Clogging of steam generators, sensitivity analysis and metamodel validation

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Table of contents

Table of contents

Industrial use case

- Clogging is a complex phenomenon happening in some steam generators (SGs) of pressurized water reactors (PWRs).
- Due to long operation times and corrosion of the secondary water circuit.
- Overtime, it can increase the risk of mechanical and vibrations on tube bundles and internal structures $\rightarrow$ affects the SG response to hypothetical transients.

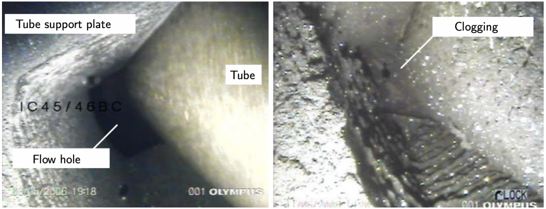
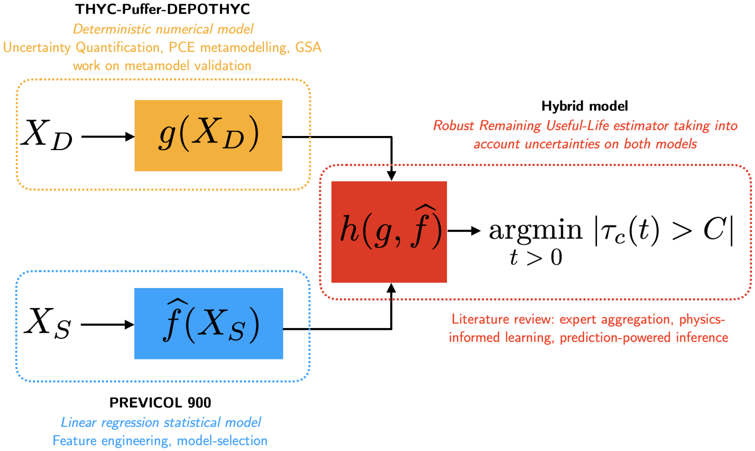


Figure: Example of video examination during a PWR outage (© EDF).

Industrial use case

- This phenomenon is controlled by chemical cleaning maintenances performed during PWR outages.
- To better address this maintenance planning, EDF R&D has worked on deploying models for enhancing the prediction of the clogging rate: τ_c.
- Two predictive models exist, a *numerical physics model* - THYC-Puffer-DEPOTHYC - and a *data-driven statistical model* - PREVICOL 900 - relying on operational data.
- The ambition of this thesis is to provide a pathway for *hybridizing* the two approaches in order to robustify the estimation.

Objective of the thesis



The physics of clogging

- Original clogging model/code: DEPOTHYC, developed by [Prusek, 2012] → mixed ODE-PDE system → accounts for short-time clogging evolution
- This model relies on the physical-validity of stationary thermohydraulic quantities → not guaranteed on long periods of time
- For the long-time evolution of clogging, multi-physics model: THYC-Puffer-DEPOTHYC, developed by [Feng et al., 2023] → takes into account chemical conditioning (pH) of the fluid.

THYC-Puffer-DEPOTHYC (TPD)

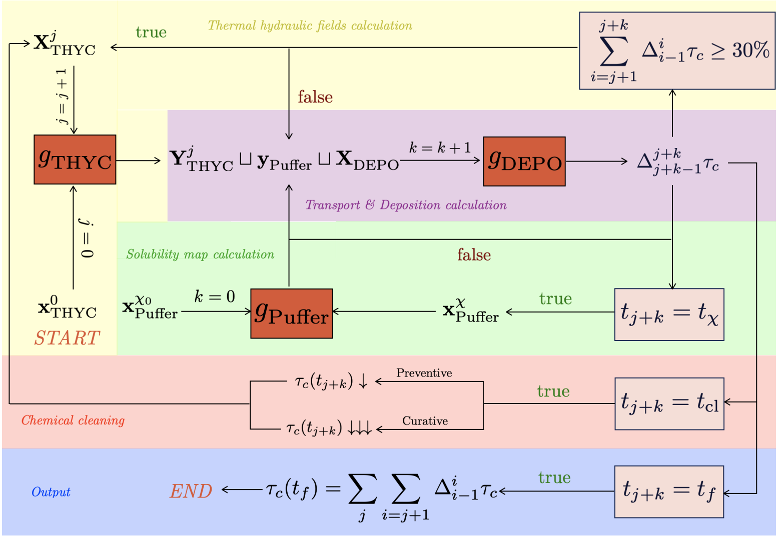


Figure: TPD architecture.

