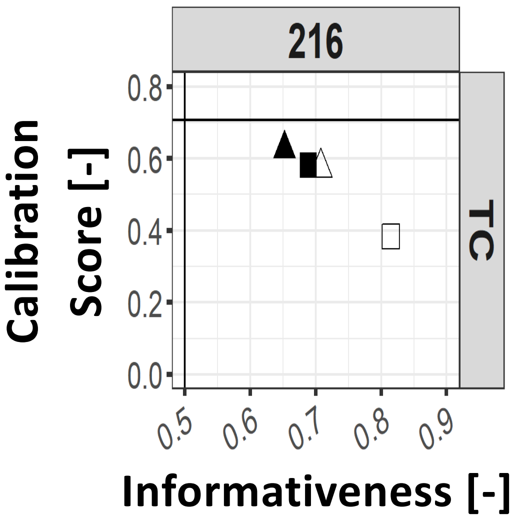
$P_{\text{sys}} = 4.1\ [\text{bar}]$
$V_{\text{inlet}} = 3.8\ [\text{cm. s}^{-1}]$

Calibration Scheme

- □ All Parameters, Correlated
- ■ All Parameters, Independent



Removing a Highly Correlated Influential Parameter from the Calibration

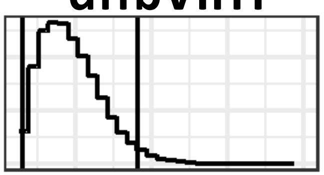


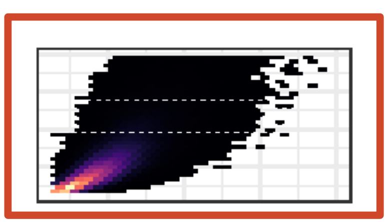
$P_{sys} = 4.1$ [bar]
$V_{inlet} = 3.8\ [\mathrm{cm.s^{-1}}]$

Calibration Scheme

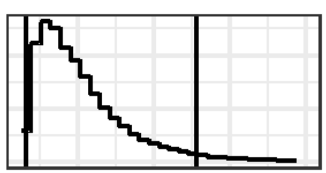
- □ All Parameters, Correlated
- ■ All Parameters, Independent
- △ Excl. dffbVIHT, Correlated
- ▲ Excl. dffbVIHT, Independent

dffbVIHT — Vapor-Interface HTC of the DFFB

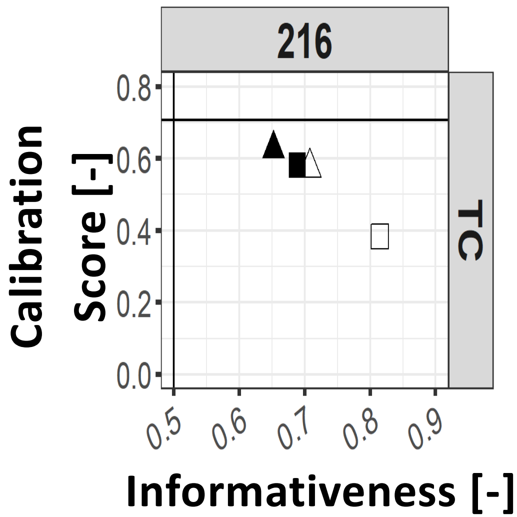




dffbIntDr — Interfacial drag of the DFFB



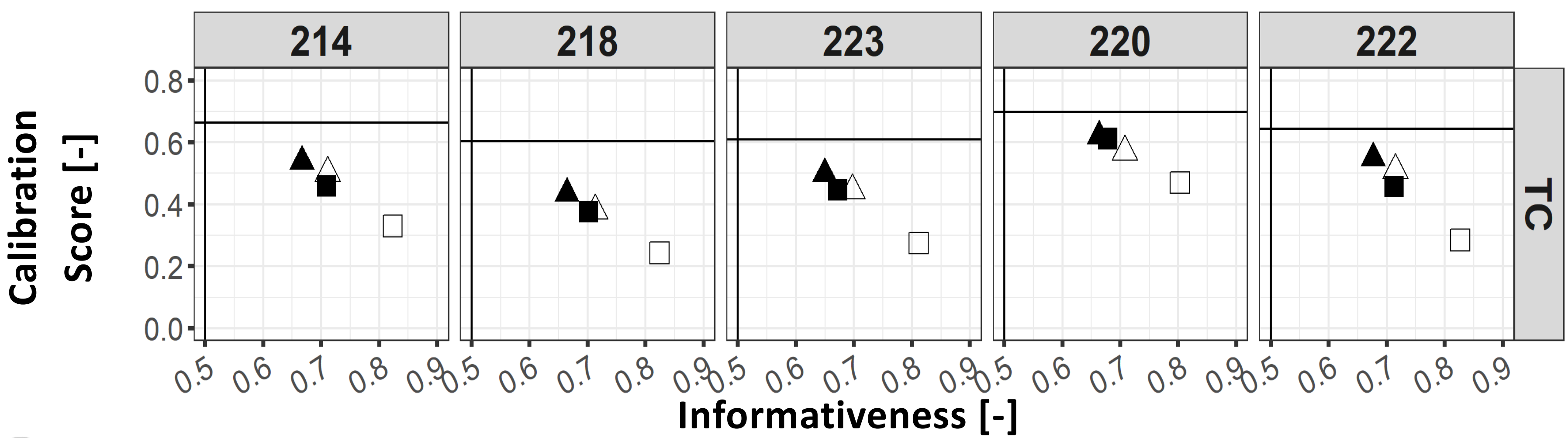
Effects of Experimental Conditions on Posterior Prediction Uncertainty



$P_{sys} = 4.1$ [bar]
$V_{inlet} = 3.8$ [cm. s^{-1}]

Calibration Scheme

□ All Parameters, Correlated
■ All Parameters, Independent
△ Excl. dffbVIHT, Correlated
▲ Excl. dffbVIHT, Independent



Conclusion

Motivation:

Uncertainty in physical model parameters are often derived mainly based on expert-judgment and on a particular experimental data

Objectives:

Given data from a separate effect test facility, develop a methodology to systematically quantify the uncertainty of the parameters in the TRACE code

Contribution:

Consolidation, implementation, and application of tools
based on statistical framework
for quantifying the physical model parameters in the TRACE code

Contributions: Demonstration of the Methodology on the FEBA TRACE Model

How to select important model parameters?

