Simulation-based and statistical tools for uncertainty quantification in a digital twin of a steam generator

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Clogging of steam generators (SGs)

- Clogging of SGs is a complex multiphysics phenomenon that occurs following long operational periods in pressurized-water reactors (PWR) of the French nuclear fleet → undermines performance & weakens the structures → *may require chemical cleanings*

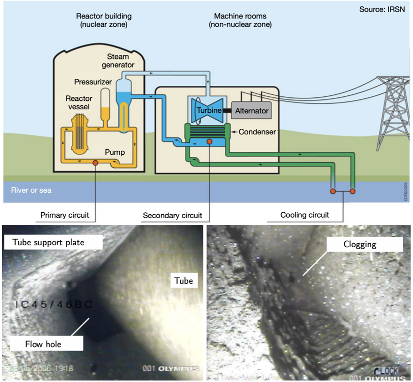

Figure: PWR scheme, and example of video examination during an PWR outage (© IRSN, EDF)

Clogging of SGs

- No state-of-the-art model allowing for ground insights on diagnosis and prognosis of clogging rate τ_c $\rightarrow$ very hard to model & challenging to create reproducible lab experiment for model validation + not a lot of literature [Srikantiah and Chappidi, 2000; Prusek et al., 2013; Girard, 2014; Yang et al., 2017]
- Available scarce video field data as well as indirect measurements $\rightarrow$ allow to construct data-driven regression algorithms [Pinciroli et al., 2021] $\approx$ not enough data to have robust predictive models
- Another tool is the physical clogging model developed by [Prusek et al., 2013] $\rightarrow$ subsequent numerical model THYC-Puffer-DEPO [Feng et al., 2023] $\approx$ lack of enough trustworthy field data for precise validation
- Necessary decision-making on chemical cleaning planning under uncertainty $\rightarrow$ ***how to make use of the available knowledge and models for achieving reliable predictions?***

Towards digital twins (DTs) in nuclear industry

- Growing interest of creating digital twins for nuclear industry → many industrial challenges to address

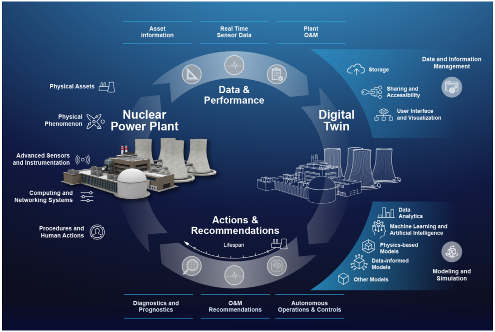

Figure: DT methodologies for nuclear reactors [Vaibhav and al., 2023]

- Stepping stone towards the elaboration of DT for SGs at EDF → **more details in E. Remy's talk - MS018D on Friday morning**

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The long-term clogging model

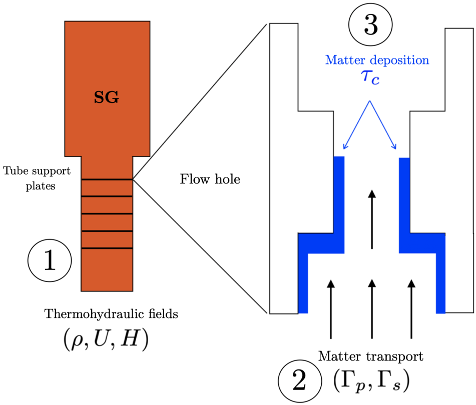

Figure: Clogging physical model

- Clogging results from two main mechanisms → *vena contracta* & *flashing* [Prusek et al., 2013]
- Long-term clogging model [Feng et al., 2023] → must change stationary thermohydraulics + compute chemical conditioning

The numerical model: THYC-Puffer-DEPO

- THYC-Puffer-DEPO (TPD) is the chaining of 3 codes $\rightarrow$ allows to simulate SG clogging on entire lifespan of the asset integrating past chemical cleanings and predicting future τ_c states $\rightarrow$ takes into account the chemical pH of the secondary fluid
- THYC [Petit, 1991] is based on a finite-volume numerical scheme for the two-phase conservation equations
- Puffer is an in-house chemical code allowing to compute the solubility of iron oxides as a function of pH $\rightarrow$ used in the deposit model
- DEPO [Prusek et al., 2013] is the deposit module, solving the transport and clogging equations with iterative finite-differences schemes methods
- The chaining of these three codes is made on different criteria, more details are found in [Jaber et al., 2024]$\rightarrow$ unitary call is $\sim$ 5h on HPC infrastructure