Uncertainty quantification of TPD

- Expert advice outlined the presence of uncertainty in the parameters $\boldsymbol{X}_{\text{DEPO}}$ of DEPOTHYC.
- Preliminary analysis performed by [Lefebvre et al., 2023]: building of a neural-network based metamodel + estimation of Sobol' sensitivity indices + Bayesian calibration.
- However, the long-time sensitivity analysis of the THYC-Puffer-DEPOTHYC model has not yet been analyzed. This is what we address in [Jaber et al., 2023b].
- Use of metamodels requires assessing the quality of the approximation $\rightarrow$ use of validation metrics [Demay et al., 2022]
- Approach for quantifying the Gaussian Process (GP) metamodel quality with conformal prediction methods [Vovk et al., 2005; Angelopoulos and Bates, 2023] proposed in [Jaber et al., 2023a] $\rightarrow$ tested for GP metamodelling of TPD

Table of contents

Design of experiment

- Experts outlined $d = 7$ uncertain independent input variables of the clogging module:

$$\boldsymbol{X}_{\text{DEPO}} = \boldsymbol{X} = (\alpha, \beta, \epsilon_e, \epsilon_c, d_p, \Gamma_p(0), a_v) \sim \mathbb{P}_{\boldsymbol{X}} = \otimes_{i=1}^{d} \mathbb{P}_{X_i},$$

  and provided the supports of their distributions.

- $n = 1000$ crude Monte-Carlo samples on the inputs are drawn according to the distributions in the table below.
- Focus is given on the output on the hot leg (HL) of the SG at the top in z_{max}.

Variable	Signification	Distribution
α	First empirical correlation parameter	$\mathcal{N}(101.6, 4.0)$
β	Second empirical correlation parameter	$\mathcal{N}(0.0233, 0.0005)$
ϵ_e	Porosities of the fouling deposits	$\mathcal{T}(0.2, 0.3, 0.5)$
ϵ_c	Porosities of the clogging deposits	$\mathcal{T}(0.01, 0.05, 0.3)$
d_p	Iron oxide particle diameter (m)	$\mathcal{T}(0.5, 5.0, 10.0) \times 10^{-6}$
$\Gamma_p(0)$	Initial data for solid mass transport equation	$\mathcal{T}(1.0, 4.5, 8.0) \times 10^{-9}$
a_v	Calibration parameter	$\mathcal{T}(0.1, 7.8, 12) \times 10^{-4}$

Table: Uncertain variable signification and corresponding distributions.

Design of experiment

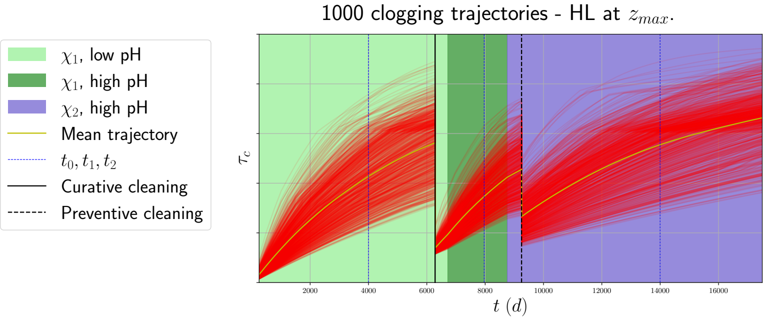


Figure: Clogging simulation trajectories.

The output is a time-discretized function:

$$g_{\text{TPD}}(\boldsymbol{X}) = (g_{\text{TPD}}(t_1, z_{\max}, \boldsymbol{X}), \ldots, g_{\text{TPD}}(t_N, z_{\max}, \boldsymbol{X})) \in \mathbb{R}^N, \ N = 75.$$

Polynomial chaos expansion (PCE) metamodel

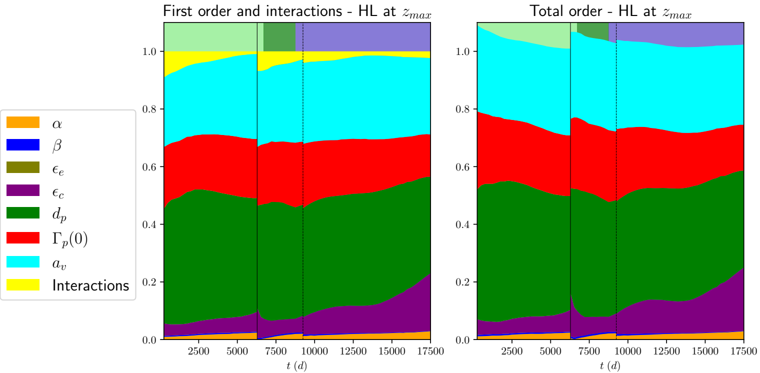
- Here $g_{\text{TPD}} =: g$. Computing Sobol' indices → byproduct of a polynomial chaos expansion (PCE) metamodel [Sudret, 2008].
- This means choosing an orthonormal polynomial Hilbert basis $\{\varphi_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathbb{N}^d}$ of L^2 and making use of the truncated decomposition:

$$g(\boldsymbol{X}) \simeq \widetilde{g}(\boldsymbol{X}) = \sum_{|\boldsymbol{\alpha}|\leq p} g_{\boldsymbol{\alpha}}\varphi_{\boldsymbol{\alpha}}(\boldsymbol{X}),\; g_{\boldsymbol{\alpha}} \in \mathbb{R}^N,\; \forall \boldsymbol{\alpha}. \tag{1}$$

