

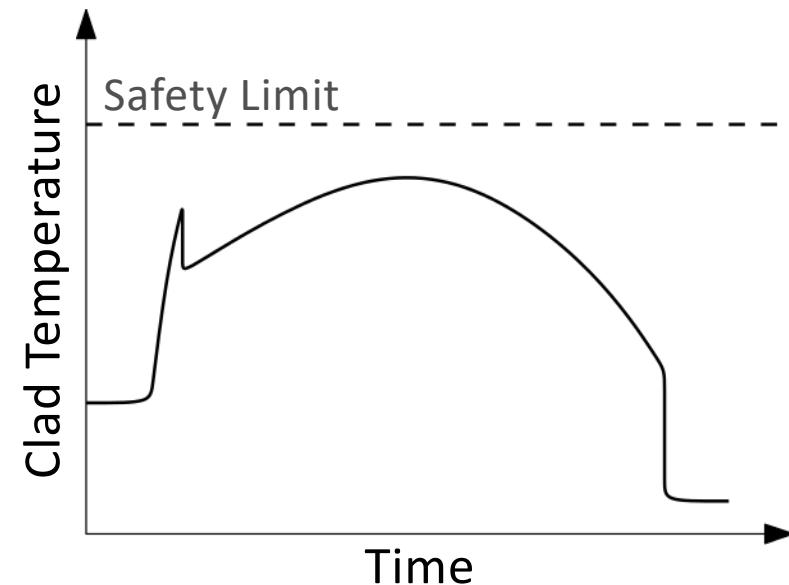
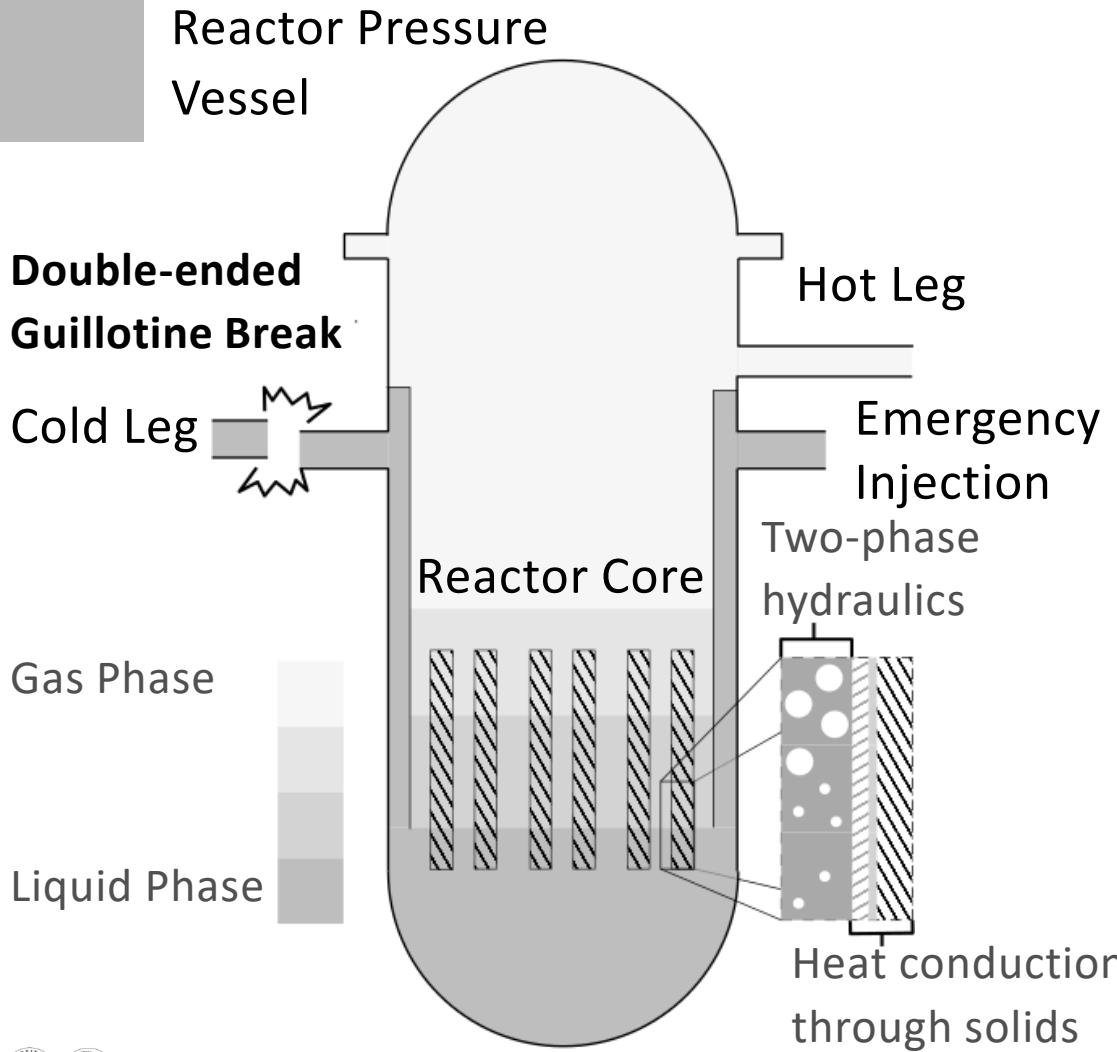


Damar Wicaksono (Thesis Directors: Prof. A. Pautz & Mr. O. Zerkak)

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

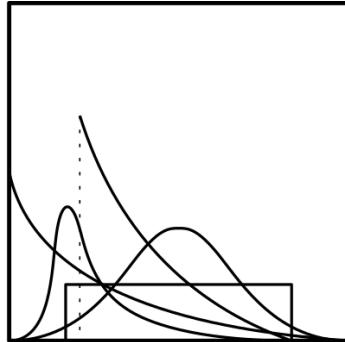
PhD Defense, EPF Lausanne, 19.01.2018

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



Forward Uncertainty Quantification:

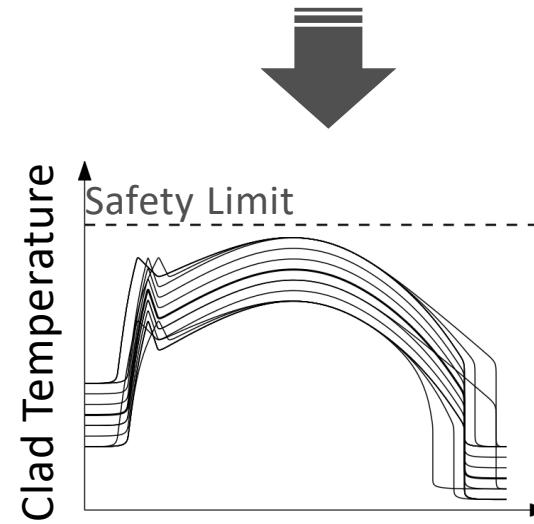
Uncertain Inputs \Rightarrow Uncertain Outputs



Uncertain Inputs
(random variables)

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

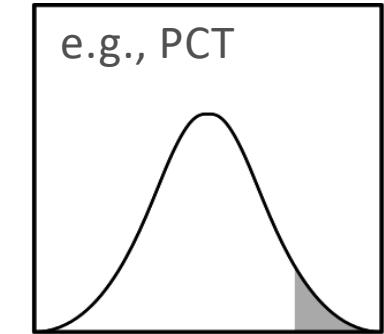
Forward Model (Code)
 $f: x \mapsto y$



Uncertain Outputs

Monte Carlo simulation
(multiple code runs)

Statistical Analysis
of ``Quantities of Interest''



Decision Making

Safe/Fail, Accept/Reject, etc.

