

## ENC-2024-XXXX

# Data-Driven Bayesian Modeling Using Approximate Bayesian Computation for Heat Exchanger Monitoring

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**Abstract.** For monitoring the operation of heat exchanger by measuring the temperature data is essential to have a digital replica that communicates with the process control. Bayesian calibration tools oriented by these data are a welcome way to carry out this identification, as a heat exchanger has many uncertain parameters and requires stochastic modeling, especially when estimating the overall heat transfer coefficient. The Approximate Bayesian Computation (ABC) method is one likelihood-free technique that has gained popularity. In this context, this paper aims to implement this method for a reduced-order heat exchanger model. The overall heat transfer coefficient is calibrated, alongside an analysis of a distance metric estimated based on observed data, to estimate the parameter's probability distribution. The results of the chosen parameter calibration are presented, along with the system responses obtained through the calibration, represented by the temperature curves of the hot and cold fluids. Additionally, the validation data are exhibited, demonstrating the model's efficiency.

**Keywords:** Heat Exchanger, System identification, Approximate Bayesian Computation (ABC), Data-driven, Bayesian Modeling

## 1. INTRODUCTION

Since heat exchangers are essential equipment in various industrial processes, it is important to ensure adequate life-cycle management, reducing costs and increasing efficiency through maintenance and scheduled shutdowns only when necessary (Sheriff *et al.*, 2022; Jonsson *et al.*, 2007; Muenthong *et al.*, 2020). Many methods are used to monitor the operation of heat exchangers, and the availability of measurement and data storage, especially flow and temperature data, has increasingly allowed for the implementation of digital models that function as accurate replicas of heat exchangers in supervisory control and process monitoring systems. Currently, the use of digital twins has been widely documented in the literature (Ritto and Rochinha, 2021), where communication between the physical plant (heat exchanger) and the digital model (the identified model) is interconnected and can bring actions and parameter changes in both directions (Gong *et al.*, 2022; Chen *et al.*, 2023; Yu *et al.*, 2022).

Moreover, data-driven modeling, which harnesses data from industrial plants, is a game-changer. It eliminates the need for costly or time-consuming implementation of phenomenological models. These data-driven models, identified using parameter calibration techniques, are particularly effective in dealing with uncertainties. Bayesian modeling approaches, widely used in the analysis and identification of thermal systems, are instrumental in this. They help address inherent uncertainties, whether stemming from a lack of knowledge or systematic errors during operation or temperature variable measurements, thereby enhancing the reliability of the models.

A popular Bayesian calibration is the Markov Chain Monte Carlo (MCMC). However, the MCMC generally involves likelihood functions to assess the probability of specific temperature fields occurring, given known parameters to calibrate and entail residuals and poorly known statistical distributions (da S Raqueti *et al.*, 2022). Unfortunately, several applications do not have a simple way to define a likelihood function. Therefore, this paper applies a likelihood-free approach, the approximate Bayesian computation (ABC), to propose a calibration in a heat exchanger. This approach, widely used in cases where a dataset has intractable likelihood functions, holds significant promise. The results of our study demonstrate that, even with limited measurement knowledge of temperature, it is feasible to calibrate a satisfactory data-driven model. This not only validates the potential of the ABC approach but also underscores its role in facilitating decisions regarding

the heat exchanger's operational status, instilling hope for its wider application in heat exchanger management.

## 2. HEAT EXCHANGER MODELING

The heat exchanger, a crucial equipment facilitating thermal energy transfer between two fluids at different temperatures, is a key focus of our simulation. The chosen model, a concentric Shell-and-Tube heat exchanger operating in countercurrent with water as the fluid in both the shell and the tube, was selected for its simplicity. This model plays a pivotal role in generating the necessary data to calibrate the parameters of the simplified model, which forms the foundation for the proposed digital model:

- Variation in fluid properties with temperature is considered negligible;
- The heat exchanger is considered adiabatic, meaning there is no heat exchange with the environment;
- Initially, effects of the conduction phenomenon were disregarded, with heat exchange in the exchanger being exclusively between the fluids and through convection;
- Variation in kinetic and potential energy is insignificant;
- The heat exchanger operates under steady-state conditions.

