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DATA-DRIVEN BAYESIAN MODELING USING APPROXIMATE BAYESIAN COMPUTATION FOR DETECTION OF HEAT EXCHANGER FOULING

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Abstract. Fouling is a chronic issue in heat exchanger operation, degrading performance over time. Tracking the global heat transfer coefficient throughout the operational cycle is particularly effective among various monitoring strategies. This study presents a Bayesian calibration algorithm to assess fouling in heat exchangers using sparse temperature data, a configuration commonly recorded in real thermal plant operations. A reduced-order model, serving as a digital representation of the heat exchanger plant, represents the global heat transfer coefficient and its exponential decay coefficient as random variables to account for the inherent uncertainties of the system. The associated inverse problem is addressed through Bayesian calibration. Given the complexity of real systems, where likelihood functions are often unknown, we employ Approximate Bayesian Computation (ABC) within a sequential Monte Carlo method to accelerate the calibration process while eliminating the need for explicit likelihood functions. The reduced-order model simulations were conducted using a representative shell-and-tube heat exchanger. In this approach, the outlet temperatures of the heat exchanger were determined by solving the system's governing ordinary differential equations, which describe its dynamic thermal behavior. This stochastic representation enabled a more comprehensive analysis of the exchanger's performance under varying operating conditions, forming the foundation for the Bayesian calibration process. Additionally, numerical simulations were performed to validate the proposed data-driven approach, generating representative data and estimating the model's accuracy. Hence, the digital shadow model will be capable of estimating the heat transfer coefficient and the degree of fouling present in the plant based on temperature data typically collected in industrial environments, providing valuable insights into its operational condition.

Keywords: Data-Driven Modeling, Bayesian Modeling, Approximate Bayesian Computation (ABC), Heat Exchanger Monitoring

1. INTRODUCTION

Heat exchangers play a vital role in a wide range of industrial processes, where operational efficiency and cost-effectiveness are closely linked to the equipment's thermal performance and maintenance strategy (Sheriff *et al.*, 2022; Jonsson *et al.*, 2007; Muenthong *et al.*, 2020). As fouling progressively degrades heat transfer capacity, continuous monitoring becomes essential for life cycle management and the planning of preventive interventions. However, developing accurate and robust monitoring tools is still challenging due to the limited availability of commissioning data, sensor inaccuracies, and the inherent uncertainties in real-world operating conditions (Davoudi and Vaferi, 2018). In this context, data-driven modeling has emerged as a promising alternative to first-principles models, as it enables the creation of digital replicas—or digital shadows—of heat exchangers using process data such as temperature and flow rate, which are routinely collected by industrial control systems (Gong *et al.*, 2022; Brunton and Kutz, 2019).

Recent advances have highlighted the potential of digital twins in predicting system behavior and assessing equipment health (Ritto and Rochinha, 2021; Yu *et al.*, 2022). However, for such models to be reliable, especially under uncertainty, a probabilistic framework is required. Bayesian inference has been increasingly adopted for this purpose due to its ability to incorporate uncertainty stemming from limited knowledge, sensor noise, and modeling assumptions (Strzelczyk *et al.*, 2024). While the Markov Chain Monte Carlo (MCMC) method is a common choice for Bayesian calibration, its reliance on explicitly defined likelihood functions often poses limitations in complex or ill-posed problems (da S Raqueti *et al.*, 2022).

To address this challenge, we propose a likelihood-free approach based on Approximate Bayesian Computation (ABC)

for calibrating a reduced-order model of a shell-and-tube heat exchanger. Still, the Sequential Monte Carlo (SMC) method was adopted as the sampling strategy for the ABC calibration. The SMC samplers offer notable advantages over MCMC, such as improved convergence and the ability to handle complex, likelihood-free problems. Their flexibility and efficiency make them particularly suitable for the probabilistic estimation of system parameters in uncertain and dynamic environments (Del Moral *et al.*, 2006). This developed model is designed to estimate the overall heat transfer coefficient ($\mathbb{U}$) as a stochastic parameter, reflecting the system's evolving condition due to fouling. The ABC method enables probabilistic calibration directly from operational data without the need for a likelihood function or large labeled datasets, as typically required by conventional machine learning approaches (Ritto *et al.*, 2023). The result is a flexible and interpretable model that acts as a digital shadow, allowing real-time condition monitoring of heat exchangers. This approach demonstrates strong potential for practical applications in industrial environments, particularly in scenarios where measurement data are sparse and reliable diagnostics are crucial.