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

Mass

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

Closure Laws

Parametric
models

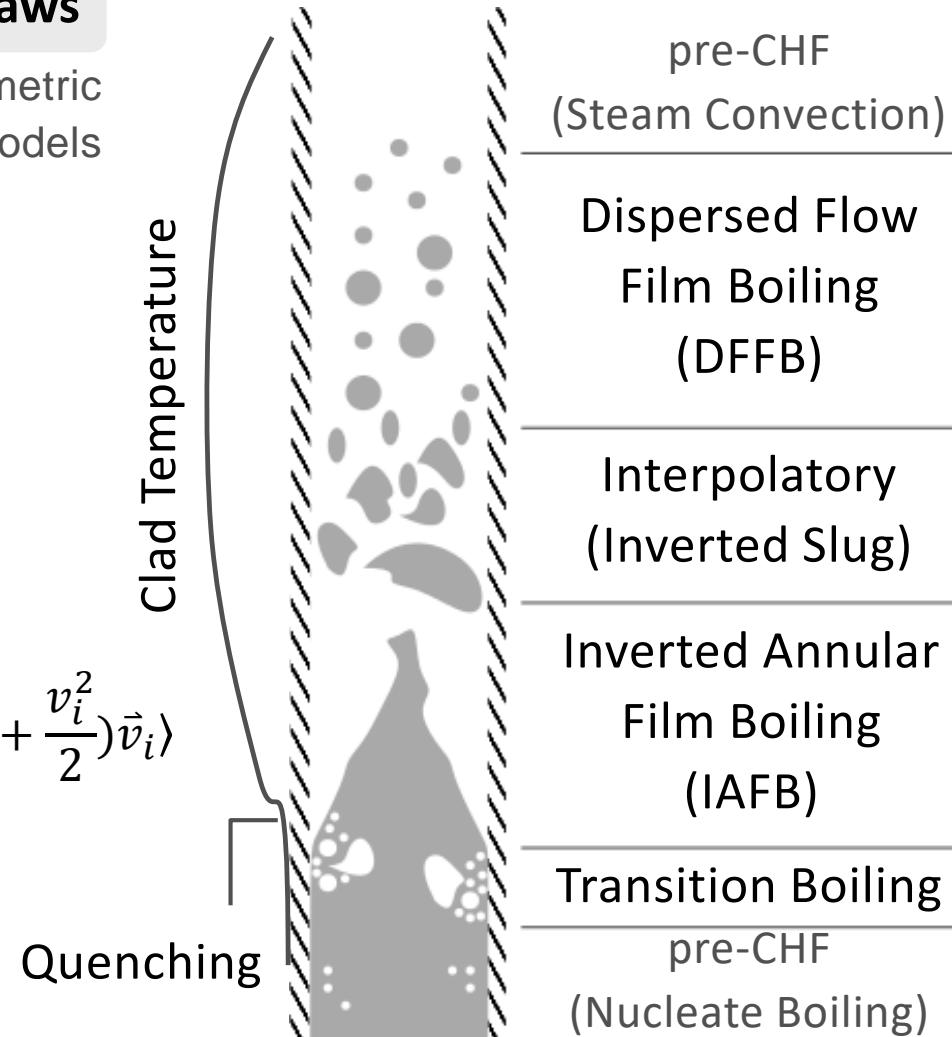
Momentum

$$\begin{aligned} \frac{\partial \langle \alpha_i \rho_i \vec{v}_i \rangle}{\partial t} + \langle \nabla \cdot \alpha \rho_i \vec{v}_i \vec{v}_i \rangle + \langle \alpha \nabla P \rangle \\ = -\langle \vec{f}_{\text{int}} \rangle + \langle \vec{f}_{w_i} \rangle + \langle \alpha \rho_i \vec{g} \rangle + \langle \Gamma_{\text{int}} \vec{v}_i \rangle \end{aligned}$$

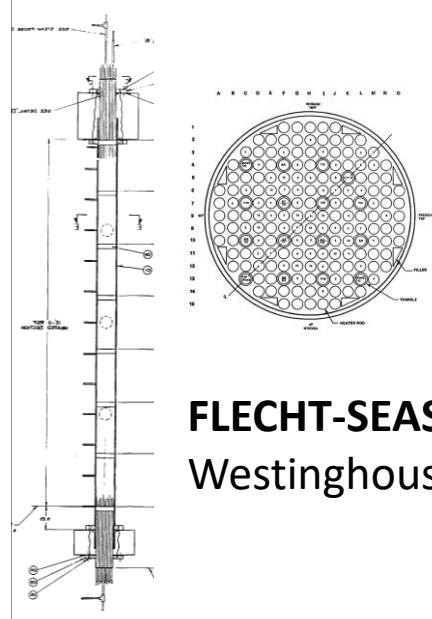
Energy

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

$i = G$ (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 $\frac{3}{4}$ to better match FLECHT-SEASET** high flooding rate reflood data, so...” (pp. 166)

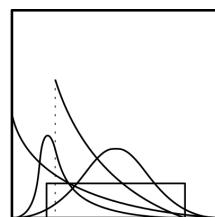
No statement of uncertainty on these parameters

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.



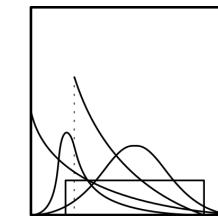
Pre-calibration
uncertainties



Calibration

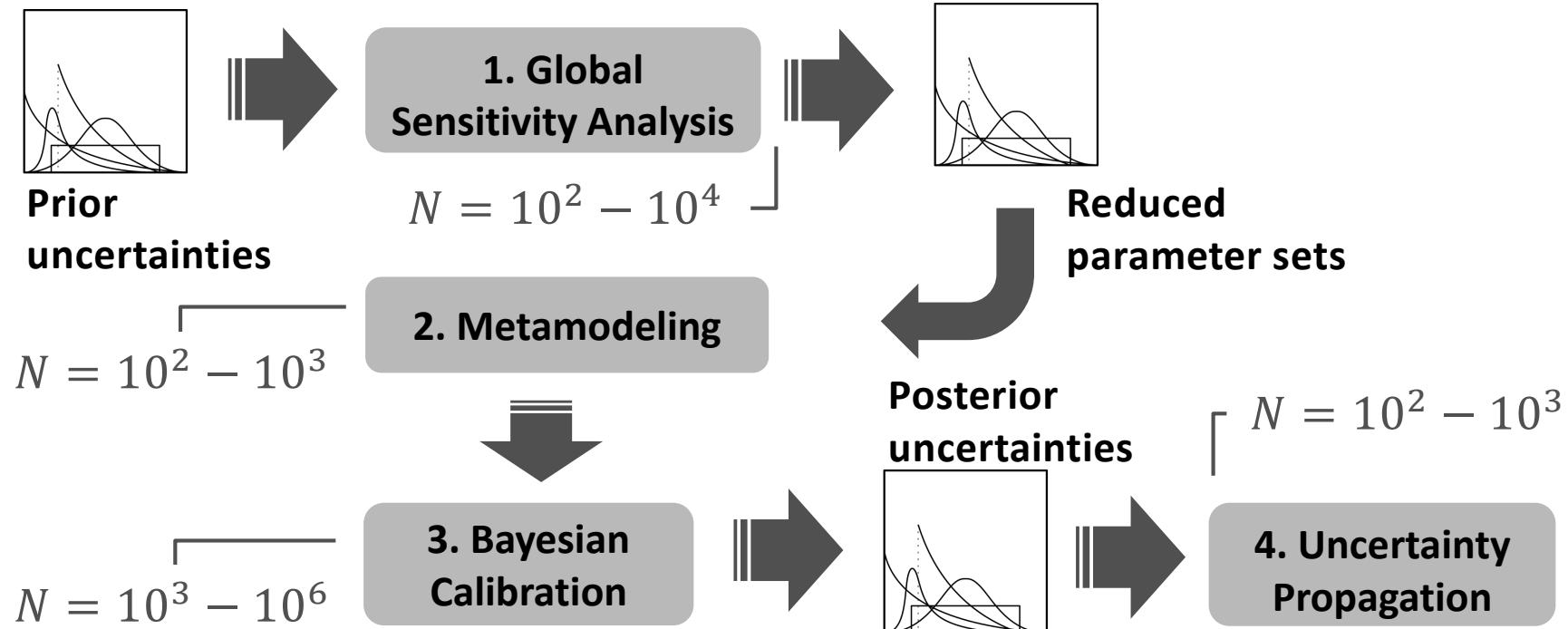


Experimental
Data from SETF



Post-calibration
uncertainties

Scope of Research (1/2): Statistical Framework



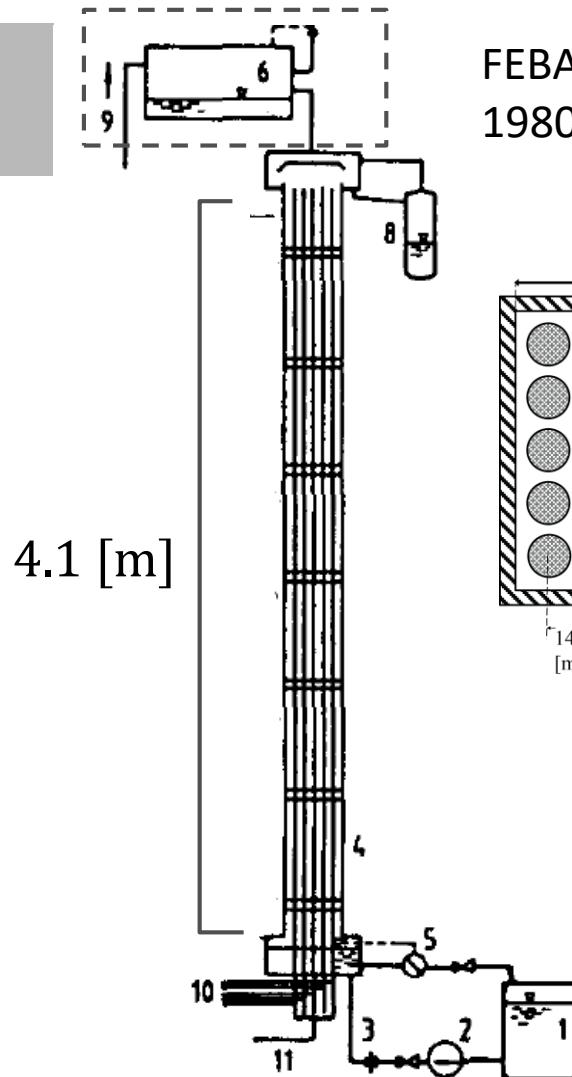
- Methods are non-intrusive
- Methods require less assumptions about the underlying model
- Results conform with probabilistic framework for UQ

- Methods tend to be expensive (require numerous code runs)



Scope of Research (2/2):

FEBA Separate Effect Test Facility (SETF)