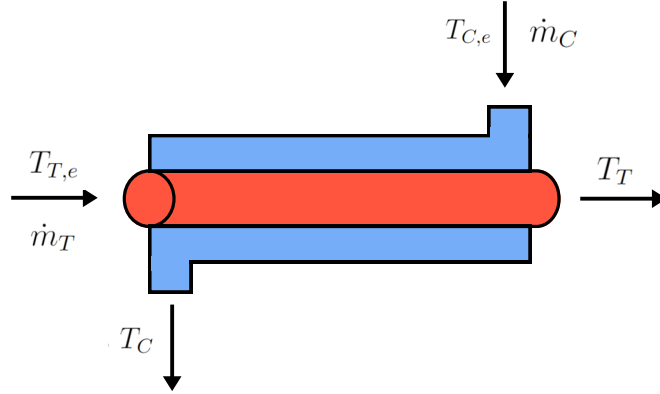


Figure 1. Schematic diagram of the Heat Exchanger

In the system, the hot fluid enters the inner tube at a temperature  $T_{T,e}$  of 90°C at a constant flow rate  $\dot{m}_T$  [ $\frac{kg}{s}$ ] and exits at temperature  $T_T$  [°C] on the opposite side; the cold fluid enters at a temperature  $T_{C,e}$  of 20°C at  $\dot{m}_C$  [ $\frac{kg}{s}$ ] and exits at  $T_C$  [°C]. The heat lost by the water in the tube is gained by the water in the shell, with the former fluid being cooled.

Considering the system equations, constitutive relations, and most importantly, the energy balances, we obtain the differential equations that describe the system dynamics. These energy balances play a crucial role in ensuring the accuracy of our analysis.

$$\frac{d}{dt}(T_T) = \frac{1}{\rho_T V_T C_{P,T}} [\dot{m}_T C_{P,T} (T_{T,e} - T_T) - U_{CT} A_{CT} (T_T - T_C)], \quad (1)$$

$$\frac{d}{dt}(T_C) = \frac{1}{\rho_C V_C C_{P,C}} [\dot{m}_C C_{P,C} (T_{C,e} - T_C) + U_{CT} A_{CT} (T_T - T_C)]. \quad (2)$$

The first term in both differential equations, which relates the flow rate-  $\dot{m}_T$  and  $\dot{m}_C$ - to the difference between the inlet temperatures and the temperatures of each fluid, refers to the transport of enthalpy due to the fluid flow. The second term, relating the overall heat transfer coefficient  $U_{CT}$  [ $\frac{W}{m^2 \cdot ^\circ C}$ ], the heat exchange area  $A_{CT}$  [ $m^2$ ], and the temperature difference between the fluids, corresponds to the heat transfer between the fluids. Table 1 provides the parameter values used.

Considering that the thermodynamic properties are defined concerning a temperature close to that assumed for the fluid, this resolution approximates the actual model, and many variables were not assumed. Such approximations are adopted to simplify the system's resolution, even though they result in some distortion of the simulation compared to the actual model. However, these approximations are integrated and analyzed through stochastic modeling to be presented later. It should be noted that the discrepancies between the simplified model and the dynamics present in the experimental data can be incorporated into uncertainty propagation and quantification, i.e., within confidence intervals in the data.

Table 1. Nominal values of parameters

| Parameters (Heat exchanger) |                                |                       | Parameter (fluid) |                  |                       |
|-----------------------------|--------------------------------|-----------------------|-------------------|------------------|-----------------------|
| Parameter                   | Unit                           | Value                 | Parameter         | Unit             | Value                 |
| $m_T$                       | $\frac{kg}{s}$                 | $6.99 \times 10^{-2}$ | $C_{P,TeC}$       | $\frac{J}{kgK}$  | 4186.80               |
| $A_{CT}$                    | $m^3$                          | $1.73 \times 10^{-1}$ | $\mu_a$           | $Pa \cdot s$     | $7.97 \times 10^{-4}$ |
| $V_T$                       | $m^3$                          | $2.0 \times 10^{-3}$  | $\rho_{TeC}$      | $\frac{kg}{m^3}$ | 998.21                |
| $V_C$                       | $m^3$                          | $6.0 \times 10^{-3}$  | $k_a$             | $\frac{W}{mK}$   | $6.1 \times 10^{-1}$  |
| $m_C$                       | $\frac{kg}{s}$                 | $6.0 \times 10^{-2}$  | $Pr_q$            | -                | 2.90                  |
| $U_{CT}$                    | $\frac{W}{m^2 \cdot ^\circ C}$ | 71.74                 | $Pr_f$            | -                | 6.14                  |

### 3. STOCHASTIC MODELING

A numerical model serving as a digital replica must communicate with process control systems to monitor the operation of heat exchangers in industrial environments. However, heat exchangers present numerous uncertain parameters and necessitate stochastic modeling, particularly in estimating the overall heat transfer coefficient. Moreover, stochastic modeling will form the basis for developing Bayesian calibration and system identification. This approach will be presented in the subsequent chapters of this work.