In this study, the methodology was validated using synthetically generated data that emulate the dynamic behavior of a heat exchanger undergoing progressive fouling. By modeling an exponential increase in fouling over time, we estimated $\mathbb{U}$ at successive time points, enabling an analysis of the degradation pattern and an assessment of the model's ability to capture the decline in thermal performance.

The paper is organized as follows: first, in section two, we present the digital shadow modeling of the heat exchanger; next, in the third section, we detail the results of the fouling detection procedure; and finally, in the fourth section, we provide concluding remarks.

2. HEAT EXCHANGER MODELING

2.1 Bayesian Modeling

In engineering problems, particularly those involving complex systems such as heat exchangers, simplified models are often used as representations of their more intricate counterparts. Then, it is crucial to assess the fidelity of these simplified models and capture how accurately they reflect the real-world problem. In this context, stochastic modeling emerges as a sophisticated tool, enabling the emulation of various scenarios by acknowledging the inherent variability in system parameters. This approach offers a more realistic representation of the physical model and provides a quantifiable measure of uncertainty.

For our stochastic modeling, we begin by considering the general regression problem used to represent data observations:

$$y = f(\theta; x) + \varepsilon, \quad (1)$$

where $y \in \mathbb{R}^D$ represents the data observations, $f(\cdot, \cdot)$ is a functional model form given a set of parameters $\theta \in \mathbb{R}^n$ and an input $x \in \mathbb{R}^D$, and $\varepsilon \in \mathbb{R}^D$ is the additive modeling error, that encompasses model and measurement errors, under the assumption of identically and independently distributed samples.

The Bayesian rule states that the updated posterior PDF (Probability Density Function) of model parameters, given observed data, can be expressed as:

$$\pi(\theta|y) = \frac{\pi(y|\theta)\pi(\theta)}{\pi(y)}, \quad (2)$$

in which $\pi(\theta|y)$ is the posterior distribution, $\pi(\theta)$ is the prior PDF, $\pi(y|\theta)$ is the likelihood function, and $\pi(y)$ is considered a normalizing constant. As mentioned, the likelihood function is defined by the predictive error model. However, if this error form is unknown, we cannot explicitly write this function.

To overcome this limitation, the Approximate Bayesian Computation (ABC) algorithm provides a framework for inferring the updated posterior distribution from Equation 2, based on a distance/metric function $d(\cdot, \cdot) : \mathbb{R}^D \times \mathbb{R}^D \mapsto \mathbb{R}$, in which:

$$\pi(\theta|d(y, f(\theta; x)) \leq \epsilon) \propto \pi(d(y, f(\theta; x)) \leq \epsilon) \times \pi(\theta), \quad (3)$$

Here, ϵ is a threshold or tolerance acceptance level for a candidate sample θ . Thus, the ABC scheme approximates $\pi(\theta|y)$. Note that if ϵ is sufficiently small, $\pi(\theta|d(y, f(\theta; x)) \leq \epsilon)$ is a good approximation for the posterior distribution. The distance/error metric $d(\cdot, \cdot)$ can take different forms depending on the problem being addressed (Castello and Ritto, 2023). In this case, we used this error function:

$$J = \mathbf{D} - \mathbf{M}(\theta) \quad (4)$$

were $\mathbf{D}$ represents the measured data, and $\mathbf{M}(\theta)$ is the output obtained from the mathematical model.