Design of experiments

- Some experts exhibited a number of uncertain variables in the clogging model $\rightarrow$ prior work done in [Lefebvre et al., 2023]
- In the DEPO module model, variables $\boldsymbol{X} = (X_1, \ldots, X_d) \in \mathbb{R}^d$, with $d = 7$ $\rightarrow$ how these parameters affect the long term τ_c prognosis uncertainty? $\rightarrow$ sensitivity analysis - work done in [Jaber et al., 2024]
- Assume $\boldsymbol{X} \sim \mu = \mathcal{U}(I_1) \otimes \ldots \otimes \mathcal{U}(I_d)$ with support intervals given by experts and code designers $\rightarrow$ use Latin Hypercube Sampling to draw $n = 10^3$ points and build

$$\mathrm{DoE}_{\mathrm{LHS}}^{\mathrm{TPD}}(\boldsymbol{X}) = \{(\boldsymbol{X}^{(i)}, g(\boldsymbol{X}^{(i)}))\}_{i=1}^{n} \quad (1)$$

- Output is a vector $g(\boldsymbol{X}) = (g(\boldsymbol{X}, t_1), \ldots, g(\boldsymbol{X}, t_N))$ of reduced dimension $N \sim 10^2$

Uncertainty propagation numerical results

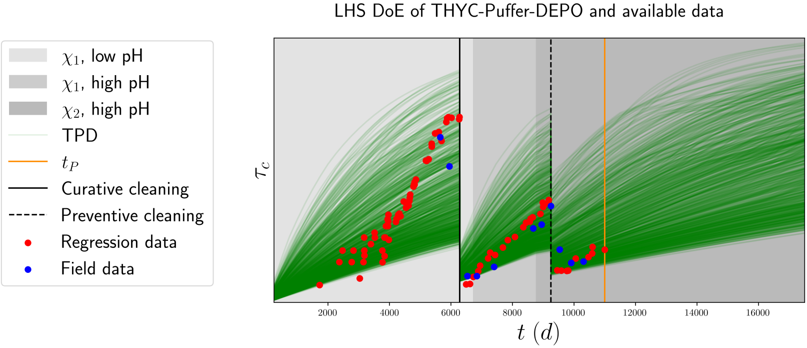

Figure: Illustration of output of $\mathrm{DoE}^{\mathrm{TPD}}_{\mathrm{LHS}}(\boldsymbol{X})$ on a specific SG for a given simulation time, available field and regression data, the present time t_P is highlighted in orange

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Bayesian calibration methodology for RUL update

- Sensitivity analysis results highlight potential dependence on the output of $X_7 = \theta \rightarrow$ parameter related to the *vena contracta* phenomenon in the deposit model [Prusek et al., 2013]
- *Idea*: use the available field & regression data to update the prior distribution of $\theta \rightarrow$ reduce the future prediction uncertainty

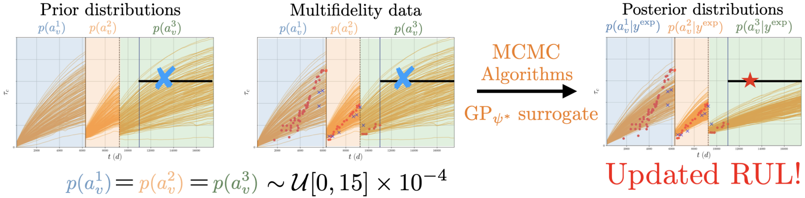

Figure: Bayesian calibration methodology for updating the RUL $\rightarrow$ make use of Markov-Chain Monte-Carlo (MCMC) algorithm with optimized Gaussian process surrogate (GP) of the code. The multifidelity data comprises field data (FD) and regression data (RD)

Bayesian calibration formalism

- Three distributions of θ are calibrated for each period $\rightarrow$ before *curative cleaning* (CC), between *curative cleaning and preventive cleaning* (CC-PC), and after *preventive cleaning* (PC) $\rightarrow$ choice justified by the observed change in kinetics after a chemical cleaning
- Build, optimize & use a GP surrogate model $\widetilde{g}_{\mathrm{TPD}}$ for fast sampling (since actual model calls are time-prohibitive) $\rightarrow$ procedure based on $m = n + 1$ calibrations where n is the number of cleanings performed on a SG (in this example $m = 3$)
- Data between the k-th and $k+1$-th chemical cleaning:

$$\{\boldsymbol{y}_k^* = (y_{k,1}^*, \ldots, y_{k,n_k}^*)\} \subset \{\boldsymbol{y}_1^*, \ldots, \boldsymbol{y}_m^*\} \tag{2}$$