#### 3.1 Approximate Bayesian Computation

Figure 2 provides a graphical summary of the calibration process. This process is instrumental in developing a data-driven reduced-order physical model, which plays a key role in supporting decision-making regarding the state of a heat exchanger.

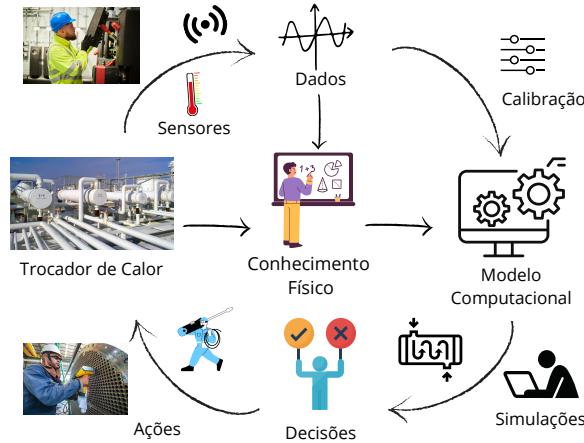


Figure 2. Graphical abstract of data-driven

Consider the following general regression problem to represent data observations:

$$y = f(\theta; x) + \varepsilon, \quad (3)$$

where  $y \in R^D$  represents data observations,  $f(\cdot, \cdot)$  is a functional model form given a set of parameters  $\theta \in R^n$  and an input  $x \in R^D$ , and  $\varepsilon \in R^D$  is the additive modeling error.

The Bayesian approach states that:

$$\pi(\theta|y) = \pi(y|\theta)\pi(\theta)\pi(y), \quad (4)$$

in which  $\pi(\theta|y)$  is the updated posterior probability density function of model parameters given observed data,  $\pi(\theta)$  is the prior probability density function,  $\pi(y|\theta)$  is the likelihood function, and  $\pi(y)$  is considered as a normalizing constant. As mentioned, the likelihood function is given by the model of the predictive error. For accurate models, errors  $\varepsilon$  do not depend on model parameters – therefore, if a Gaussian distribution is assumed to fully describe the density of  $\varepsilon$ , the posterior distribution is fully tractable. However, as stated beforehand, digital shadow models might face missing physics, which turns the likelihood untractable and we cannot explicitly marginalize this function to obtain the posterior distribution.

To overcome such limitation, the ABC algorithm provides a framework for inferring the updated posterior distribution from Eq. 4 based on a distance/metric function  $d(\cdot, \cdot) : R^D \times R^D \mapsto R$ , in which:

$$\pi(\theta|d(y, f(\theta; x)\epsilon)) \propto \pi(d(y, f(\theta; x)\epsilon)) \times \pi(\theta), \quad (5)$$

where  $\epsilon$  is a threshold or tolerance acceptance level for a candidate sample  $\theta$ ; thus, the ABC scheme approximates the  $\pi(\theta|y)$ . Note that if  $\epsilon$  is sufficiently tiny,  $\pi(\theta|d(y, f(\theta; x)\epsilon))$  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, such as the  $L_2$  norm and the  $L_1$  norm, among others.

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 data observations. 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 until convergence on the posterior distribution is achieved. This strategy is the classic ABC approach, called the ABC rejection sampler (Castello and Ritto, 2023).

Note that problems can occur with this approach. On the one hand, if the threshold chosen is small, there is a slight possibility of obtaining successful candidates in the posterior function. On the other hand, the space of candidates comprising the prior function can be large, and traversing it in search of candidates that satisfy the threshold can be exhausting, reducing the algorithm's efficiency.

#### 4. RESULTS

Experimental data were emulated from a Gamma distribution of the parameter  $U$  with a standard deviation of 5 % for calibration initiation. Two hundred experimental samples were generated, and additional data were emulated with the same distribution for subsequent validation.

A uniform prior distribution with a 15% variation centered around the mean value 71.7 was set as input for the calibration. This mean value represents the global heat transfer coefficient calculated for the average adopted properties. The model is solved to obtain the system's response for the proposed  $U$  values, resulting in the tube and shell outlet temperatures. A metric is then calculated between the experimental data and the model response for the proposed values. Based on the analysis of this metric, which represents the comparative residual between the responses, the ABC algorithm determines whether the proposed value from the prior distribution is accepted. If accepted, it contributes to the posterior distribution of the calibrated parameter. Thus, the resulting distributions are presented in Figure 3, showing the calibrated parameter's prior, posterior, and experimental (target) distributions.