To solve this problem, a set of candidates is generated from the prior distribution of the model parameters. The model's response is calculated, and the distance metric is estimated based on the observed data. In the classical ABC approach, known as the ABC rejection sampler (Lye *et al.*, 2021), if this difference is smaller than the proposed acceptance level, these candidates are accepted to compose the posterior distribution; otherwise, they are rejected. This procedure is carried out, achieving convergence on the posterior distribution.

However, this method incurs a high computational cost in some cases, mainly because of the complex sampling space imposed by prior distribution, necessitating numerous simulations before it converges to yield satisfactory results. Moreover, if the chosen acceptance level is too small, the probability of obtaining successful candidates for the posterior function becomes low. Meaning that, the candidate space in the prior function can be broad, searching for candidates that satisfy the limit, exhausting and diminishing the algorithm's efficiency.

With these challenges in mind, the SMC method offers a more efficient alternative (Green *et al.*, 2022). It involves an iterative updating of the probability distribution from which the data are sampled. This approach substantially accelerates the calibration process, addressing the issue of computational cost while still avoiding the need to calculate a likelihood function.

In the SMC algorithm, parameters are sampled from a prior distribution, and a weight $\mathbf{W}$ is computed based on a chosen kernel, which is then associated with each sample. This weight guides the subsequent update of the distribution. After updating the distribution, the sampling process is repeated iteratively until the calibration results are satisfactory. The kernel function used in this case is based on the same error metric as before, and the weights were calculated as:

$$\mathbf{W} = \frac{1}{\mathbf{D} - \mathbf{M}(\theta)}. \quad (5)$$

In this case, based on the use of measured temperature data that will be described in the next sections, the likelihood function is maximized in the case of the MCMC method, while in the ABC methodology, the calculated metric is minimized, seeking to align the heat exchanger model's predictions with real data as closely as possible. With the model properly calibrated, simulations and analyses can be conducted to assess the current state of the heat exchangers.

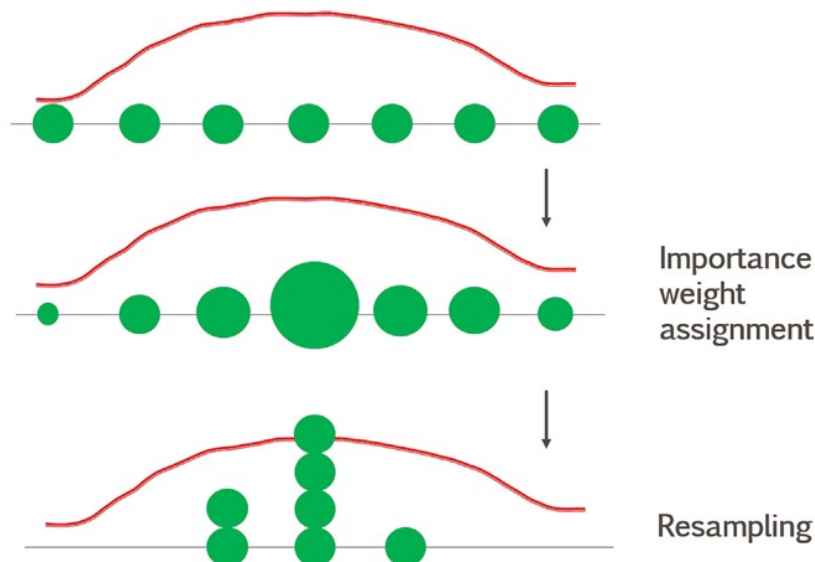


Figure 1. Illustration of SMC Method from Lye *et al.* (2021)

Figure 1 is an illustration of how the resampling process is carried out, where the red curve represents the statistical weight function and the samples are in green.

2.2 Stochastic Modeling of Heat Exchangers

The heat exchanger, a fundamental component in thermal systems, enables the exchange of thermal energy between two fluids at different temperatures. In this work, a concentric shell-and-tube heat exchanger operating in counter-flow was selected due to its conceptual simplicity and relevance for controlled thermal transfer processes. Both fluids—water in this case—circulate through the shell and tube sides, respectively.