  $\{g_{\boldsymbol{\alpha}}\}$ computation → [Blatman and Sudret, 2011].
- Validation of PCE hyperparameters with predictivity coefficient Q^2 → K-fold cross-validation.
- Rearranging the coefficients → Sobol' sensitivity indices:

$$S_{\gamma}(t_k) = \frac{\sum_{\boldsymbol{\alpha}\in\mathcal{J}_{\gamma}}(g_{\boldsymbol{\alpha}}^k)^2}{\sum_{|\boldsymbol{\alpha}|\leq p}(g_{\boldsymbol{\alpha}}^k)^2},\; \forall k \in \{1,\dots,N\}, \boldsymbol{\gamma} \in \mathbb{N}^d. \tag{2}$$

Time-dependent Sobol' indices



- The hierarchy of the influential variables is preserved and similar to what is uncovered in the prior analysis [Lefebvre et al., 2023].
- A new phenomenon discovered is the influence of the clogging porosity ϵ_c in high-pH, high-clogging regime.

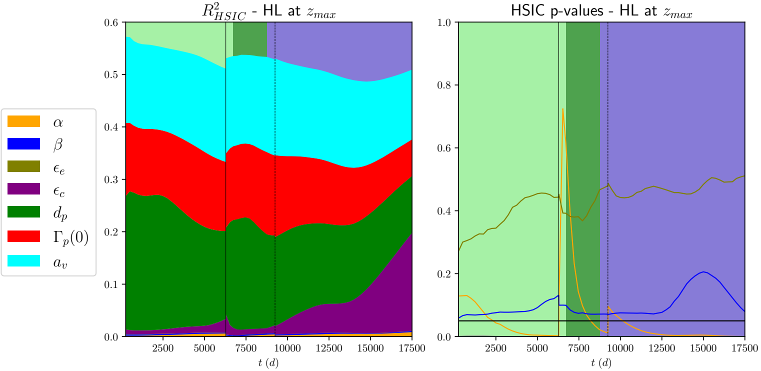
HSIC sensitivity index

- Complementary approach robustifying the Sobol' analysis $\rightarrow$ computation of different HSIC indices.
- Hilbert-Schmidt Independence Criterion (HSIC) [Gretton et al., 2005; Da Veiga, 2015], kernel method $\rightarrow$ evaluates sensitivity of a *single input* in a given-data context.
- Theoretical result for all $i \in \{1, \ldots, d\}, k \in \{1, \ldots, N\}$:

$$\mathrm{HSIC}(X_i, g_k(X_i)) = 0 \iff X_i \perp g_k(X_i). \tag{3}$$

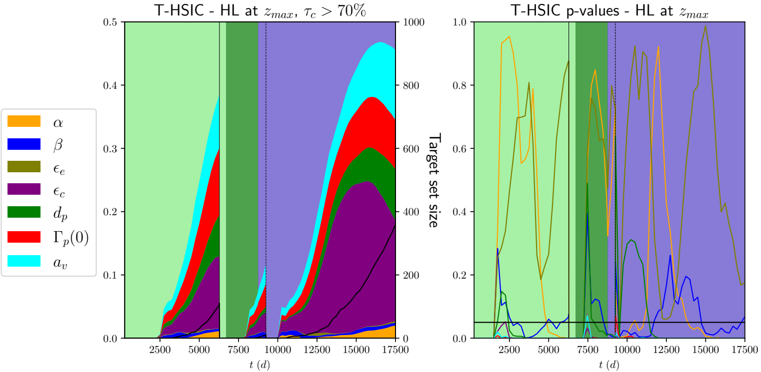
- The index disposes of U-stat and V-stat estimators that are easily computable in a limited-budget context, and a hypothesis testing with corresponding p-value.
- Moreover, it allows for easy evaluation of local target and conditional indices, for given target regions.

