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Bayesian and ultrasonic sensor aided multi-objective optimisation for sustainable clean-in-place processes

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ABSTRACT

In food and drink manufacturing, clean-in-place procedures are essential for hygienic and efficient operations but often over-clean process equipment leading to unnecessary use of energy, water, and chemicals. Previous attempts in the literature to optimise clean-in-place processes have focused on trialling cleaning over a range of parameter (e.g. temperature and chemical concentration) combinations or modelling the process using equations. However, these methods do not aim to minimise the number of experimental trials that a manufacturer must conduct and only determine the optimal cleaning parameters for the average fouling condition. In this work, Bayesian optimisation is used to minimise the number of cleaning parameter combinations that require trialling thereby reducing the disruption to a manufacturing process during the optimisation procedure. Secondly, ultrasonic sensors are used to monitor the cleaning process and enable real-time optimisation of the parameters to adapt to variations in the fouling condition. Multi-objective optimisation was used in both tasks to simultaneously minimise the economic cost, carbon footprint, and water usage of a clean-in-place process. Bayesian optimisation was able to optimise the process after trialling only nine cleaning parameter combinations (achieving between 98.7% and 100% optimisation of the objective function compared with the global optimum). Bayesian optimisation displayed a small advantage (0.0–4.7% decrease in the objective function) compared with methods used in previous literature. Real-time optimisation of the cleaning parameters using ultrasonic sensor data improved the optimisation objective function by 0.0 – 4.8% for all fouling instances tested when utilising results from ten trials conducted during the Bayesian optimisation procedure along with five additional cleaning processes under normal operation.

Abbreviations: CIP, Clean-In-Place; DoE, Design of Experiment; PC, Principal component; PCA, Principal Component Analysis; US, Ultrasonic

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1. Introduction

In food and drink manufacturing, Clean-In-Place (CIP) processes are conducted to maintain hygienic production, prevent contamination, and ensure equipment is operating under optimal conditions. CIP systems consist of tanks, pumps, and spraying mechanisms that automatically clean the internal surfaces of process equipment without requiring them to be dismantled. Cleaning is completed via a combination of mechanical force, chemical concentration, temperature, and time (Fryer et al., 2006). Therefore, a significant environmental burden is imposed by cleaning owing to the water, energy, and chemicals used. CIP processes are often conducted for a pre-defined duration that has been chosen and validated to eliminate cleaning failure and thereby leads to substantial over-cleaning for most fouling instances. It is thought that cleaning is responsible for between 9 (Jude and Lemaire, 2014) and 30 (Eide et al., 2003) % of energy use in the dairy sector and in brewing approximately 70% of incoming water is discharged to drain most of which has been used for cleaning purposes (Brewery Vivant, 2013; Braeken et al., 2004). Furthermore, cleaning processes account for around 20% of time use across food and drink manufacturing and thereby represent significant lost production time for factories (Jude and Lemaire, 2014). Despite this, the results from an informal poll suggest that only 12% of food and drink manufacturers think that their cleaning processes are efficient and only 18% have investigated cleaning process optimisation (Jude and Lemaire, 2014). For example, it has been estimated that the UK brewing sector could save 1% of its total carbon emissions by implementing real-time cleaning verification (Carbon Trust, 2011).

Several works have investigated the optimisation of cleaning processes by trialling a range of cleaning parameter combinations or by using equations to model the cleaning process. Palabiyika et al. (2015) developed a two-step CIP protocol by investigating the cleaning of adhesive material at varying temperature and velocity of cleaning fluid. This reduced the overall energy consumption and volume of wastewater. Piepiórka-Stepuk et al. (2016) optimised the flow velocity, pressure, temperature of water, and cleaning time of a CIP process for a plate heat exchanger contaminated with hot milk. The cleaning efficacy was maximised whilst minimising the energy usage. A 5-level experimental design of the cleaning parameters was used to find the optimal combinations. Piepiórka-Stepuk et al. (2021) optimised the parameters during the pre-rinsing stage of a CIP process to remove milk impurities from a plate heat exchanger. A 5-level experimental design was used to vary the water temperature, flow rate, and cleaning process time. Cleanliness was used as the objective function. Brooks and Roy (2022) optimised cleaning effectiveness for a heat exchanger by trialling over a range of cleaning fluid flowrates and mechanisms. Pettigrew et al. (2015) modelled cleaning transport phenomena to simulate a water reuse system and Deponte et al. (2020) used parameters such as the Reynolds number and density of the fouling material to predict the cleaning time.

However, there are two limitations to these approaches. Firstly, the optimised cleaning parameters are only devised for a single instance of fouling and are not adaptable if the quantity or difficulty of fouling were to vary. Therefore, industrial implementation of these approaches necessitates the optimised cleaning parameters to be selected to clean the most difficult fouling encountered. This would result in over-cleaning for most fouling instances, offering limited improvements to current approaches. Secondly, the collection of cleaning results over many cleaning parameter combinations or the development of simulations would require significant time investment and may cause unacceptable disruption to a manufacturing process. The process may be disrupted during the trials of parameter combinations that fail to clean or when collecting the data via sampling to develop and validate the simulations. Whilst Design of Experiment (DoE) methods were used in Palabiyika et al. (2015), Piepiórka-Stepuk et al. (2016), Piepiórka-Stepuk et al. (2021), Brooks and Roy (2022), and Deponte et al. (2020) to reduce the number of experiments conducted, these methods are not designed to minimise the number of trials by selecting those that are the most informative to the optimisation procedure. Therefore, a method is required that optimises cleaning parameters for varying fouling instances whilst minimising the time investment required during its deployment by selecting parameter combinations to trial that are most advantageous.