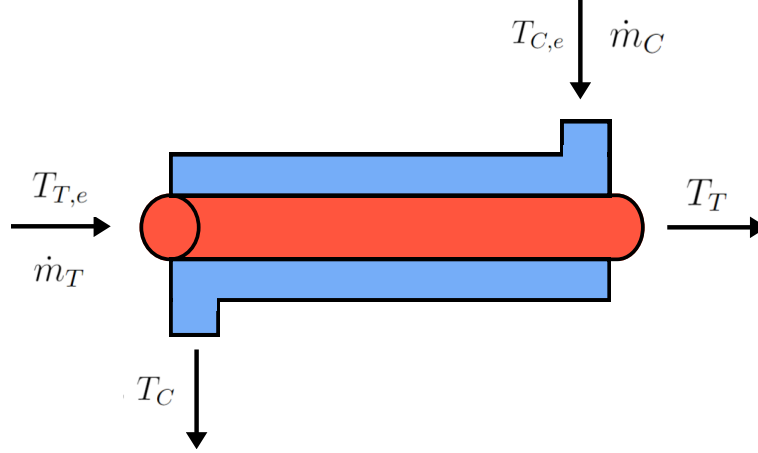


Figure 2. Schematic diagram of the Heat Exchanger

To construct a dynamic, reduced-order model commonly adopted in literature and enough to describe and identify the system with the Bayesian calibration, a set of simplifying assumptions was adopted. Thermophysical properties of the fluids are considered constant (temperature-independent); the system is thermally insulated from the environment (adiabatic walls); heat transfer occurs solely by convection between the fluids, with conduction effects neglected; changes in kinetic and potential energy are negligible; the system operates under steady-state flow conditions.

A schematic diagram of the heat exchanger is shown in Figure 2. The hot fluid enters the inner tube at a constant mass flow rate $\dot{m}_T$ [$\frac{\text{kg}}{\text{s}}$] and inlet temperature $T_{T,e}$ of 90°C, while the cold fluid enters the shell at a temperature $T_{C,e}$ of 20°C at $\dot{m}_C$ [$\frac{\text{kg}}{\text{s}}$]. Both fluids undergo heat exchange along the length of the exchanger, resulting in outlet temperatures T_T [°C] and T_C [°C] for the hot and cold streams, respectively. The cold fluid entirely gains the energy lost by the hot fluid.

Based on energy conservation and the relevant constitutive relations, the governing differential equations that describe the dynamic behavior of the outlet temperatures are:

$$\frac{dT_T}{dt} = \frac{1}{\rho_T V_T C_{P,T}} [\dot{m}_T C_{P,T} (T_{T,e} - T_T) - \mathbb{U}A(T_T - T_C)], \quad (6)$$

$$\frac{dT_C}{dt} = \frac{1}{\rho_C V_C C_{P,C}} [\dot{m}_C C_{P,C} (T_C - T_{C,e}) + \mathbb{U}A(T_T - T_C)]. \quad (7)$$

The first term in each equation represents the enthalpy transport resulting from mass flow and a temperature difference. In contrast, the second term corresponds to the convective heat exchange between the fluids, characterized by the overall heat transfer coefficient $\mathbb{U}$ and the heat exchange area A [m^2].

The nominal parameter values used in the model are summarized in Table 2, and were defined based on the geometric and thermal characteristics of the physical system.

The overall heat transfer coefficient was computed from convective heat transfer coefficients of the hot (h_H) and cold (h_C) fluids using:

$$U = \left(\frac{1}{h_H} + \frac{1}{h_C} \right)^{-1}, \quad (8)$$

where h_H and h_C were estimated using the Dittus–Boelter correlation:

$$Nu = 0.023 \cdot Re^{0.8} \cdot Pr^{0.4}, \quad (9)$$

and the Nusselt number is related to the heat transfer coefficient by:

$$Nu = \frac{hD_h}{k}, \quad (10)$$

with D_h being the hydraulic diameter, k the thermal conductivity, and Re, Pr the Reynolds and Prandtl numbers respectively.