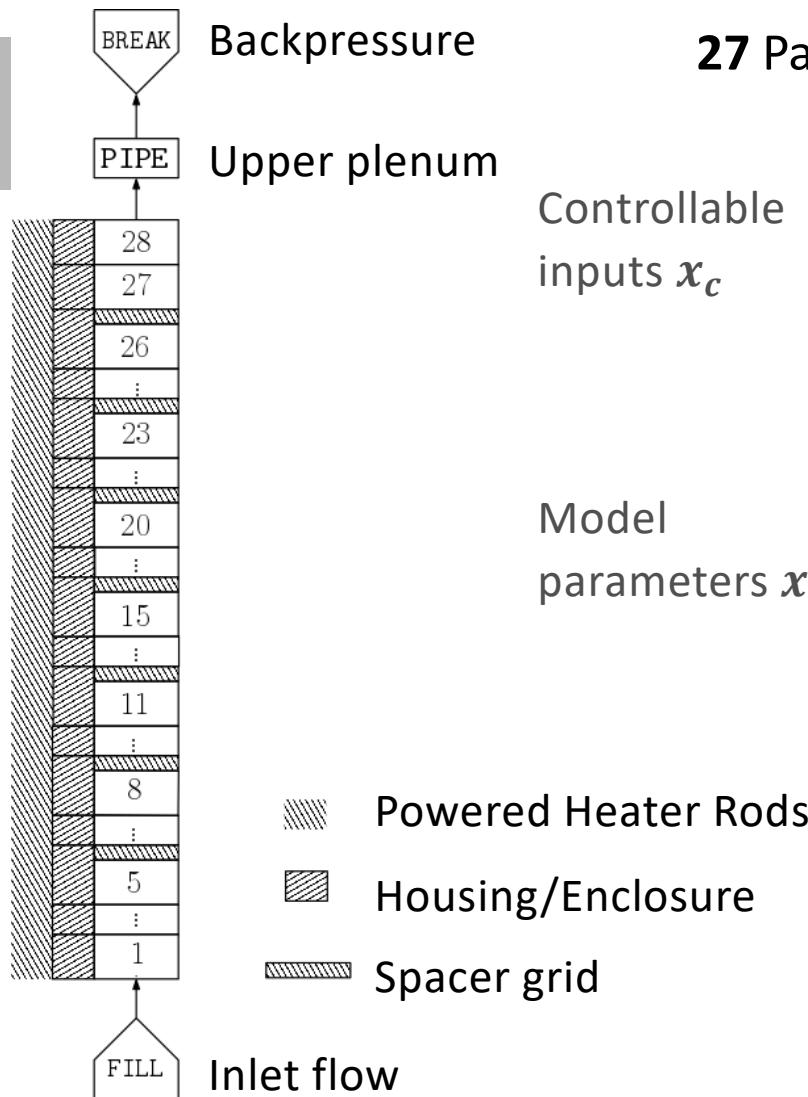
FEBA Reflood Tests were conducted at Kfz Karlsruhe (KIT) during 1980s for investigating bottom reflood using rod simulators (NiCr)

Main analyses are based on Test No. 216:

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

Three types of measurements were taken:

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



27 Parameters are required to specify the model:

- (4) Experimental boundary conditions (P_{sys} , V_{inlet} , etc.)
- (9) Material properties (k , C_p , etc.)
- (2) Spacer grid model (HTC_{enh.}, ΔP)
- (10) Post-CHF closure relations (IAFB wall HTC, DFFB interfacial drag, etc.)
- (1) Quench temperature
- (1) Transition boiling HTC

With flat independent uncertainties,
either in linear or log scales

Statistical Framework (1/4): Global Sensitivity Analysis

How to select the important parameters?

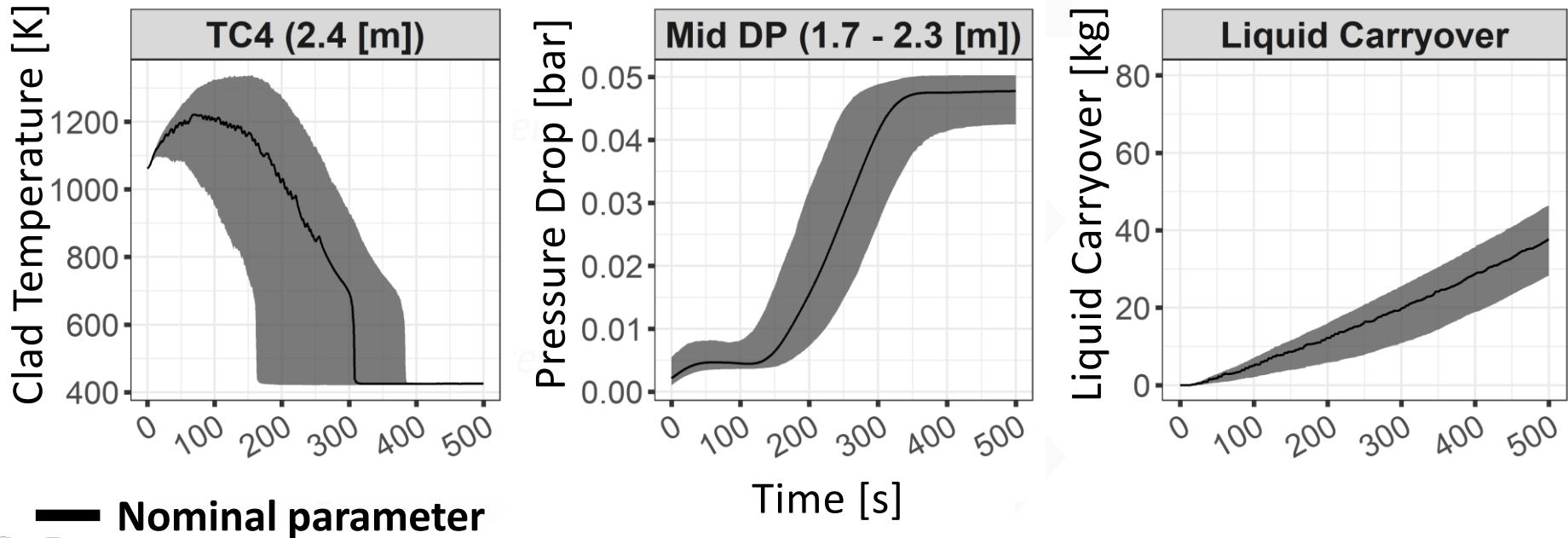
**1. Global
Sensitivity Analysis**

**27 initial
parameters**

**Identify the least
influential parameters,
and exclude them**

How to approximate the input/output of the forward model?

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

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

Grid size

320 replications \Rightarrow 8'960 code runs

Sobol' total-effect index for x_d :

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

10^3 samples \Rightarrow 29'000 code runs

Sensitivity Measure

Results on TC4 output

Morris (radial)

Morris (trajectory)

Sobol' (total-effect)

Number of Replications / Samples

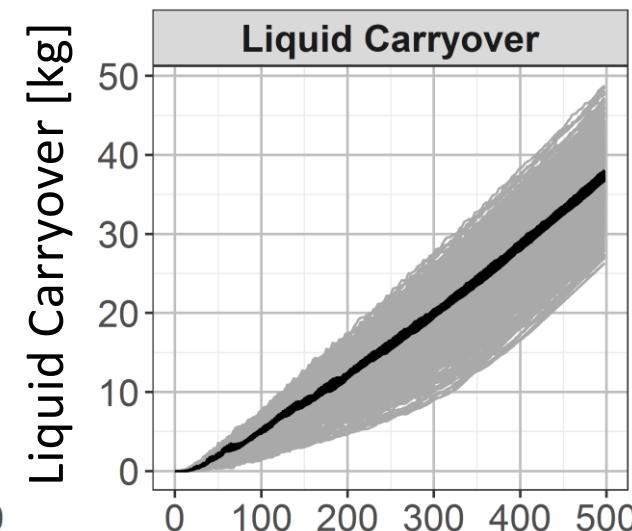
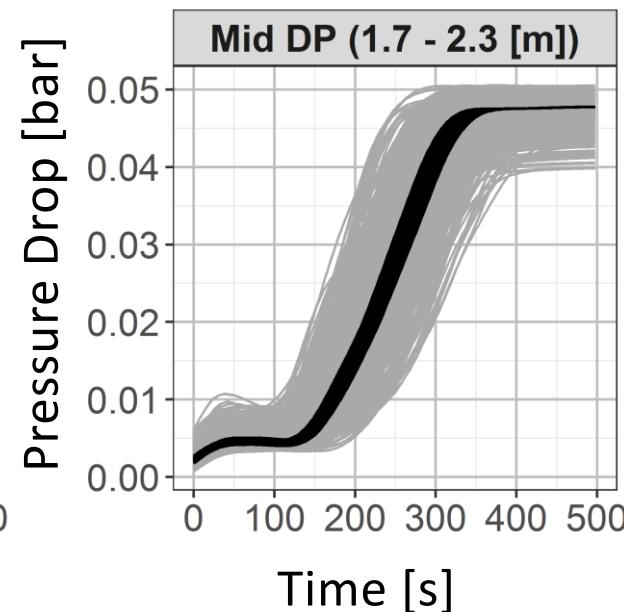
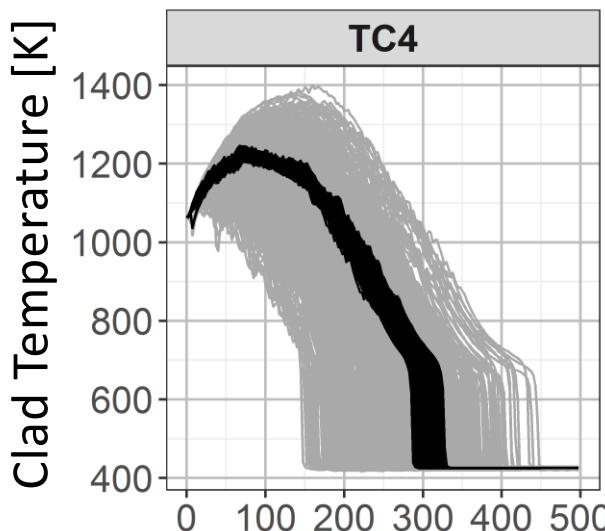
Uncertainty Propagation using Influential vs. Non-Influential Parameters