$\mathcal{J}_{*,k}$ are the respective time step indices, $n_{*,k} := |\mathcal{J}_{*,k}|$ with $* = \{\mathrm{FD}, \mathrm{RD}\}$

Bayesian calibration formalism

- Without model discrepancy, assume [Carmassi et al., 2019] for $k = 1, \ldots, m$, with $* = \{\mathrm{FD}, \mathrm{RD}\}$:

$$\boldsymbol{y}_k^* = \boldsymbol{\mathcal{G}}_k^*(\theta_k) + \boldsymbol{\eta}_k^*, \quad \boldsymbol{\eta}_k^* \sim \mathcal{N}(0, \sigma_*^2 I_{n_{*,k}}) \tag{3}$$

  where $\boldsymbol{\mathcal{G}}_k^*$ applies the projection of the outputs of the surrogate model $\widetilde{g}_{\mathrm{TPD}}$ onto time steps of the $*$-th data between the k-th and $k+1$-th chemical cleaning

- Choice of priors for all k:
  - $\theta_k \sim \mathcal{U}[0, 15] \times 10^{-4}$
  - Jeffreys prior for $\upsilon := 1/\sigma_*^2$, $p(\upsilon) = 1/\upsilon$
  - θ_k and $\boldsymbol{\eta}$ are independent $\rightarrow$ residuals give a Gaussian likelihood

- If all field data have the same standard deviation, then we can show that [Keller et al., 2022]:

$$p(\theta_k | \boldsymbol{y}_k^*) \propto \|\boldsymbol{y}_k^* - \boldsymbol{\mathcal{G}}_k^*(\theta_k)\|^{-n_{*,k}} \tag{4}$$

Bayesian calibration formalism

- This posterior distribution can be generalized for q groups of multifidelity data $(\boldsymbol{y}^{\mathrm{exp},1}, \ldots, \boldsymbol{y}^{\mathrm{exp},q})$ with different variances (in our case $q = 2$ since FD and RD have different variances) for $k = 1, \ldots, m$:

$$p(\theta_k | \boldsymbol{y}_k^{\mathrm{FD}}, \boldsymbol{y}_k^{\mathrm{RD}}) \propto \|\boldsymbol{y}_k^{\mathrm{FD}} - \mathcal{G}_k^{\mathrm{FD}}(\theta_k)\|^{-n_{\mathbf{FD},k}} \times \|\boldsymbol{y}_k^{\mathrm{RD}} - \mathcal{G}_k^{\mathrm{RD}}(\theta_k)\|^{-n_{\mathbf{RD},k}}$$

- Weight associated with the $*$ data type $\rightarrow$ related to the number of data points $n_{\mathrm{FD},k}, n_{\mathrm{RD},k}$.
- MCMC algorithm of the Random-Walk Metropolis-Hastings type [Rubinstein and Kroese, 2011] in OpenTURNS Python library $\rightarrow$ sampling from distributions $p(\theta_k | \boldsymbol{y}_k^{\mathrm{FD}}, \boldsymbol{y}_k^{\mathrm{RD}})$ + Gelman-Rubin convergence test for Markov chains

Numerical results

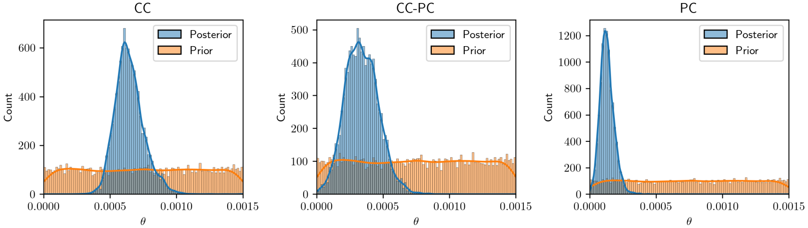

Figure: Prior and MCMC-sampled posterior distributions of the calibration parameter $\theta \rightarrow$ different modes after the different chemical cleaning actions $\rightarrow$ confirms the prior operational knowledge and informs the physical model $\rightarrow$ **hybrid approach!**