To construct the stochastic model, the overall heat transfer coefficient U was treated as a random variable, denoted here as $\mathbb{U}$. Based on the deterministic model, the prior distributions and experimental distribution mean for the initial value of $\mathbb{U}$ were defined by the deterministic value estimated - presented in Tab. 2. For the prior distribution of the parameter, a uniform distribution with a $\pm 10\%$ variation around the mean was adopted. This choice represents a non-informative prior, as no prior knowledge about the parameter's behavior was assumed. In contrast, the synthetic data were generated using a Gaussian distribution with a standard deviation of 5%, providing a probabilistic characterization of the system behavior.

This reduced-order model, governed by two first-order ODEs, forms the core of the Bayesian calibration process by capturing the dominant thermal dynamics of the system. While simplifications introduce model discrepancies, these can be quantified and addressed through stochastic modeling and uncertainty propagation in the calibration stage.

3. FOULING DETECTION METHOD

A parameter calibration was conducted using Bayesian modeling and the SMC method, as previously discussed, for a thermal system represented by a shell-and-tube heat exchanger. To emulate the fouling process, an exponential decay function was adopted to simulate the consequence of fouling, resulting in a time-dependent coefficient and a stochastic process (Fig.3 and Eq.11). Based on this decaying behavior, synthetic temperature data were emulated based on the experimental distribution of $\mathbb{U}$. These temperature data, result of the random process, represent uncertainty in the system and served as the experimental observations for the calibration process.

$$\mathbb{U}(t) = \mathbb{U}_0 \cdot e^{-\frac{t}{\lambda}}, \quad (11)$$

where $\mathbb{U}_0$ is the random variable representing the initial value of $\mathbb{U}$ in the absence of fouling, λ is the fouling coefficient, and t is the simulation time. The values used in the simulation are presented in Tab 1 and 2.

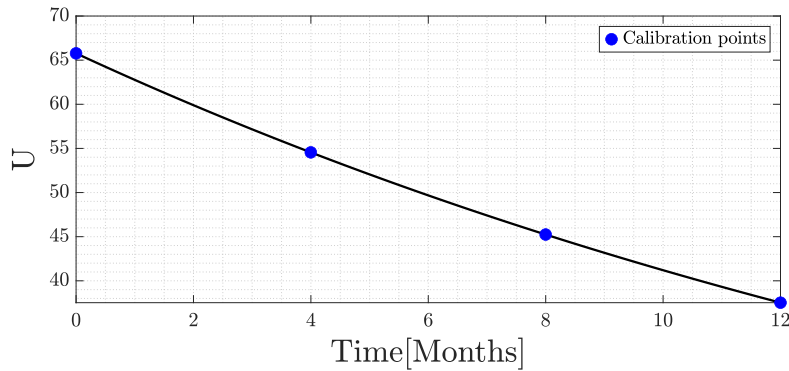


Figure 3. U decay

Table 1. Parameters - decay function

$\mathbb{U}_0 \left[\frac{W}{m^2K} \right]$	$\lambda [s]$
65.78	-1.03×10^3

The Bayesian inference procedure aimed to estimate the value of $\mathbb{U}$ at four distinct time points over one simulated year. A prior distribution was defined as uniform, also centered on the deterministic mean value of U , representing an initial state of knowledge before observing the data.

The SMC method was implemented using 8 sequential updates of the prior distribution. In each step, 120 samples of the parameter space were drawn, and their corresponding weights W (Eq. 5) were calculated based on a predefined distance metric J (Eq. 4), inversely proportional to the deviation between the observed and simulated outputs. These weights guided the resampling and propagation of the distributions across iterations, progressively refining the posterior estimation of $\mathbb{U}$.

As a result of the simulations, the posterior distributions of the calibrated parameter at each time point were obtained, as shown in Fig. 4. The evolution of the PDF can be observed, indicating the decay of $\mathbb{U}$ over time as a consequence of fouling accumulation. The chain was updated from the prior to the posterior distribution through the simulation steps.