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”

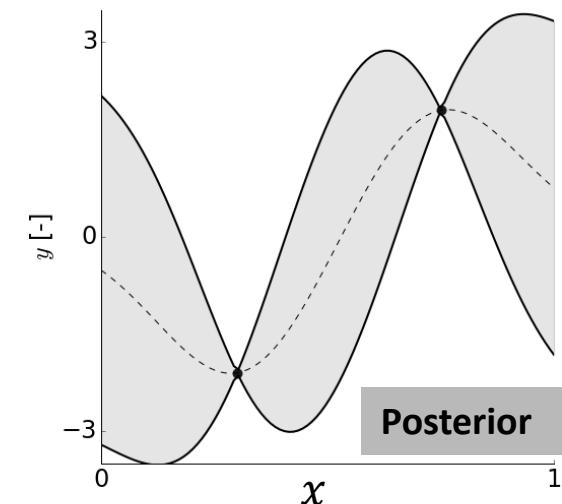
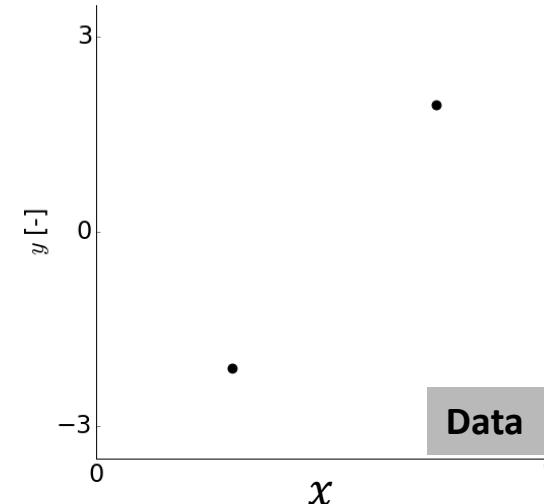
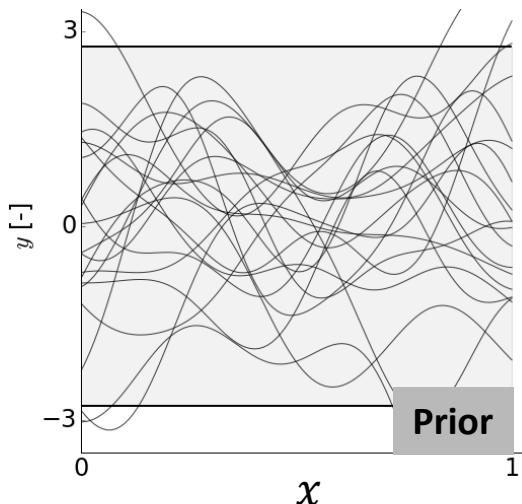
Gaussian Process (GP) Metamodel

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

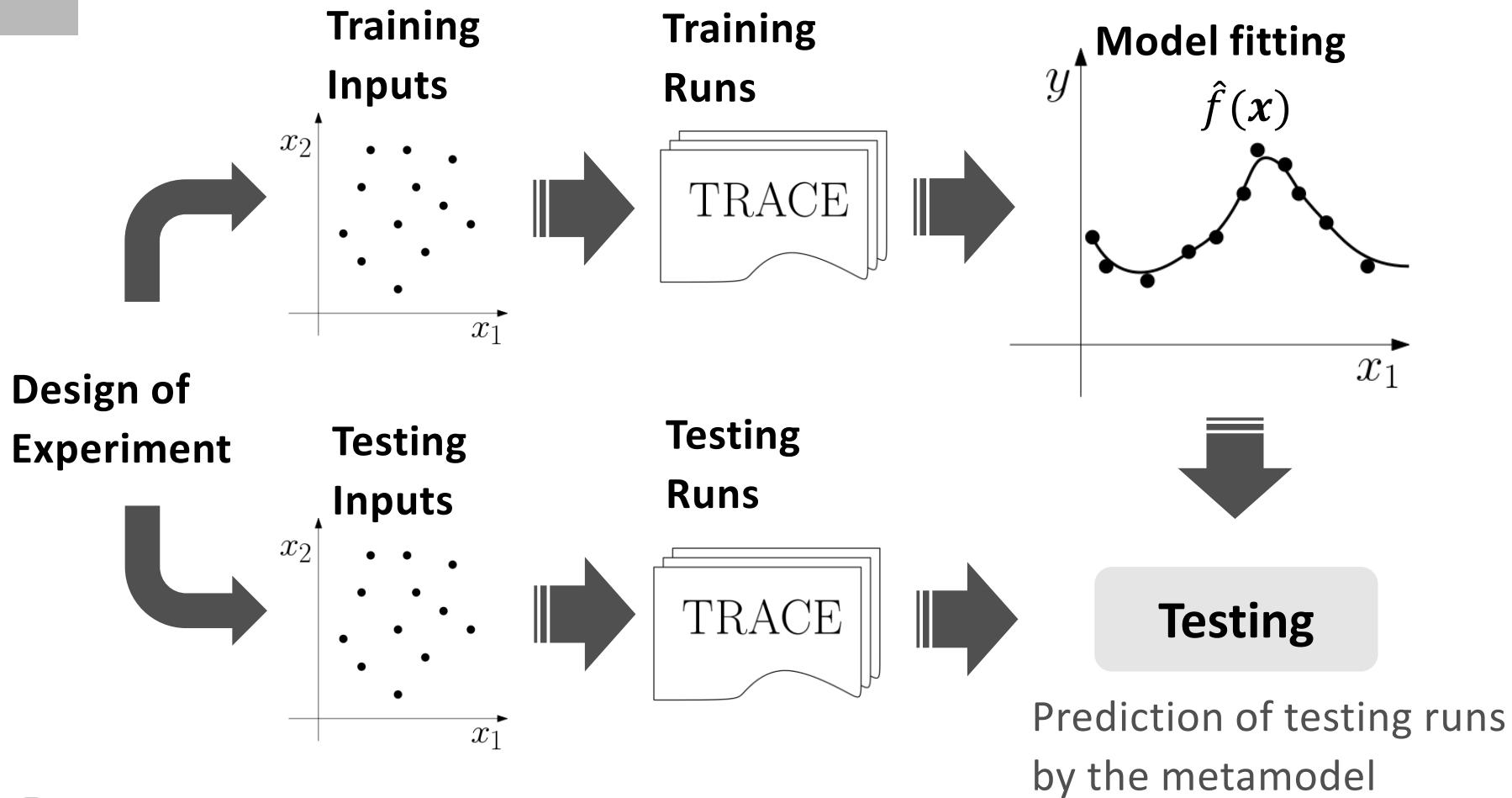
$$Y(x) \sim GP(m(x), \sigma^2 k(x, x^*))$$

Gaussian Process process variance
 Probability distribution of functions mean function
 correlation (kernel) function $k(x, x^*) \equiv \text{Cov}[Y(x), Y(x^*)]$