Bayesian optimisation is a common optimisation method for functions that are expensive to evaluate (e.g. time, computational, or economic resources). In this work, Bayesian optimisation is used to minimise the number of cleaning parameter combinations to trial and thereby minimise disruption to a manufacturing process. The Expected Improvement acquisition function is used to determine the next set of cleaning parameters to trial by balancing exploration of low confidence regions and exploitation of high value parameter combinations (Frazier, 2018). Secondly, Ultrasonic (US) sensor measurements are used to monitor fouling in real-time and enable adaptive cleaning parameter optimisation to variations in fouling instances. US sensors monitor the interaction of materials with mechanical sound waves and have previously been used to monitor cleaning in heat exchangers (Wallhäußer et al., 2011), pipes (Escrig et al., 2019), and duct sections (Chen et al., 2019). US sensors can be applied non-invasively allowing them to be externally retrofitted to existing process equipment. A neural network surrogate model was trained using experimental data from a CIP process to conduct both optimisation tasks. Surrogate models map input-output relationships of more complex systems that are demanding to evaluate in terms of time or computational resources (McBride and Sundmacher, 2019). In this work, the surrogate model mapped the inputs (cleaning parameters and US sensor measurements) to the outputs (whether cleaning was successful) of the experimental CIP process. The surrogate model enabled different combinations of process parameters to be trialled during the optimisation tasks in place of an experimental set-up and simulate the trajectory of the US features during the cleaning process. The surrogate model provided labelled data for the Bayesian optimisation procedure by indicating whether the plate would be cleaned based on the inputted cleaning parameter combinations. Three objective functions were minimised for both tasks: the economic cost, the carbon footprint, and the water use of the CIP process whilst ensuring cleanliness of the equipment. The novelty of this work is: 1) The optimisation of a CIP process for three objective functions (economic cost, carbon footprint, and water use). 2) The use of Bayesian optimisation to minimise the number of parameter combinations to trial during cleaning optimisation thereby reducing disruption to a manufacturing process during method deployment. 3) The use of in-line US sensors to perform real-time optimisation of cleaning processes to adapt to variations in fouling instances.

2. Materials and methods

2.1. *Cleaning experiments*

Experimental work was conducted to obtain the data to train the surrogate model for the optimisation tasks. In the experimental work, malt extract (Coopers, Irish Stout) was used as the fouling material and was cleaned from a 304 stainless steel sheet (Fig. 1). This represents cleaning of fouling material from the internal walls of processing equipment. The ingredients of the malt extract included malted barley, hops, yeast and water. The CIP process was repeated 30 times whilst being monitored using a US sensor positioned on the opposite side of the plate to the fouling. Each CIP process consisted of three stages: a preliminary water rinse (Rinse 1), cleaning with sodium hydroxide solution (Chemical Cleaning), and a final water rinse (Rinse 2). The combination of process parameters used for each repeat were randomly selected within the ranges provided in Table 1. The parameter ranges were selected to produce a combination of successful and failed cleaning repeats. In total, this led to 13 repeats that produced a fully clean plate and 17 repeats where the plate was not fully cleaned. Visual examination was used to determine whether the plate was fully cleaned. The metal sheet was positioned at an angle to allow the cleaning fluid to be directed towards a drain. Approximately 15 g of the malt extract was placed onto the metal sheet at the location of the US sensor prior to cleaning commencing. The fluid for each cleaning stage was prepared in a container and poured at a consistent flowrate at a marked location at the top of the metal sheet above the location of the fouling. The chemical solution was prepared by dissolving sodium hydroxide pellets into a volume of water. The temperature was increased using a hot plate and monitored using a thermometer.

A magnetic US sensor (5 MHz central resonance, M1057, Olympus) was attached to the underside of the metal sheet. The sensor was attached to an adhesive magnetic strip and coupling gel (Dow Corning High Vacuum Grease) was applied between the sensor and strip. A non-invasive, reflection-mode, pulse-echo sensing technique was used to monitor the

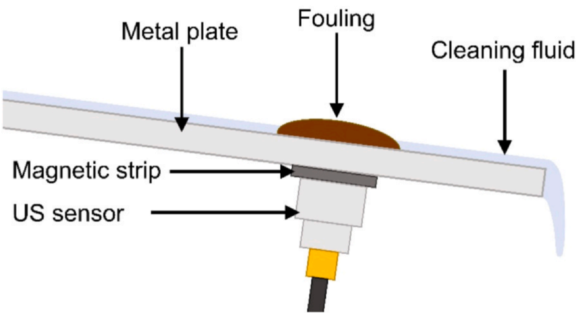

Fig. 1 – A diagram of the experimental set-up. Approximately 15 g of malt extract was used as the fouling material and was cleaned from a 304 stainless steel sheet. An US sensor was positioned on the opposite side of the plate to monitor the cleaning processes. The metal sheet was positioned at an angle to allow the cleaning fluid to be directed towards a drain.