Updated uncertainty propagation

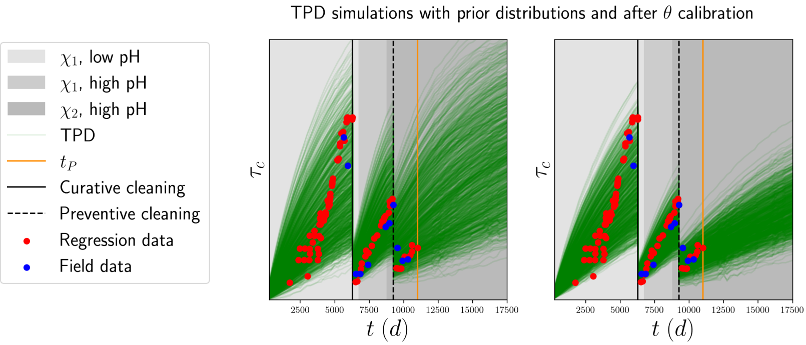

Figure: Uncertainty propagation with regular $\mathcal{U}(I_1) \otimes \ldots \otimes \mathcal{U}(I_d)$ vs. updated posterior $\mathcal{U}(I_1) \otimes \ldots \otimes \mathcal{U}(I_{d-1}) \otimes p(\theta | \mathbf{y}^{\mathrm{RD}}, \mathbf{y}^{\mathrm{FD}}) \rightarrow$ dispersion next to t_P is highly reduced $\rightarrow$ decision-making more robust!

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Summary

- Clogging of SGs in PWR is a degradation phenomenon requiring diagnosis and prognosis for chemical cleaning planning $\rightarrow$ complex phenomenon, hard to model
- Making use of available knowledge to help decision-making in uncertain field $\rightarrow$ UQ methodology + Bayesian calibration allow to give more robust predictions
- Build controllable predictive machine learning algorithms that could be pilotable $\rightarrow$ based on sensor time-series operational data placed on the SG and the PWR $\rightarrow$ *work in progress*
- Hybrid methodology could be generalized to other degradation phenomena to provide decision-making assistance for predictive maintenance

Thank you for your attention!
Any questions?

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Sensitivity analysis: HSIC

- Hilbert-Schmidt Independence Criterion (HSIC) [Gretton et al., 2005], kernel method → evaluates sensitivity of a single-input in a given-data context, no need for surrogate models
- Theoretical result for all $i \in \{1, \ldots, d\}, k \in \{1, \ldots, N\}$:

$$\mathrm{HSIC}(X_i, g(\boldsymbol{X}, t_k)) = 0 \iff X_i \perp g(\boldsymbol{X}, t_k) \tag{5}$$

- The index disposes of U-stat and V-stat estimators + hypothesis testing with corresponding p-value → implemented in the OpenTURNS
- The normalized R^2_{HSIC} index is better suited for interpretation:

$$R^2_{\mathrm{HSIC}}(X_i, g(\boldsymbol{X}, t_k)) = \frac{\mathrm{HSIC}(X_i, g(\boldsymbol{X}, t_k))}{\sqrt{(\mathrm{HSIC}(X_i, X_i)\mathrm{HSIC}(g(\boldsymbol{X}, t_k), g(\boldsymbol{X}, t_k)))}} \in [0, 1]$$

- Empirical evidence suggests show that R^2_{HSIC} can be used confidently for variable ranking → HSIC-ANOVA decompositions also exist *but* only pathological cases create stark differences (see [Sarazin et al., 2023])

Prior HSIC results

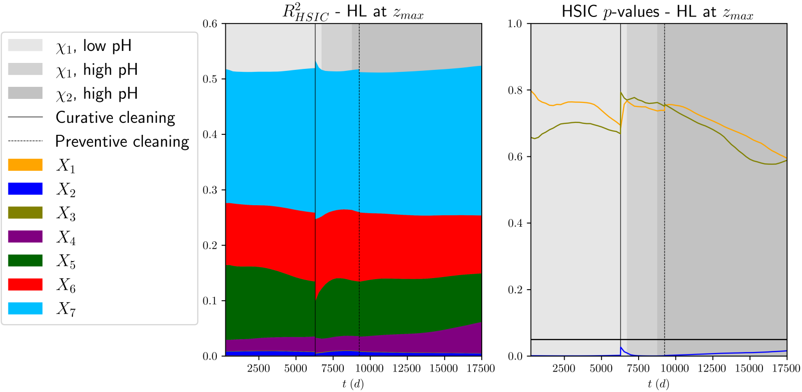

Figure: Normalized HSIC index time variation, ranking displays a potential strong dependence of X_7 on the output $\rightarrow X_7 = \theta$ is the calibration parameter of the DEPO model $\rightarrow$ drives the τ_c kinetics