Application in Regression

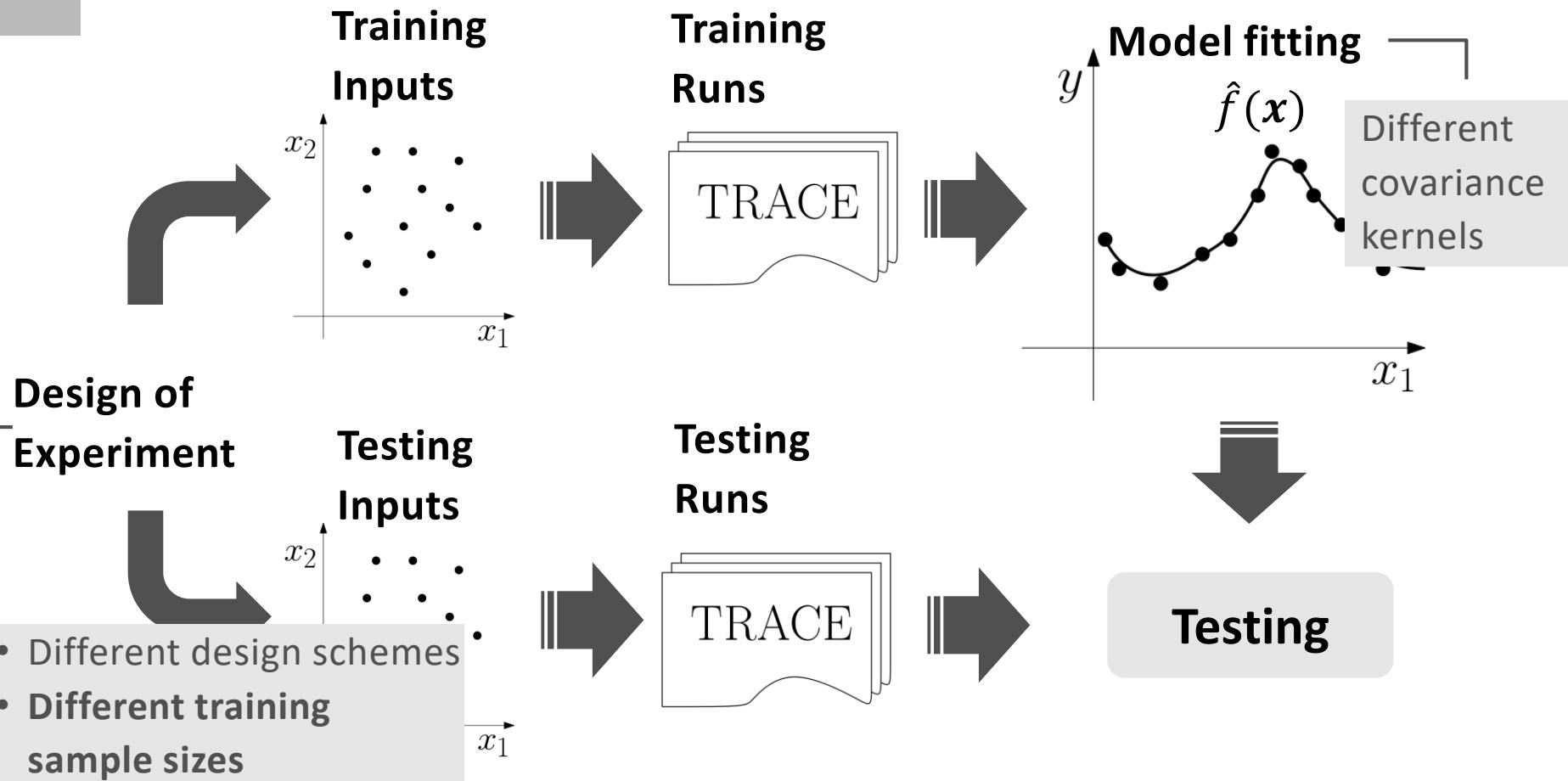


Constructing GP Metamodel: Training and Testing



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**.

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

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

Y' | W
 | | |
 Concatenate Eigenvectors PC scores
 and centered (principal components)

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

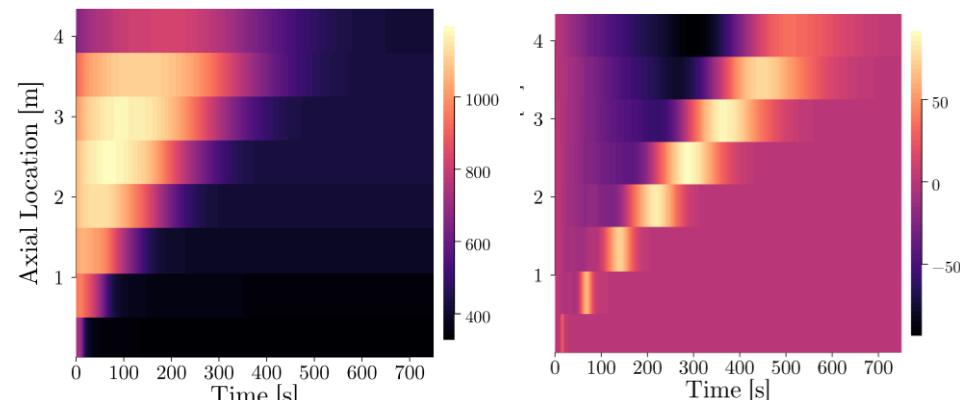
$\bar{y}^{\text{model}}(z, t)$ |
 the mean |
 of output

$$Q_{TC} = 7$$

$$Q_{DP} = 10$$

$$Q_{CO} = 5$$

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

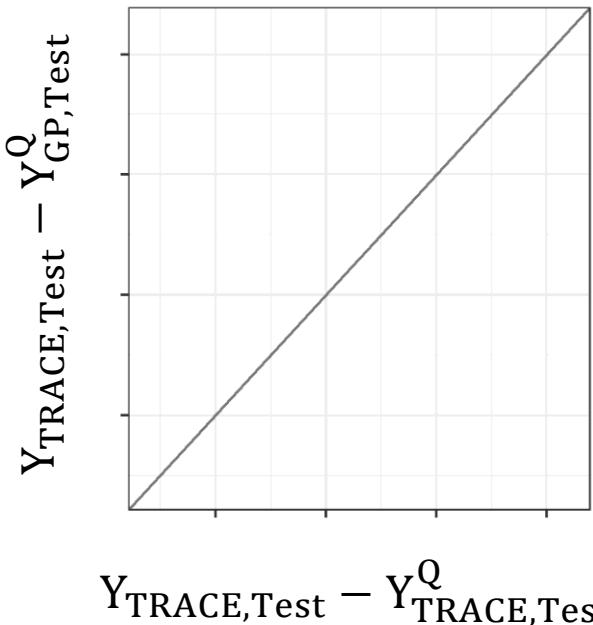


Mean and 1st PC of
clad temperature output

PC scores,
predicted by GP metamodel

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: $Y_{\text{TRACE},\text{Test}} - Y_{\text{TRACE},\text{Test}}^Q$

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

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

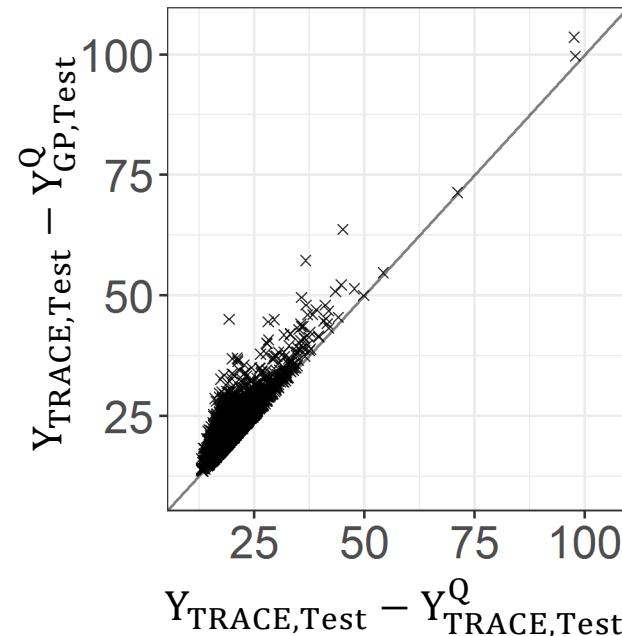
- Dimension reduction error **and** GP error
- Due to (also) **miss-prediction of PC scores**

Both are in terms of RMSE

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

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

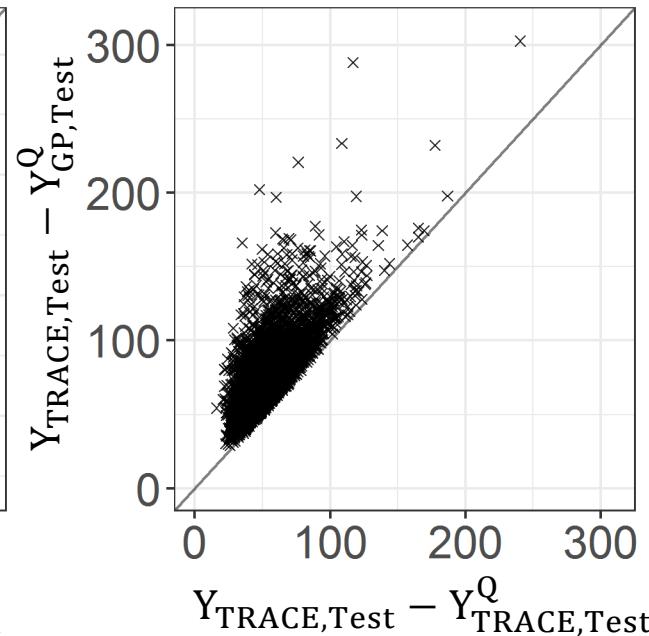
Clad Temperature [K]



GP PC RMSE 22.4 [K]

Testing Samples σ 254. [K]
(< 9%)

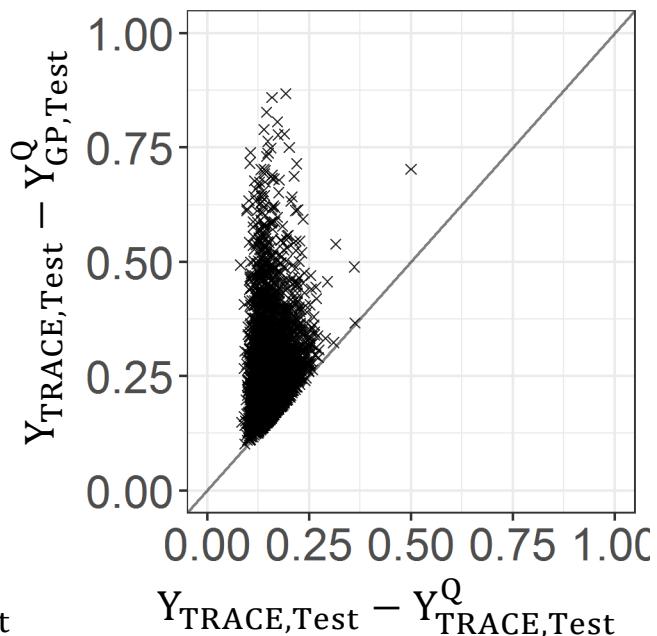
Pressure Drop [Pa]