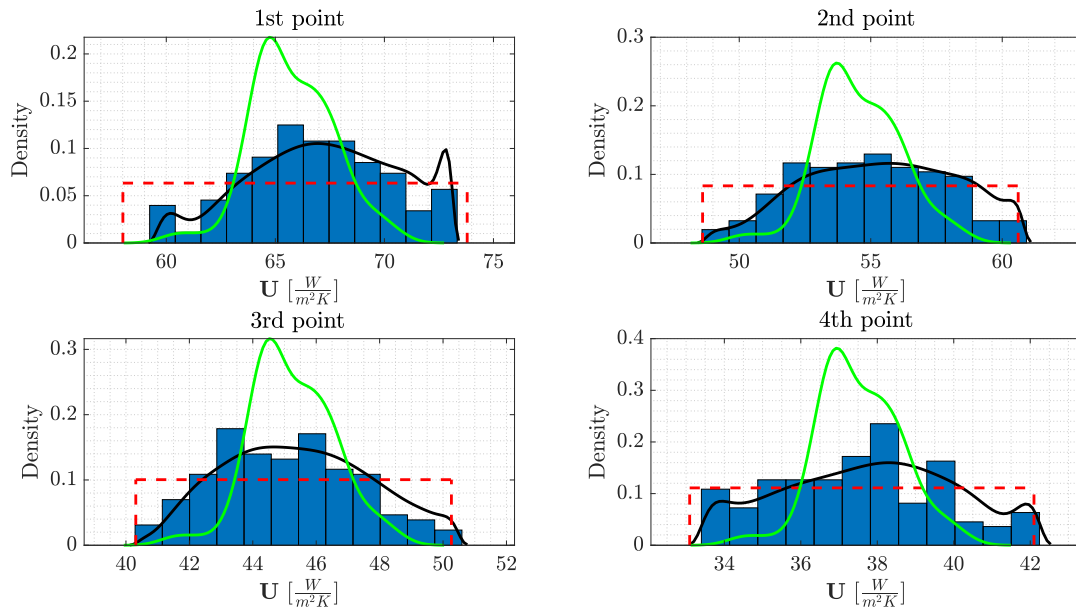


Figure 4. Posterior distributions in wich point of calibration - Posterior (blue), EPDP achieved (black), Prior (red), Target (green).

Notably, the means of these distributions—characterized by the peaks of the (PDFs)—are closely aligned with the target distribution, indicating that the calibration procedure was consistent and effective in capturing the expected parameter behavior.