Table 1 – The ranges of the cleaning parameters used for the three cleaning stages: a preliminary water rinse (Rinse 1), cleaning with sodium hydroxide solution (Chemical Cleaning), and a final water rinse (Rinse 2). The CIP process was repeated 30 times with the parameters randomly varied between the ranges presented. In total, this led to 13 repeats that produced a fully clean plate and 17 repeats where the plate was not fully cleaned. The grid search granularity represents the fineness of the cleaning parameter search used to determine optimal combinations from the machine learning models.

Stage	Parameters	Range	Grid search granularity
Rinse 1	Water volume (L)	1–3	0.25
	Temperature (°C)	25–45	2.5
Chemical Cleaning	Sodium hydroxide concentration (% wt)	0–2	0.25
	Water volume (L)	1–3	0.25
	Temperature (°C)	25–45	2.5
Rinse 2	Water volume (L)	1–3	0.25
	Temperature (°C)	25–45	2.5

sound wave reflected from the interface between the plate surface and the process material as used in Bowler et al. (2020) and Escrig et al. (2019). Therefore, it can be externally attached to process equipment to monitor cleaning. The process material at the plate surface is either the fouling or the cleaning fluid depending on the process stage. An US box (Lecoeur Electronique) was used to excite the transducers and digitise the received sound waves. The US box was connected to a laptop and a bespoke MATLAB software controlled the hardware components and acquired the data.

2.2. *Machine learning*

2.2.1. *US feature extraction*

Each US waveform consisted of 2000 sample point amplitudes collected at a sampling rate of 160 MHz. During the cleaning process, the waveform is affected by two phenomena: changes in temperature to the system (the metal plate and fouling material) and the removal of the fouling material from the plate surface. Variations in temperature affect the speed of sound through the metal plate and therefore the arrival time of the waveform oscillations in returning to the transducer. Furthermore, changes in temperature affect the acoustic impedance, the product of the sound velocity and material density, of the metal plate and fouling material and thereby alter the magnitude of the sound wave reflected at this interface (Awad et al., 2012). The removal of fouling changes the material located at the measurement interface and therefore alters the acoustic impedance and magnitude of the sound wave reflected. As the phenomena of interest in this study was the removal of fouling, a moving average was applied to the absolute amplitudes of the US waveforms to overcome the effect of the waveform shifting in the time domain due to the changing temperature of the metal plate. A window size of 30 sample points was chosen for the moving average by inspecting the change in the waveforms during the cleaning process (Fig. 2). Principal Component Analysis (PCA), in scikit-learn, was utilised to extract two Principal Components (PCs) from the 2000 input variables (the waveform sample points following

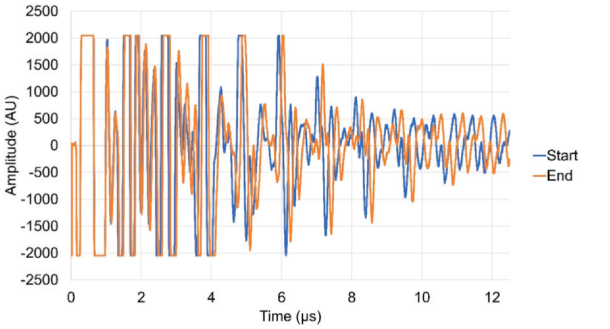

Fig. 2 – A comparison between the US waveforms at the beginning and end of the first repeat of the cleaning process. The maximum shift in the US waveform peaks in the time domain is approximately 30 sample points in the region between 12 and 12.5 μs. Therefore, this was the value used to perform a moving average of the absolute amplitudes of the US waveforms.

application of the moving average). PCA linearly transforms input variables into new, uncorrelated features called PCs (Khalid et al., 2014). Each input variable was scaled to have a minimum of zero and a maximum of one to ensure all variables contributed equally to the PCA results. Two PCs were extracted to identify the two phenomena affecting the magnitude of the reflected waveform: temperature variations and the removal of the fouling material from the plate surface. The first and second PCs explained 39.0% and 25.9% of the variance. Despite the low total contribution of these two extracted PCs, additional PCs did not follow consistent trends across all cleaning repeats and were therefore not used. Furthermore, during the real-time optimisation procedure using US sensor measurements, only a small dataset size is available due to the requirement to minimise disruption to a manufacturing process. Therefore, the selection of two PCs also minimised the complexity of the models.