77.95 [Pa]

9'200 [Pa]
(< 0.9%)

Liquid Carryover [kg]



0.27 [kg]

30.4 [kg]
(< 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) \Rightarrow Uncertain Inputs Updated

Controllable inputs
(w.r.t experiment)

x_c
 x_m

Forward Model
 $M: (x_c, x_m) \mapsto Y$

Uncertain
model parameters
(prior)

Experimental
Data from SETF

D

Probability of observing
data given parameters

Likelihood
 $p(D|x_m, x_c)$

Additional
sources of uncertainty

Uncertain
model parameters
(posterior)

Bayes' Theorem

Normal Likelihood

Experimental Data	Model prediction	Model bias	Measurement error
$y^{\text{exp}}(z, t) = y^M(x_m; z, t) + \delta(z, t) + \epsilon$			
given	GP	GP	Gaussian
unknown			
Likelihood			
Multiple sources of variance			
$p(y^{\text{exp}} x_m) \sim N\left(\tilde{y}^M + m_b, \underbrace{V \Sigma_w V^T}_{\substack{\text{GP} \\ \text{metamodel}} + \underbrace{V_{>P_{tr}} S_{>P_{tr}} V_{>P_{tr}}^T}_{\substack{\text{Principal Comp.} \\ \text{truncation}} + \underbrace{\Sigma_b}_{\substack{\text{Model} \\ \text{bias}}} + \underbrace{\sigma_{\text{exp}}^2 I}_{\text{measurement}}\right)$			

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 x_m is fully specified by $p(x_m|\{y^{\text{exp}}\})$, the posterior pdf.

Bayes' Theorem

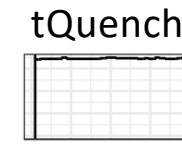
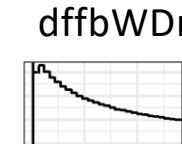
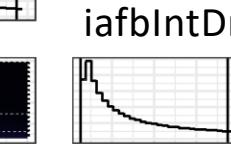
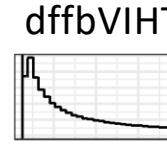
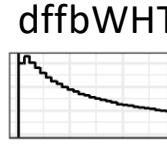
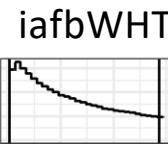
$$\begin{array}{ccc}
 \text{Posterior} & \text{Likelihood} & \text{Prior} \\
 | & | & | \\
 p(x_m|\{y^{\text{exp}}\}) & = \frac{p(\{y^{\text{exp}}\}|x_m) \times p(x_m)}{\int_{x_m} p(\{y^{\text{exp}}\}|x_m) \times p(x_m) dx_m}
 \end{array}$$

How $p(x_m|\{y^{\text{exp}}\})$ 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)

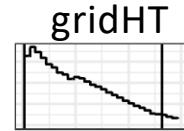
Markov Chain
 Monte Carlo
(MCMC)
 Simulation

Prior uncertainty of the model parameters

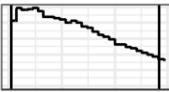
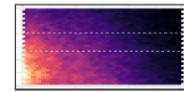


- **Diagonal panels:** univariate marginal PDFs
- **Off-diagonal panels:** pairwise correlation plots (bright color = concentrated samples)

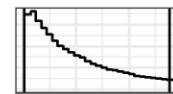
The posterior uncertainty based on pressure drop data only ($\approx 10^6$ samples)



iafbWHT



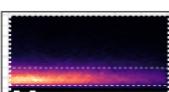
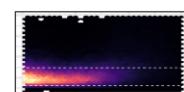
dffbWHT



dffbVIHT



iafbIntDr

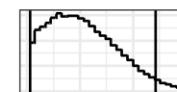


Interfacial drag of the
inverted annular
flow regime

dffbIntDr



dffbWDr



tQuench

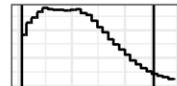


Posterior on all types of data ($\approx 10^6$ samples)

gridHT

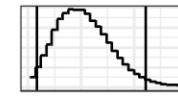
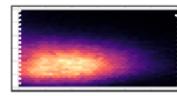
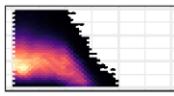


iafbWHT



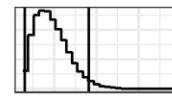
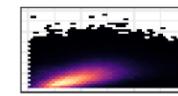
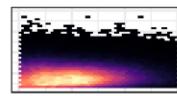
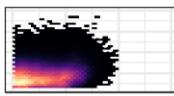
Wall HTC of the DFFB

dffbWHT

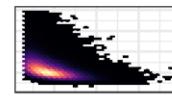
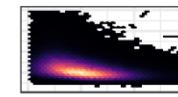
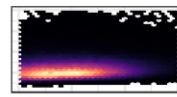
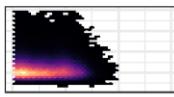


Vapor-Interface HTC of the DFFB

dffbVIHT

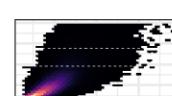


iafbIntDr

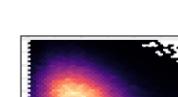
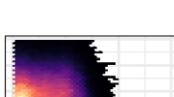


Interfacial drag of the DFFB

dffbIntDr



dffbWDr



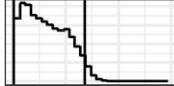
dffbWDr



tQuench

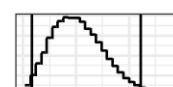
Posterior on all types of data ($\approx 10^6$ samples)

gridHT



iafbWHT

dffbWHT

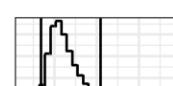


dffbVIHT



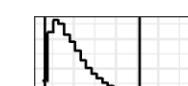
Vapor-Interface HTC of the DFFB

iafbIntDr



Interfacial drag of the DFFB

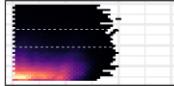
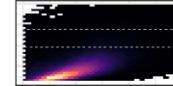
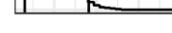
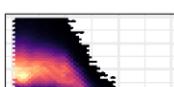
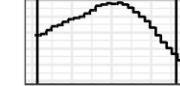
dffbIntDr



dffbWDr

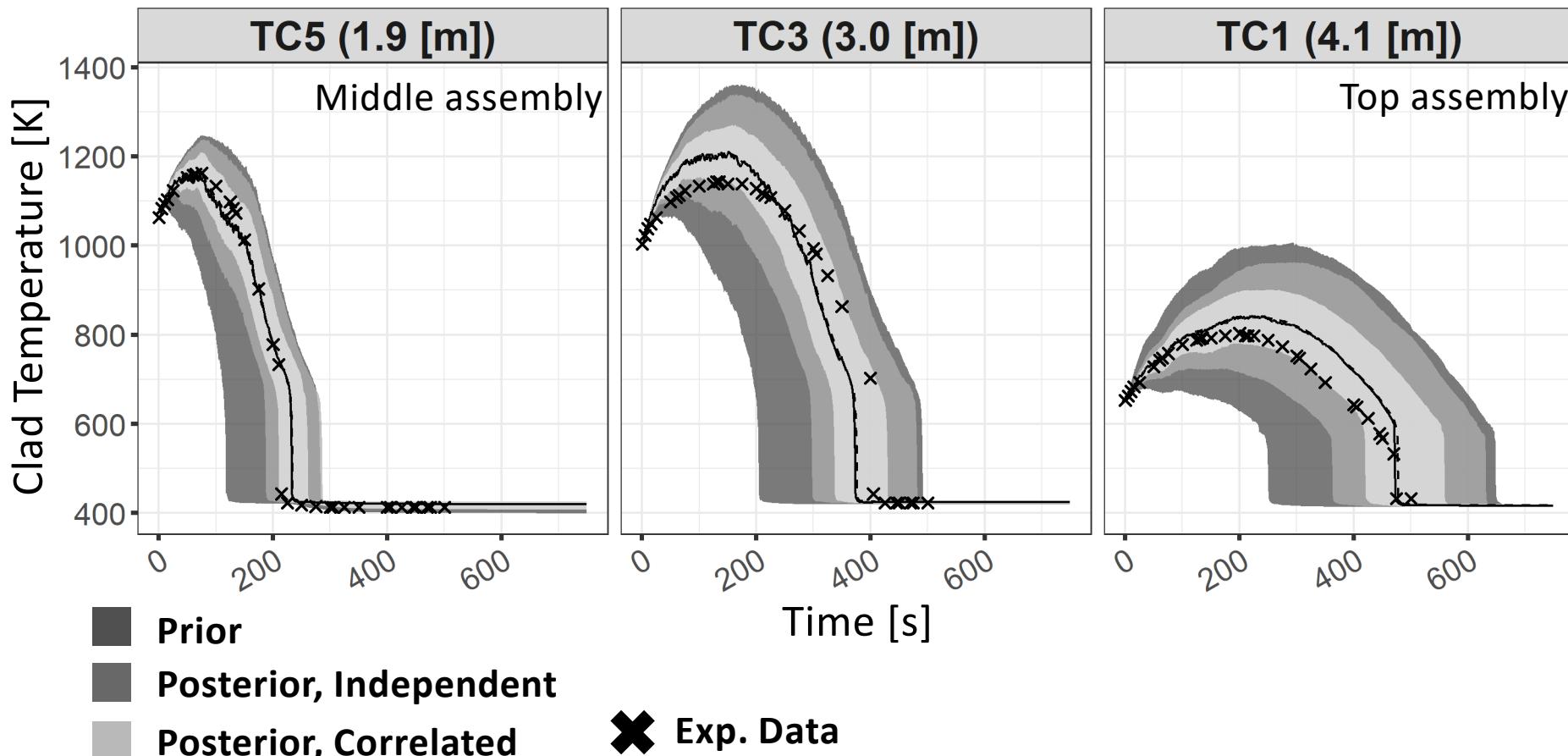


tQuench



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

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



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

How to make the uncertainty quantification?