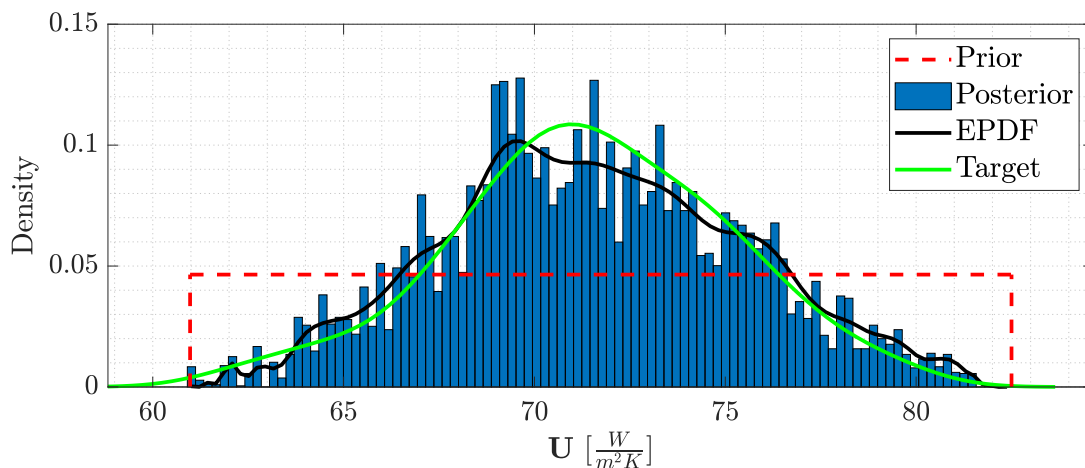


Figure 3. Results for Approximate Bayesian Computation

It can be observed that the probability distribution of the calibrated parameter, initially uniform, is now very close to the experimental distribution after updating, indicating that the parameter was successfully calibrated.

The system's response to the calibrated overall heat transfer coefficient, as depicted in Figure 4, falls within the 95% interval of the temperature curves for both the cold and hot fluids. This alignment with the validation data, which accurately represents the system's actual response, confirms the precision of our calibration process.

All validation data falls within the confidence interval predicted by the calibrated model. This gives us confidence in the digital model, even when based on a reduced-order replica. It effectively handles the inherent uncertainties of the physical process and quantifies them efficiently, predicting the temperature curves with a high level of accuracy.

Ten thousand samples were proposed using the Monte Carlo method to calibrate. Convergence of the method was