Posterior HSIC indices

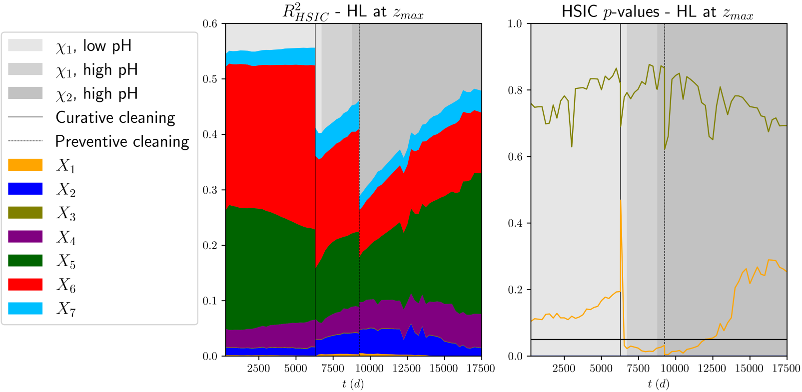

Figure: Normalized HSIC index time variation after calibration $\rightarrow$ displays consequent influence reduction of the X_7 calibration component on the output

References I

Carmassi, M., Barbillon, P., and Chiodetti, M. (2019). Bayesian calibration of a numerical code for prediction. *Journal de la Societe Francaise de Statistique*, 160(1).

Feng, Q., Nebes, J., Bachet, M., Pujet, S., You, D., and Deri, E. (2023). Tube support plates blockage of PWR steam generators: thermalhydraulics and chemical modeling. Proceedings of the International Conference on Water Chemistry in Nuclear Reactor Systems (NPC 2023), Juan-les-Pins.

Girard, S. (2014). *Clogging of Recirculating Nuclear Steam Generators*. Springer International Publishing.

Gretton, A., Bousquet, O., Smola, A., and Scholkopf, B. (2005). *Measuring Statistical Dependence with Hilbert-Schmidt Norms*. Lecture Notes in Computer Science, Algorithmic Learning Theory, 63–77. Springer.

References II

Jaber, E., Chabridon, V., Remy, E., Baudin, M., Lucor, D., Mougeot, M., and Iooss, B. (2024). Sensitivity analyses of a multi-physics long-term clogging model for steam generators. *International Journal for Uncertainty Quantification*.

Keller, M., Damblin, G., Pasanisi, A., Schumann, M., Barbillon, P., Ruggeri, F., and Parent, E. (2022). Validation of a computer code for the energy consumption of a building, with application to optimal electric bill pricing. *Econometrics*, 10(4).

Lefebvre, L., Segond, M., Spaggiari, R., Le Gratiet, L., Deri, E., Iooss, B., and Damblin, G. (2023). Improving the Predictivity of a Steam Generator Clogging Numerical Model by Global Sensitivity Analysis and Bayesian Calibration Techniques. *Nuclear Science and Engineering*, 197(8):2136–2149.

Petit, G. (1991). *THYC: a 3D thermal-hydraulic software for flows in tube bundles*. EDF.

References III

Pinciroli, L., Baraldi, P., Shokry, A., Zio, E., Seraoui, R., and Mai, C. (2021). A semi-supervised method for the characterization of degradation of nuclear power plants steam generators. *Progress in Nuclear Energy*, 131:103580.

Prusek, T., Moleiro, E., Oukacine, F., Adobes, A., Jaeger, M., and Grandotto, M. (2013). Deposit models for tube support plate flow blockage in Steam Generators. *Nuclear Engineering and Design*, 262:418–428.

Rubinstein, R. and Kroese, D. (2011). *Simulation and the Monte Carlo Method*. Wiley Series in Probability and Statistics. Wiley.

Sarazin, G., Marrel, A., Da Veiga, S., and Chabridon, V. (2023). New insights into the feature maps of Sobolev kernels: application in global sensitivity analysis. *Preprint HAL cea-04320711*, pages 1–78.

References IV

Srikantiah, G. and Chappidi, P. (2000). Particle deposition and fouling in PWR steam generators. *Nuclear Engineering and Design*, 200(1-2):285–294.

Vaibhav, Y. and al. (2023). Technical challenges and gaps in integration of advanced sensors, instrumentation, and communication technologies with digital twins for nuclear application. Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States).

Yang, G., Pointeau, V., Tevissen, E., and Chagnes, A. (2017). A review on clogging of recirculating steam generators in pressurized-water reactors. *Progress in Nuclear Energy*, 97:182–196.