2.2.2. *Surrogate model*

The surrogate model was trained using experimental data to represent the CIP system. The surrogate model mapped the input- (cleaning parameters and US sensor measurements) output (whether cleaning was successful) relationship of the CIP process. The surrogate model was used in both optimisation tasks: Bayesian optimisation and real-time optimization using US sensors. In the Bayesian optimisation procedure, the surrogate model helps to trial different combinations of process parameters in place of an experimental set-up and simulate the trajectory of the US features during the cleaning process. This enables the evaluation of the selected parameter combinations without requiring real experimental runs. The surrogate model provided labelled data for the Bayesian optimisation procedure by indicating whether the plate would be cleaned based on the inputted cleaning parameter combinations. When applying Bayesian optimisation within a manufacturing environment, an iterative approach would be taken between trialling parameter combinations and conducting the optimisation procedure which would select the next set of parameters to trial. Similarly, the data used to train the real-time optimisation models would be collected from experimental runs. The surrogate model also enabled the cleaning parameters that produced the global minima to be determined and therefore evaluate the optimisation procedures. The granularity of the grid search procedure to determine the global optima from the surrogate model is included in Table 1. While a finer grid search may identify further reductions in the objective function, the granularity used in this work is sufficient for industrial processes.

A neural network, in Keras, was used as the algorithm for the surrogate model due to the ability to create new features in the hidden layers from combinations of the input features (Rodriguez-Galiano et al., 2015). Seventeen inputs (Table 2) were fed into the multi-task surrogate model. The outputs consisted of a classification branch to predict whether the plate would be cleaned at the end of the process, and two regression branches to predict the value of US features at the next time step. In this way, the trajectory of the US features could be simulated when trialling cleaning process parameter combinations. The predictions from the classification branch were used by both the Bayesian and real-time optimisation, whereas the regression branches were only used by the real-time optimisation. The 30 CIP process repeats (consisting of 3749 US measurements in total) were used to train and evaluate the surrogate model. Single fold validation using a training set consisting of 24 cleaning process repeats and a validation set consisting of six repeats was used to select the following optimal hyperparameters: A single hidden layer containing 128 neurons with ReLu activation; a learning rate of 0.01, a batch size of 64, and the Adam optimisation algorithm used for 2000 epochs of training; an L2 regularisation value of 0.0001; and a dropout layer with a probability of 0.1 after the hidden layer. A final model was retrained using all of the data and the optimised hyperparameters.

Table 2 – A description of the seventeen features input into the surrogate Model.

Features	Number of features	Description
Cleaning process parameters	7	The process parameters used during the three stages of cleaning (Table 1)
Cleaning stage	1	The stage of cleaning. Input as either 1, 2, or 3 representing Rinse 1, Chemical Cleaning, or Rinse 2, respectively.
Cleaning stage time step	1	The time step since the start of the cleaning stage. Input as sequential integers.
US features	2	The two PCs extracted from the US waveforms
Average since cleaning stage start of US features	2	The moving average of the US features since the start of the cleaning stage. This provides the model with information from previous time steps
Time lagged US features	4	Two sets (0.5 and 1 litre in the past) of time lagged US features. This provides the model with information from previous time steps

Table 3 – The data and assumptions used to quantify the economic cost of the cleaning parameter combinations.

Description	Value and units	Assumptions and sources
Sodium hydroxide	0.0535 p per g	Calculated using the mean European price for 2022 (ChemAnalyst, 2022) and the mean US Dollar to British Pound exchange rate for 2022 (Exchange Rates UK, 2022).
Electricity (low price)	15.5 p/kWh	Taken as the annual electricity price in the UK for 2021 for medium-sized non-domestic consumers, excluding the climate change levy (BEIS, 2022a)
Heating cleaning fluid using electricity (low price)	0.0181 p per litre per °C above 14 °C	Using a specific heat capacity of water as 4.2 kJ per kg per K and an average ambient temperature of 14 °C.
Electricity (high price)	24.6 p/kWh	Taken as the electricity price in the UK for the third quarter of 2022 for medium-sized non-domestic consumers, excluding the climate change levy (BEIS, 2022a)
Heating cleaning fluid using electricity (high price)	0.0287 p per litre per °C above 14 °C	Using a specific heat capacity of water as 4.2 kJ per kg per K and an average ambient temperature of 14 °C.
Natural gas (low price)	2.81 p/kWh	Taken as the annual natural gas price in the UK for 2021 for medium-sized non-domestic consumers, excluding the climate change levy (BEIS, 2022a)
Heating cleaning fluid using natural gas (low price)	0.00410 p per litre per °C above 14 °C	Using a specific heat capacity of water as 4.2 kJ per kg per K, an average ambient temperature of 14 °C, and the efficiency to raise steam from natural gas as 80%.
Natural gas (high price)	5.45 p/kWh	Taken as the natural gas price in the UK for the third quarter of 2022 for medium-sized non-domestic consumers, excluding the climate change levy (BEIS, 2022a)
Heating cleaning fluid using natural gas (high price)	0.00795 p per litre per °C above 14 °C	Using a specific heat capacity of water as 4.2 kJ per kg per K, an average ambient temperature of 14 °C, and the efficiency to raise steam from natural gas as 80%.
Water use	0.163 p/litre	Median English business water rate 2022/23 (AquaSwitch, 2023)
Wastewater	0.172 p/litre	Median English business water rate 2022/23 (AquaSwitch, 2023)