1. Global Sensitivity Analysis — **27 initial** parameters → **12 influential** parameters

How to approximate the input/output of a computer model?

2. Metamodeling
- $\sim$ [min]/run
- $\sim 10^2$ [MB]/run

→

- $\sim$ [s]/run
- $\sim 10^2$ [MB]

How to make the quantification?

3. Bayesian Calibration — Wide, independent prior uncertainties → Narrower, correlated posterior uncertainties

How good is the quantified uncertainty?

4. Uncertainty Propagation — Wide prior prediction uncertainties → Narrower posterior prediction uncertainties for all exp. conditions

Contributions

Developed Tools:

- `trace-simexp`
  Python3 command line utilities for conducting simulation experiment of a TRACE model of Separate effect test facility
- `gsa-module`
  Python3 module implementing various design of experiments and global sensitivity analysis methods (e.g. Morris and Sobol' indices est.)

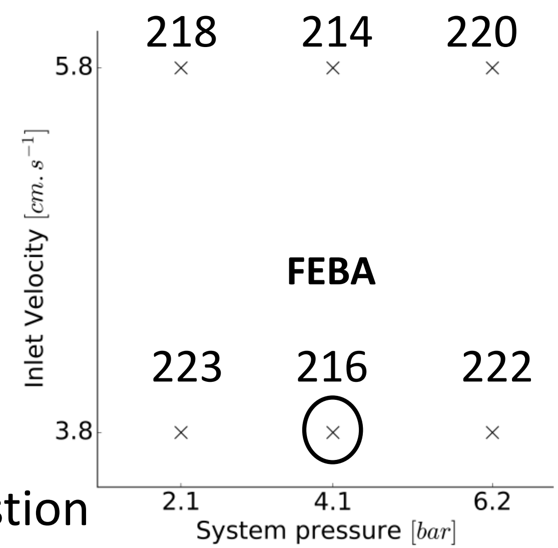
Publications and other contributions:

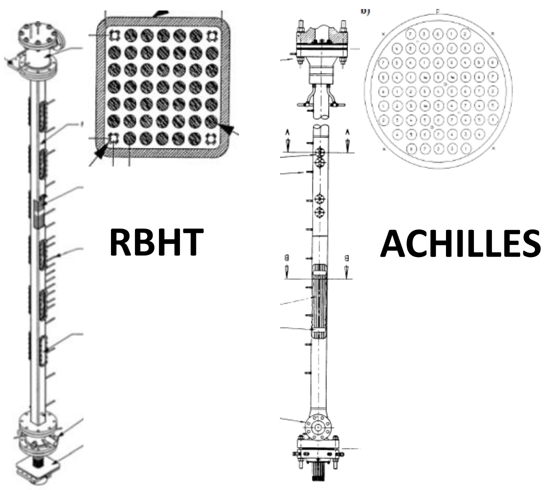
- 4 International conference papers
- 1 journal article
- 2 submissions to the OECD/NEA PREMIUM benchmark Phase 4
- 2 contributions to the OECD/NEA PREMIUM reports
- 1 PSI technical report

Upcoming Challenges

Bayesian Calibration

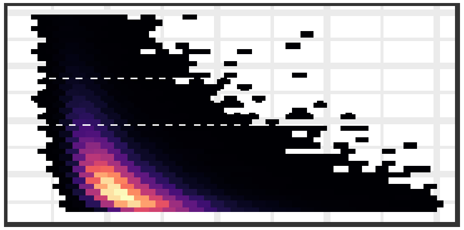
- Calibration was only done based on one dataset.
  Error structure might differ
- Sequential calibration against other SETF remains open question

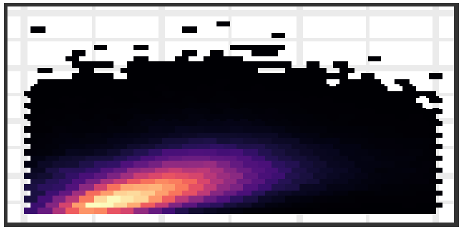




Uncertainty Propagation

How to summarize generic correlation structure of the posterior useful for downstream analysis?





Wir schaffen Wissen – heute für morgen

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1. "Global Sensitivity Analysis of Transient Code Output applied to a Reflood Experiment Model using TRACE Code," NSE, vol. 184, no. 6, 2016.
2. "Bayesian Calibration of Thermal-Hydraulics Model with Time-Dependent Output," NUTHOS-11, 2016.
3. "A Methodology for Global Sensitivity Analysis of Transient Code Output applied to Reflood Experiment Model using TRACE," NURETH-16, 2015.
4. "Sensitivity Analysis of Bottom Reflood Simulation using the Morris Screening Method," NUTHOS-10, 2014.
5. "Exploring Variability in Reflood Simulation Results: an Application of Functional Data Analysis," NUTHOS-10, 2014.

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