3. Bayesian
Calibration

Wide, independent
prior uncertainties



Narrower, correlated
posterior uncertainties

How good is the quantified uncertainty?

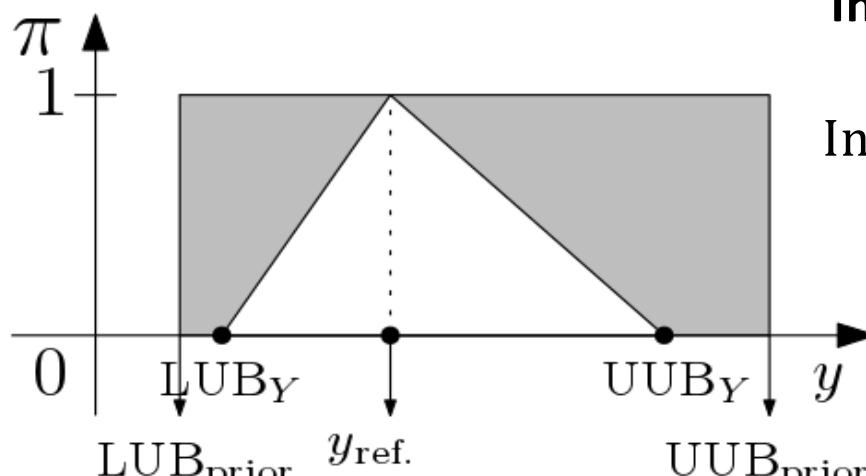
4. Uncertainty
Propagation

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

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

LUB: Lower Uncertainty Bound
(2.5th prediction percentile)

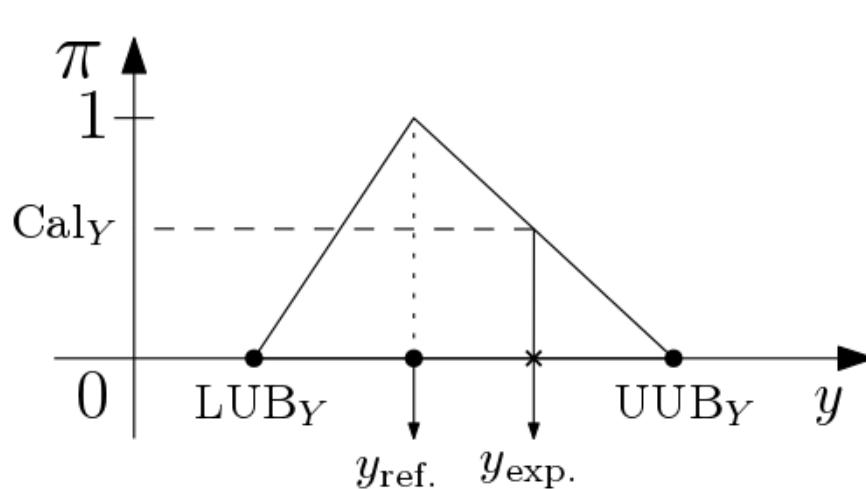
UUB: Upper Uncertainty Bound
(97.5th prediction percentile)

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

$\text{Inf}_Y = 1.0$ 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

$$\text{Cal}_Y = \pi_Y(y_{\text{exp}})$$

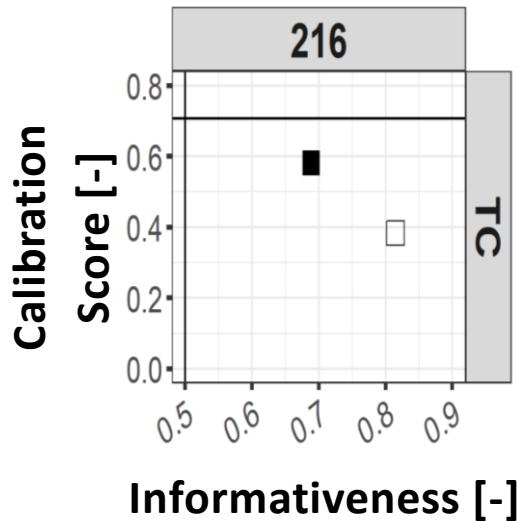
The height of the experimental data in the information triangle

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

$\text{Cal}_Y = 0.0$ Experimental data **falls outside** the uncertainty band

$\text{Cal}_Y = 1.0$ Experimental data matches the reference value **exactly**

Posterior Prediction Uncertainty in Terms of Calibration Score and Informativeness