2.2.3. *Multi-objective optimisation*

Multi-objective optimisation aims to optimise more than one objective function simultaneously (Gunantara, 2018). Usually, these objective functions conflict and a series of best points can be identified where improving one objective function degrades the others, often called Pareto optimal solutions. A common method to choose amongst the generated Pareto optimal solutions is to combine the separate objective functions into a single objective optimisation problem through scaling of each value, named the scalarisation method (Gunantara, 2018). In this work, three objective functions are minimised: the economic cost, the carbon footprint, and the water use of the CIP procedure. Four scenarios are investigated: heating the cleaning fluids with electricity or natural gas, and using both a low or high price for these energy sources. The scalarisation method is used to obtain a single objective function by assigning equal weighting for the three objective functions at the median cleaning parameter values listed in Table 1 for each scenario. The quantity of sodium hydroxide, energy required to heat the cleaning fluids, water volume, and wastewater volume were assigned costs and greenhouse gas emissions to quantify their economic cost and carbon footprint for the optimisation. The data and assumptions used to quantify the economic cost and carbon footprint are included in Tables 3 and 4, respectively. The water quantity was the total volume of water used during the three cleaning stages. The volume of water used is also representative of the lost production time for the factory during cleaning, however, this is not quantified within the economic evaluation.

2.2.3.1. *Bayesian optimisation*. Bayesian optimisation is a common method used for expensive-to-evaluate functions as it can minimise the number of trials required to find near-optimal solutions (Frazier, 2018). In this work, Bayesian optimisation is used to minimise the number of cleaning parameter combinations to trial and thereby reduce disruption to a manufacturing process during cleaning optimisation. Bayesian optimisation uses acquisition functions to balance exploration and exploitation in determining the next set of parameters to test. In this work, the Expected Improvement, the most common acquisition function, is used which calculates the probable improvement in objective function value for a given combination of cleaning

Table 4 – The data and assumptions used to quantify the carbon footprint of the cleaning parameter combinations.

Description	Value and units	Assumptions and sources
Sodium hydroxide	1.41 g CO_2 e per g	The average between 2.18 (Randall et al., 2016) and 0.633 (Thannimalay et al., 2013) g CO2 per g.
Electricity	0.193 kg CO_2 e per kWh	BEIS (2022b)
Heating cleaning fluid using electricity	0.226 g CO_2 e per litre per °C above 14 °C	Using a specific heat capacity of water as 4.2 kJ per kg per K and an average ambient temperature of 14 °C.
Natural gas	0.234 kg CO_2 e per kWh	BEIS (2022b)
Heating cleaning fluid using natural gas	0.342 g CO_2 e per litre per °C above 14 °C	Using a specific heat capacity of water as 4.2 kJ per kg per K, an average ambient temperature of 14 °C, and the efficiency to raise steam from natural gas as 80%.
Water use	0.149 g CO_2 e per litre	BEIS (2022b)
Wastewater	0.272 g CO_2 e per litre	BEIS (2022b)

parameters (Frazier, 2018). To achieve this, an ensemble of neural networks was used to produce a probability distribution of the objective function value for different parameter combinations. This allows the feature extraction capability of the neural network to be retained while the ensemble produces a probability distribution (White et al., 2021).

An ensemble of ten neural networks were trained, in Keras, using the results from the trialled parameter combinations to classify whether the plate was cleaned by the cleaning parameters. The surrogate model was used to trial the parameters combinations and determine whether the plate would be cleaned at the end of the cleaning process. These results (cleaned or not cleaned) provided the labelled data to train the neural network ensemble. From this, the neural network ensembles could be trained using the results from the trialled parameters to predict whether the plate would be cleaned using new parameter combinations. The ensembles of neural networks were trained to achieve 100% accuracy on the validation set (the most recent parameter combination trialled) and 100% accuracy on the training set (the remaining parameter combinations previously trialled). This training approach aimed to ensure the neural network ensemble could accurately classify the cleaning results from previously trialled parameter combinations for both the training and validation sets, enabling generalisation to new parameter combinations. The networks consisted of three fully-connected layers containing four neurons each with ReLu activation functions. A learning rate of 0.001, a batch size of 2, and the Adam optimisation algorithm were used for 2000 epochs of training. Two dropout layers with a probability of 0.1 were used, each located between the hidden fully-connected layers.

A grid search of cleaning parameter combinations was inputted into the train neural network ensembles. This produced a probability distribution of how likely the plate was to be cleaned by the cleaning parameter combination. The objective function value for each parameter combination was calculated by combining the economic cost, carbon footprint, and water use of the CIP procedure using the methodology detailed in Section 2.2.3 Multi-objective optimisation (Eq. 1). For exploitation, the average value of the objective function was calculated across the 10 models for each parameter combination. However, if a cleaning parameter combination was predicted to fail to clean the plate by a model, then it was assigned the maximum objective function value for that model. This discouraged the selection of cleaning parameter combinations that were predicted to fail to clean the plate. To encourage exploration, the standard deviation of the sigmoidal outputs in the neural network ensemble predictions was also calculated. The rationale being that higher standard deviation implies more disagreement among the neural networks in the ensemble, indicating increased uncertainty in this region of parameter combinations. The discrepancy between the objective function value range and standard deviation range were scaled to be equal before the components were combined. The combination of cleaning parameters which minimised the objective function whilst maximising the standard deviation were selected as the next parameters to be trialled.

$$s_E \quad E + s_C C + s_W W = OF \tag{1}$$

Where E, C, and W are the economic cost, carbon footprint, and water use totals for the cleaning parameters combination, respectively; s_E, s_C, and s_W are the scalarisation factors for the economic cost, carbon footprint, and water use, respectively; and OF is the objective function value.