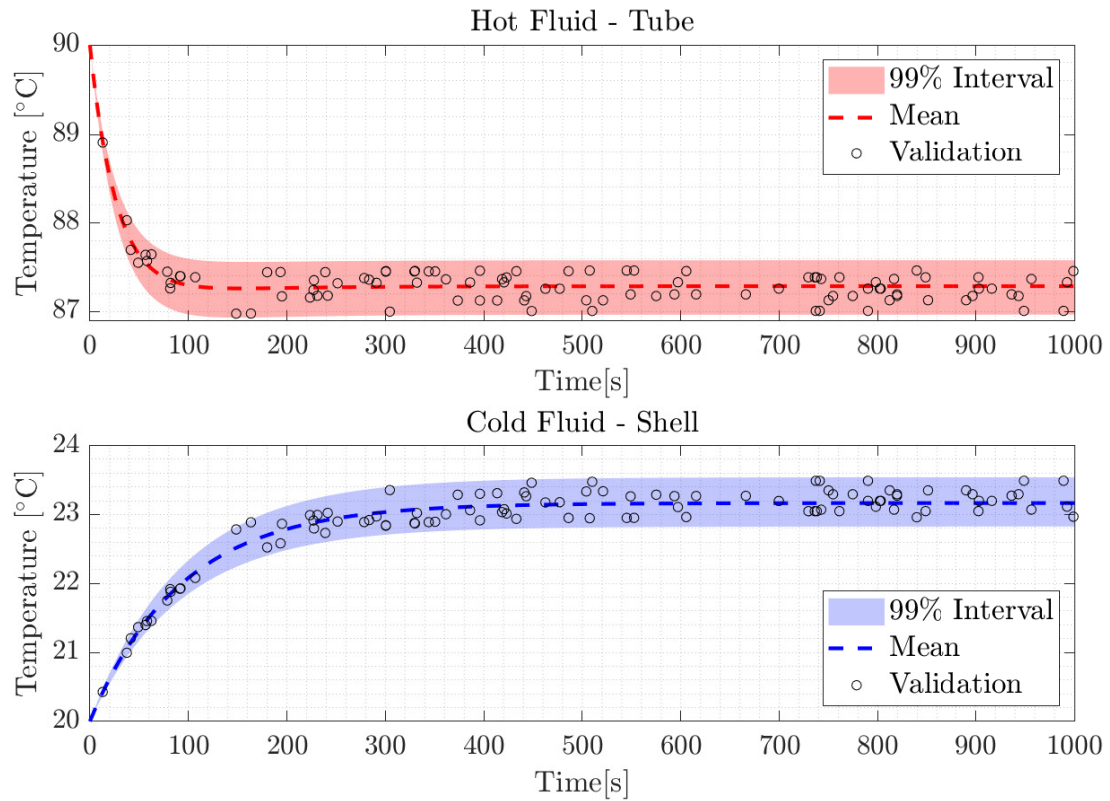


Figure 4. System responses with  $U$  as a random variable calibrated by the ABC method and validation data

ensured by analyzing the first statistical moment of the samples, as shown in the graph in Figure 5. The stabilization of the mean measurements indicates the convergence of the method.

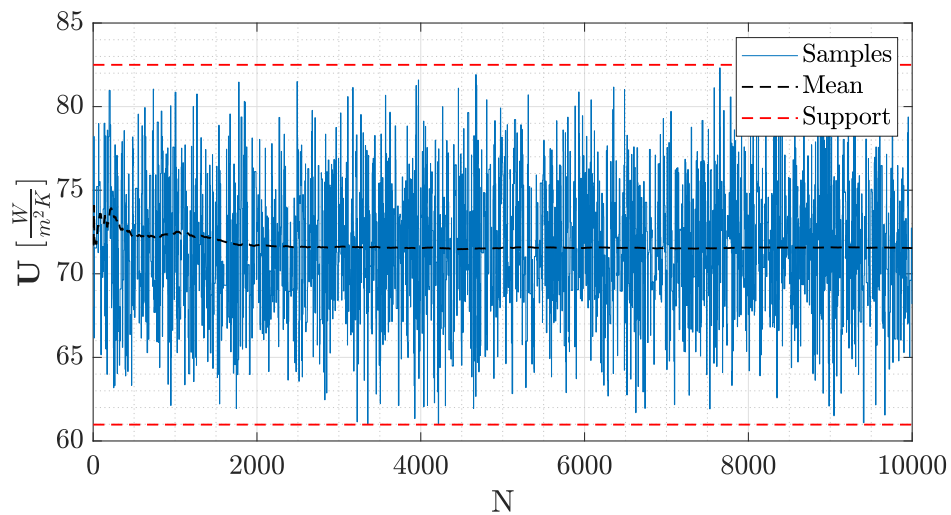


Figure 5. Observation of the first statistical moment of the samples proposed by the Monte Carlo method

## 5. FINAL REMARKS

Based on the results obtained, it was possible to successfully perform the Bayesian calibration of the parameter of overall heat coefficient, which is fundamental for the heat exchanger model under study. The posterior distribution concentrated in a range of values similar to those present in the experimental distribution, confirming the successful calibration of the parameter. Additionally, the temperature curves were represented with a 99% confidence interval and an average, providing a more comprehensive analysis of the uncertainties related to the system's behavior. As a future step, it will

calibrate several parameters to improve the model. Furthermore, actual data from a heat exchanger will be used, including fooling effects to detect the change in the overall heat coefficient automatically.

## 6. ACKNOWLEDGEMENTS

The authors thank FAPESP for the support provided by the process 2023/13794-7, as well as the BEPE scholarship associated with the grant 24/05412-0, the Institut FEMTO-ST for hosting the research internship experienced by the first author, and CNPq for grant 309467/2023-3. The authors also acknowledge the support of CNPq through Call CNPq/MCTI No. 10/2023 - Range B - Consolidated Groups, process 404475/2023-0, and the support of INCT-EIE (Instituto Nacional de Ciência e Tecnologia - Estruturas Inteligentes em Engenharia), funded by Brazilian agencies CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico) under grant number 406148/2022-8, as well as CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior) and FAPEMIG (Fundação de Amparo à Pesquisa do Estado de Minas Gerais).

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