Regular HSIC



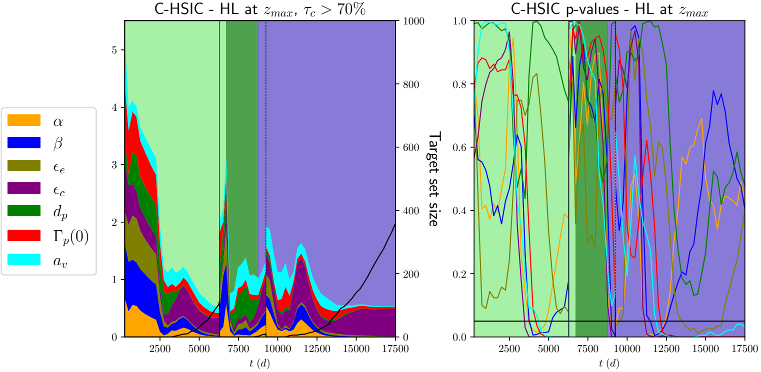
- The main conclusions from the Sobol' analysis persist, the influential variables are a_v, d_p and $\Gamma_p(0)$ in all chemical conditionings and ϵ_c becomes non-negligible in the high-pH-χ_2 conditioning.

Target HSIC



- The analysis here provides clear evidence that the clogging porosity becomes the most influential variable in high-clogging, high-pH-χ_2 regime.

Conditional HSIC



- After the preventive cleaning and under high-pH conditions in the χ_2 chemical conditioning, the clogging porosity is visibly the most influential uncertain variable, while the previously dominant variable, d_p, becomes negligible.

Summary

- THYC-Puffer-DEPOTHYC is a long-term multiphysics clogging numerical model for SGs developed by EDF R&D in which certain input variables have been exhibited as uncertain.
- Advanced sensitivity analysis tools have been deployed for assessing the influence hierarchy of these different variables and similar results as in [Lefebvre et al., 2023] hold for the long-term clogging model.
- Most notably, the findings related to the influence of the clogging porosity sheds new light on the input-output dependencies and has potential physical interpretations.
- Article submitted for review in the International Journal of Uncertainty Quantification (IJUQ) - GSA Special Issue 2023 [Jaber et al., 2023b].
- Further work would imply developing strategies for performing calibration of the parameter a_v with respect to experimental data.

Table of contents

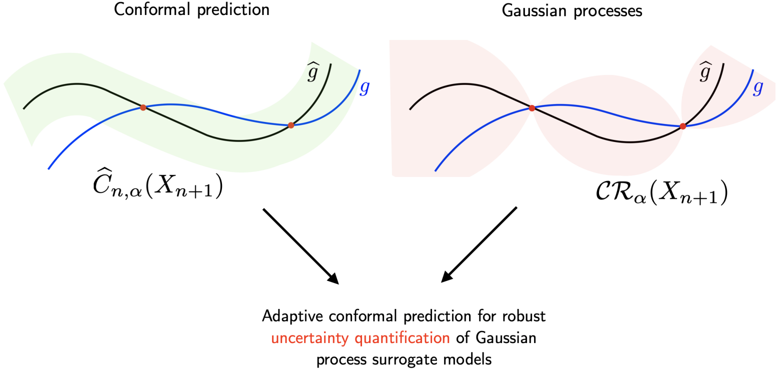
Conformal Prediction (CP)

- [Vovk et al., 2005; Angelopoulos and Bates, 2023] CP $\rightarrow$ method for performing UQ on ML algorithms $\rightarrow$ idea: apply it for metamodel validation.
- For a metamodel $\widehat{g}$, CP provides a way to build *prediction intervals* $\widehat{C}_{n,\alpha}$ s.t for a coverage level $1-\alpha \in (0,1)$, the *true value of the code* $g(X_{test})$, would be in the set with marginal probability:

$$\mathbb{P}(g(X_{test}) \in \widehat{C}_{\alpha,n}(X_{test})) \geq 1-\alpha, \tag{4}$$

  marginal meaning here that it is averaged over any realization of the training DoE.
- Generic method, not many hypothesis $\rightarrow$ idea: apply it for evaluating GP metamodel robustness $\rightarrow$ no more Gaussian assumption as with the Bayesian credibility intervals.

Adaptive GP conformal predictors



- Work project at the CEMRACS 2023.
- More details and application for the GP metamodel evaluation for THYC-Puffer-DEPOTHYC $\rightarrow$ upcoming paper [Jaber et al., 2023a]

Table of contents

Summary and upcoming work

- First year of PhD: applying UQ on methodology industrial multi-physics code THYC-Puffer-DEPOTHYC; work on learning metamodels quality assessment with CP.
- 2 papers written: [Jaber et al., 2023a] - MLJ & [Jaber et al., 2023b] - IJUQ.
- Conferences and communications: Séminaire Modélisation CB, MASCOT-NUM 2023 (poster), CJC-MA 2023 (poster), CEMRACS 2023, ETICS 2023 (talk)
- Second year: developing hybrid methods between TPD and the regression model PREVICOL 900 taking into account uncertainties.

To be continued...

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