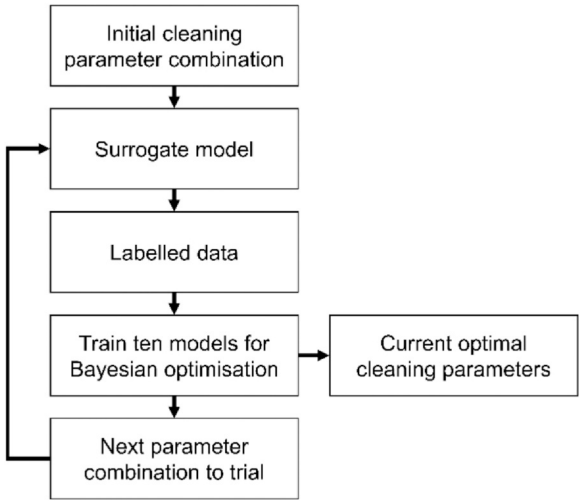

Fig. 3 – A flow diagram of the Bayesian optimisation procedure. The initial cleaning parameter used at the start of the optimisation procedure is the maximum of the ranges provided in Table 1. The surrogate model is used to obtain labelled data as to whether the plate would be cleaned by the inputted cleaning parameter combinations.

As this work uses a surrogate model in place of experimental runs, the cleaning parameter combinations to trial were input into the surrogate model to determine whether the plate would be cleaned (Fig. 3). In a manufacturing setting the combination of cleaning parameters would be trialled experimentally. To account for the variability in the fouling instances that would be observed experimentally, the starting US feature values input into the surrogate model were randomised between the ranges encountered during the experimental data collection. This alters the trajectory of the US features simulated by the surrogate model owing to natural variation of the fouling condition, adhesion, and volume encountered within the experimental data used to train the surrogate model. During data collection, the starting value for the first PC varied between 20 and 48 (no units) compared with 7 and 33 (no units) for the second PC. This is in comparison to the variation across all of the cleaning processes where the first PC varied between – 53 and 48 (no units), and the second PC between – 50 and 41 (no units).

2.2.3.2. Real-time optimisation using US sensors. The application of US sensors to enable real-time optimisation of the cleaning process was also investigated (Fig. 4). In this way, the cleaning parameters can be changed during the CIP process to adapt to variations in the fouling. Using the results from the cleaning parameter combinations trialled during the Bayesian optimisation procedure, two additional neural networks were trained in Keras: the first to predict whether cleaning would be completed based on the cleaning parameters and US features at the end of the Rinse 1 stage, and the second to predict whether the plate would be cleaned based on the cleaning parameters and the US features after the Chemical Cleaning stage. The first model could then be used to optimise the cleaning parameters for the Chemical Cleaning stage and the second for the Rinse 2 stage. The US features were the final eight features listed in Table 2 (US features, average since cleaning stage start of US

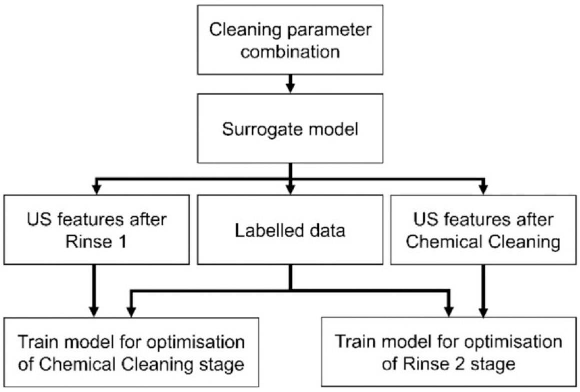

Fig. 4 – A flow diagram of the method to obtain the models for real-time optimisation of the cleaning parameters. The surrogate model is used to obtain labelled data as to whether the plate would be cleaned by the inputted cleaning parameter combinations and to simulate the trajectory of the US features during cleaning.

features, and time-lagged US features). The networks were composed of the same architecture as those used during the optimisation: three fully-connected layers containing four neurons each with ReLu activation functions. A learning rate of 0.001, a batch size of 2, and the Adam optimisation algorithm were used for 2000 epochs of training. Two dropout layers with a probability of 0.1 were used, each located between the hidden fully-connected layers. To trial the real-time optimisation method, ten new CIP processes were simulated using the surrogate model. To simulate variability in the fouling instances, the starting US feature values input into the surrogate model were randomised between the ranges encountered during the experimental data collection. After both the Rinse 1 and Chemical Cleaning stages, the US features simulated by the surrogate model were inputted into the real-time optimisation models and a grid search selected the optimal parameters for the next cleaning stage.