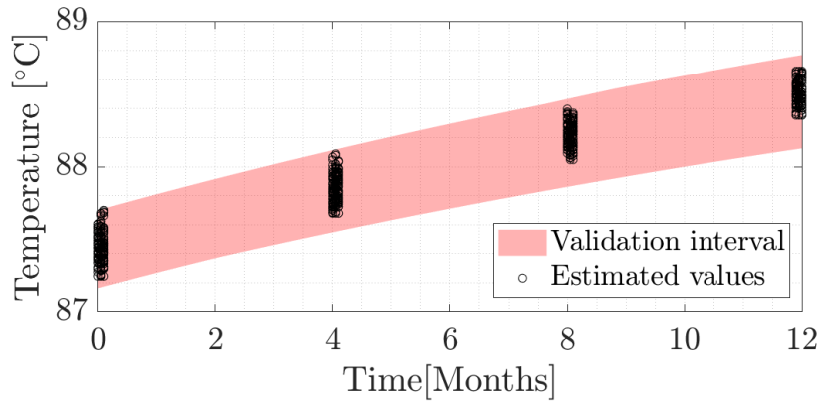


Figure 5. Hot temperature curve

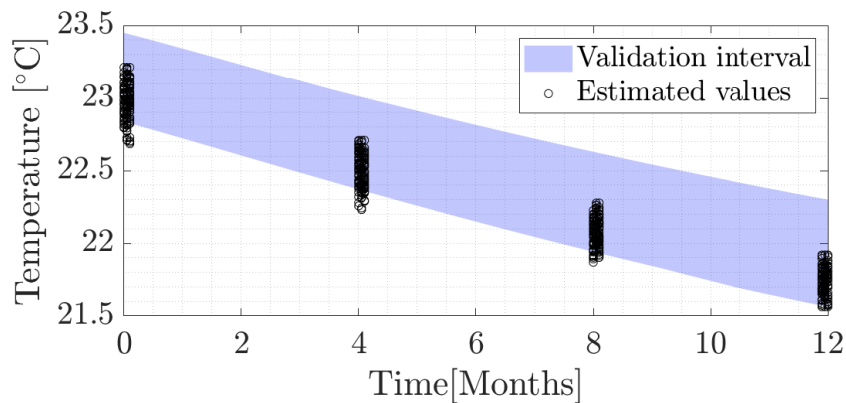


Figure 6. Cold temperature curve

In the temperature curves shown in Fig. 5 and 6, it is possible to observe the loss of efficiency of the heat exchanger over time. Moreover, the temperatures obtained through calibration—i.e., those resulting from the values of $\mathbb{U}$ estimated by the Bayesian inference process—are almost entirely within the range of values that represent the actual system. This indicates that the calibration procedure was successful in capturing the thermal behavior of the system under fouling conditions.

It can also be observed from the plots that the calibration results show better agreement for the hot fluid temperature. This occurs because the synthetic data were generated using a second-order model, which introduces a transient period that should be disregarded in simulations over a long time. Since the duration of this transient response depends on the properties and volume of each fluid, it differs between the hot and cold fluids. This discrepancy leads to greater deviation in the calibration results for the cold fluid.

Table 2. Nominal values of parameters

Parameters (Heat exchanger)			Parameters (fluids)		
Parameters	Units	Values	Parameters	Units	Values
A	m^3	1.73×10^{-1}	$C_{P,T}$	$\frac{\text{J}}{\text{kgK}}$	4186.80
ℓ	m	1.2	$C_{P,C}$	$\frac{\text{J}}{\text{kgK}}$	4186.80
D_T	m	0.0459	μ_a	$\text{Pa} \cdot \text{s}$	7.97×10^{-4}
D_H	m	0.0795	$\rho_{T,C}$	$\frac{\text{kg}}{\text{m}^3}$	998.21
V_T	m^3	2.0×10^{-3}	k_a	$\frac{\text{W}}{\text{mK}}$	6.1×10^{-1}
V_C	m^3	6.0×10^{-3}	Pr_q	-	2.90
$\dot{m}_T$	$\frac{\text{kg}}{\text{s}}$	6.99×10^{-2}	Pr_f	-	6.14
$\dot{m}_C$	$\frac{\text{kg}}{\text{s}}$	6.0×10^{-2}	Re_q	-	2.43×10^3
U	$\frac{\text{W}}{\text{m}^2 \cdot ^\circ\text{C}}$	65.78	Re_f	-	1.20×10^3

4. FINAL REMARKS

The results demonstrate that the Bayesian framework successfully captures the decay trend of $\mathbb{U}$ and closely approximates the synthetic ground truth used in the simulations. This indicates that the proposed method is capable of tracking the temporal degradation in thermal performance while providing probabilistic estimates of uncertainty, offering a robust tool for monitoring heat exchanger fouling using only basic process information available from the control system.

Although the calibration produced satisfactory results, some limitations in accuracy and efficiency can be attributed to errors inherent in the generation of synthetic experimental data. As part of future work, the methodology will be validated using data from laboratory-scale test benches and real-world heat exchanger systems, thereby enhancing its practical applicability and reliability. Furthermore, this Bayesian calibration approach, when combined with the SMC method, constitutes a powerful tool for the real-time monitoring of thermal systems. Integrating this technique into Digital Twin frameworks enables continuous assessment of equipment condition, reduction of unexpected downtime, and optimization of maintenance strategies. Such an approach has the potential to significantly reduce operational costs and support more informed decision-making through accurate and timely insights into system health.

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