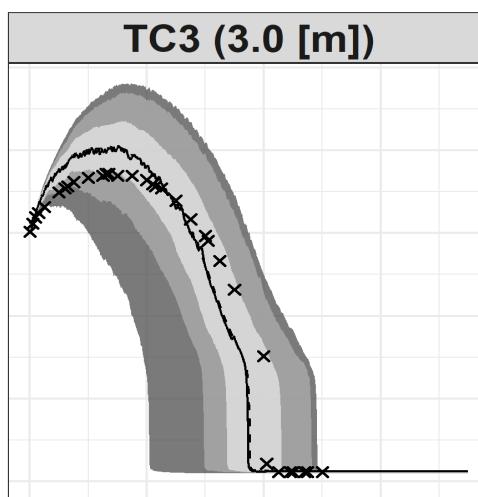


$$P_{\text{sys}} = 4.1 \text{ [bar]}$$

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

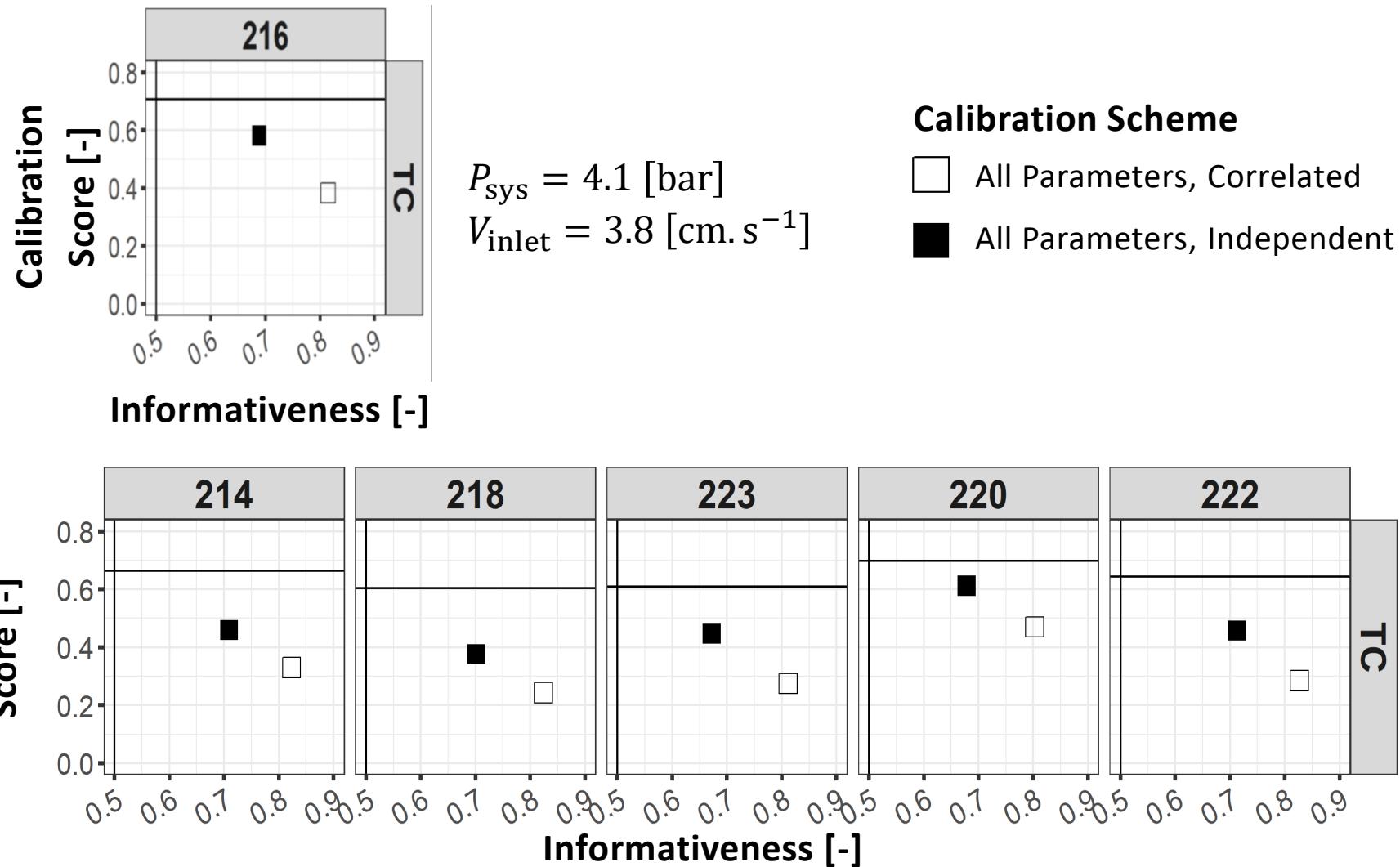
Calibration Scheme

- All Parameters, Correlated
- All Parameters, Independent

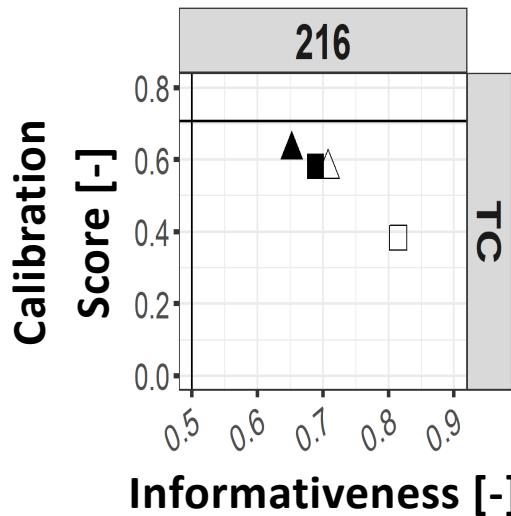


- Prior
- Posterior, Independent
- Posterior, Correlated
- ✗ Exp. Data

Effects of Experimental Conditions on Posterior Prediction Uncertainty



Removing a Highly Correlated Influential Parameter from the Calibration

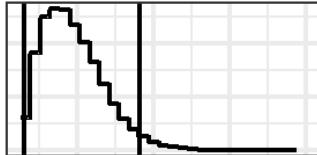


Calibration Scheme

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

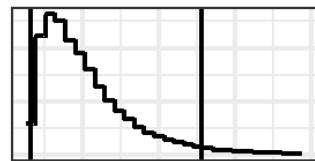
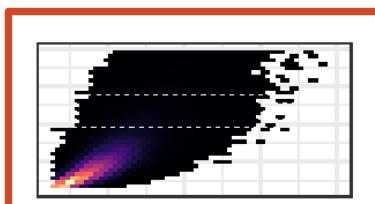
dffbVIHT

— Vapor-Interface HTC of the DFFB

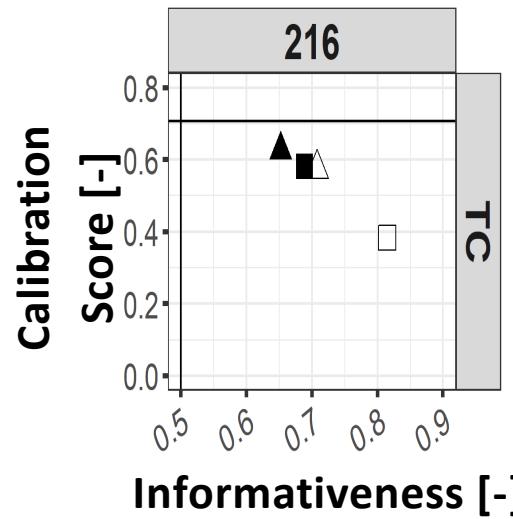


dffbIntDr

— Interfacial drag of the DFFB



Effects of Experimental Conditions on Posterior Prediction Uncertainty

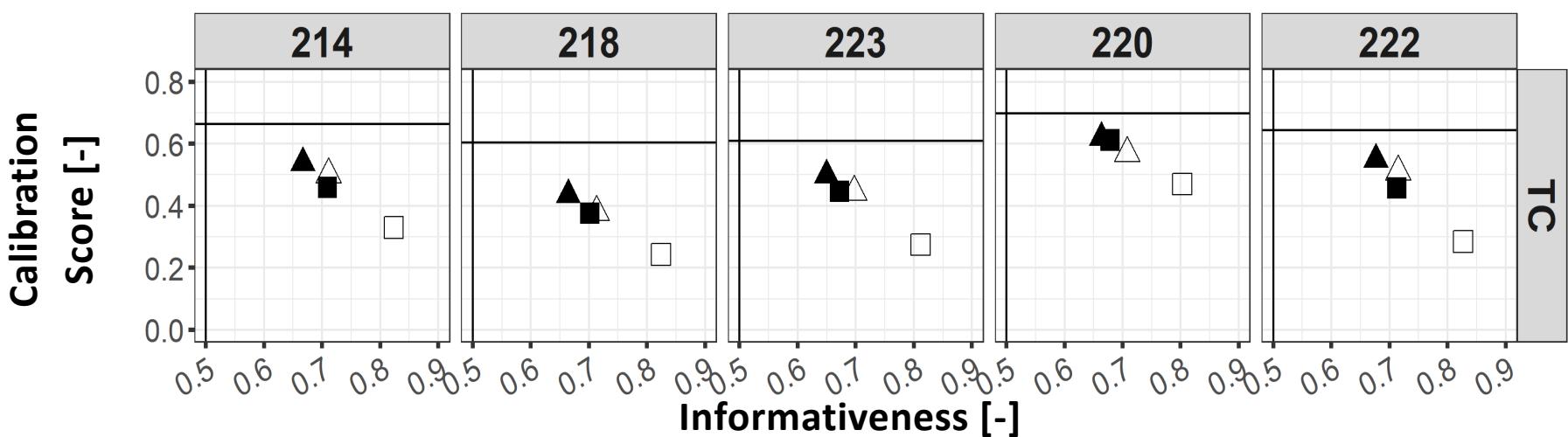


$$P_{\text{sys}} = 4.1 \text{ [bar]}$$

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

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:

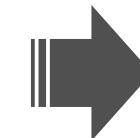
Consolidation, implementation, and application of tools
based on statistical framework
for quantifying the physical model parameters in the TRACE code

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?

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How to make the quantification?

**3. Bayesian
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Wide, independent
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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.)

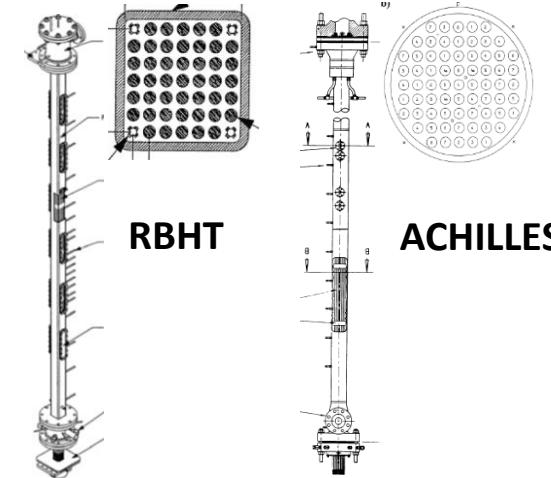
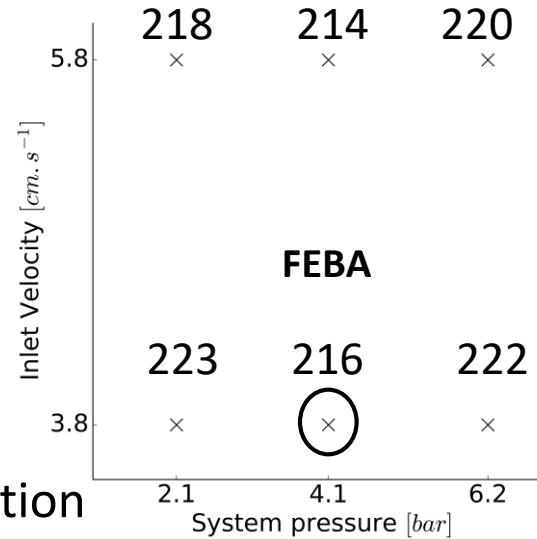
Publications and other contributions:

- 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

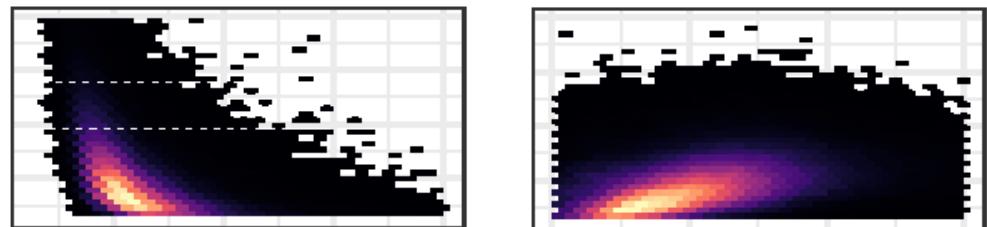
Bayesian Calibration

- 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?



**Thank you for your attention.
My sincere gratitude to:**

- Prof. A. Pautz
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- Dr. D. Rochman
- Dr. I. Clifford
- Mr. H. Ferroukhi
- Other members of STARS

The jury members:

- Dr. J. Baccou
- Prof. R. Houdré
- Prof. B. Sudret
- Dr. W. Zwermann

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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