3. Results

3.1. *Ultrasonic sensor measurements*

The US waveform consists of multiple overlapping sound waves reflected from the interface between the plate surface and the process material (either the foulant or cleaning fluid). During the cleaning process, the US waveform is affected by two phenomena: changes in temperature to the system (the metal plate and fouling material) and the removal of the fouling material from the plate surface. Two PCs were extracted from the 2000 input variables (the US waveform sample points following application of the moving average) to identify these two phenomena affecting the magnitude of the reflected waveform: temperature variations and the removal of the fouling material from the plate surface. As such, each of the extracted PCs is affected by a combination of these phenomena.

Fig. 5 depicts the two PCs extracted from the US sensor measurements. Whilst both temperature and fouling removal contribute to the extracted PCs, it was deduced that the first PC is affected mostly by the temperature change of the plate surface, whilst the second is mostly impacted by the removal of fouling. This is determined as in both Repeat 5

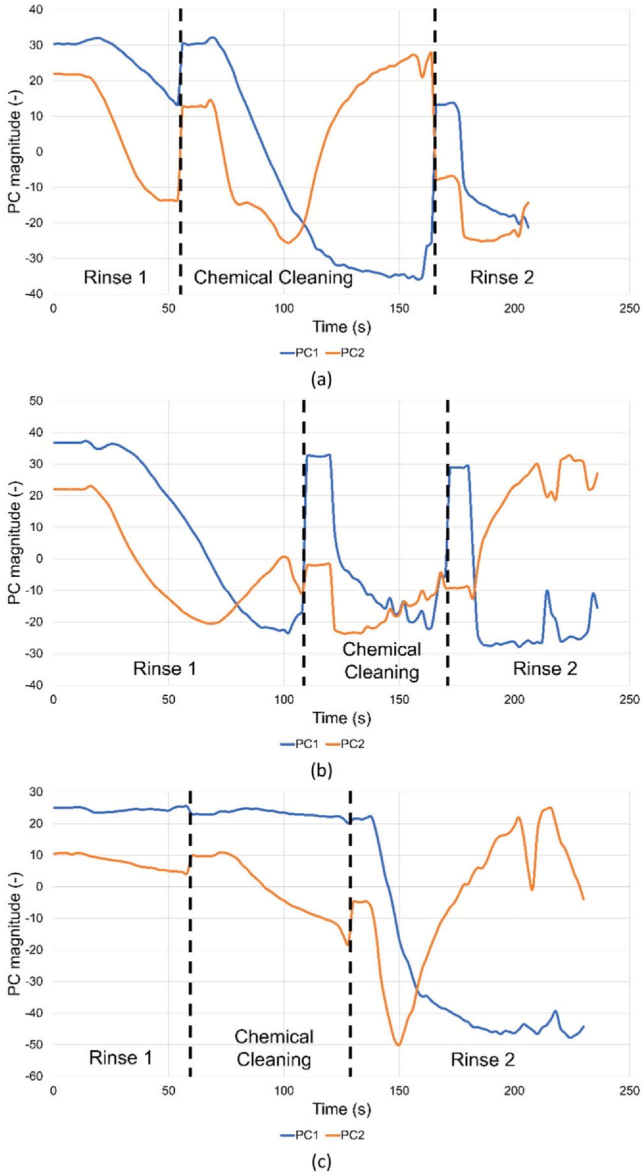

Fig. 5 – The trajectories of the PCs extracted from the US sensor measurements for Repeat 5 (Fig. 5a), 6 (Fig. 5b), and 7 (Fig. 5c) of the experimental data. The first PC follows the trend of the temperature change of the plate, while the second PC monitors the removal of fouling.

(Fig. 5a) and 6 (Fig. 5b) the plate was observed to be almost fully clean following the Chemical Cleaning stage. In contrast, Repeat 7 (Fig. 5c) experienced the most cleaning during the Rinse 2 stage. The first PC is shown to decrease in magnitude with increasing gradient during the cleaning stages for Repeats 5 and 6 showing that the temperature change of the metal plate becomes more rapid as fouling is removed from the surface. Between each cleaning stage, the plate begins to return to the environmental temperature as no fluid flows across its surface. The first PC remains unchanged during the Rinse 1 and Chemical Cleaning stages of Repeat 7 as no fouling has yet been removed from the surface and therefore prevents the plate from increasing in temperature. The second PC decreases as fouling is removed from the plate surface after which it begins to increase in magnitude. This can be observed in Repeat 5 and 6 where the second PC undergoes no further decrease during the Rinse 2 stage and undergoes the largest decrease during the Rinse 2 stage of Repeat 7. As the PCs have been extracted from US waveforms

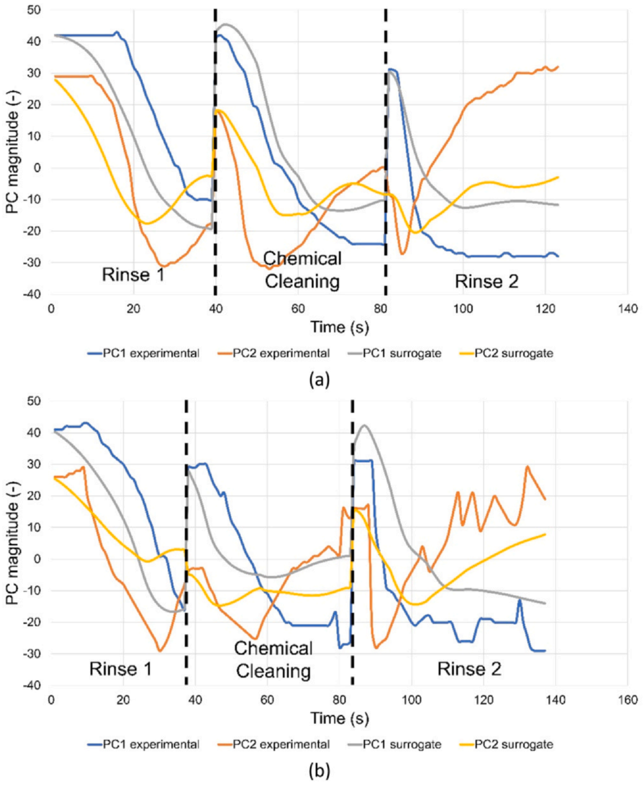

Fig. 6 – A comparison between the PC trajectories during the experimental runs and those simulated by the surrogate model. PC1 represents the first PC and PC2 represents the second PC. (a) Repeat 1 which was included in the training set of the surrogate model. (b) Repeat 4 which was included in the validation set of the surrogate model.

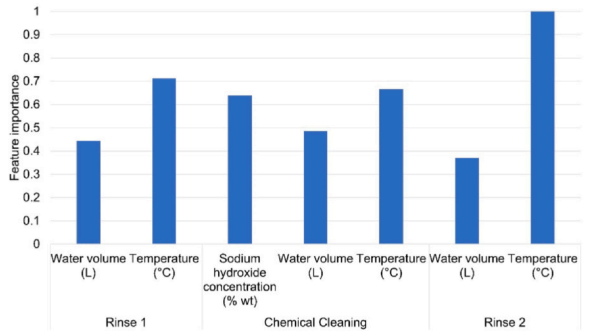

Fig. 7 – The impact of each parameter on the cleanliness of the metal plate during the CIP process. The importance of each feature has been scaled to that of the most important parameter.

consisting of multiple overlapping sound waves, the reason for the second PC increasing following removal of the fouling may be due to increased effects of temperature on the clean plate. For example, changes in temperature causes time-shifted of the peaks in the US waveform leading to altering magnitudes in the waveform sample points monitored by the second PC.

Fig. 6 compares the PC trajectories measured during experimental data collection and those simulated by the surrogate model. Fig. 6a displays PC results and simulations for Repeat 1 which was included in the training set for the surrogate model and Fig. 6b displays those for Repeat 4 which was included in the surrogate model's validation set. Single fold validation using a training set consisting of 24 cleaning process repeats and a validation set consisting of six repeats was used to select the following optimal hyperparameters: A single hidden layer containing 128 neurons with ReLu activation; a learning rate of 0.01, a batch size of 64, and the Adam optimisation algorithm used for 2000 epochs of training; an L2 regularisation value of 0.0001; and a dropout layer with a probability of 0.1 after the hidden layer. A final model was retrained using all of the data and the optimised hyperparameters.

3.2. *Cleaning parameter importance*

Fig. 7 displays the importance of each parameter in cleaning the malt extract from the metal plate during the cleaning process. These scores are determined by evaluating the impact of the cleaning parameters on the prediction obtained from the surrogate model. The scores have been normalised against the most important parameter. A permutation-based feature importance method was used which randomly shuffled the cleaning parameter values of the experimental data the surrogate model was trained on. The values of each cleaning parameter were shuffled independently and the variation in classification score was assessed (Molnar, 2022). The most important feature therefore causes the largest change to the classification predictions when shuffled. The three most important parameters were the fluid temperatures of each cleaning stage. This is due to the malt extract being a cohesive foulant which is cleaned through dissolution, as found previously in Escrig et al. (2020). Cohesive fouling is removed through breaking the forces that bind the material together and is limited by mass transfer, solubility, or by heat transfer (Fryer and Asteriadou, 2009). Higher temperatures increase the solubility of the fouling, promote phase change, and increase the kinetic energy of the molecules to increase mass transfer, thereby increasing the rate of cleaning (Fryer and Asteriadou, 2009). Furthermore, the fourth most important parameter was the concentration of sodium hydroxide during the Chemical Cleaning stage which also increases the solubility of organic foulants (Fryer and Asteriadou, 2009). The final, Rinse 2, cleaning stage fluid temperature was the most important parameter. This is mostly likely due to an artefact of the Rinse 1 and Chemical Cleaning stages having increased the solubility and promoted phase change of the fouling. This therefore facilitates the cleaning during Rinse 2, enabling the temperature to have a greater impact.

3.3. *Optimisation*

Fig. 8 displays the results of the Bayesian optimisation procedure. The results from the first parameter combination trials are omitted as these represent the unoptimised system, located at 0% optimised. The fully optimised system (100% optimised) refers to the global optima determined using the surrogate model through a grid search procedure. Overall, the four cleaning fluid heating scenarios evaluated (electricity low price, electricity high price, natural gas low price, natural gas high price) all approached the optimal solution after nine parameter combination trials, with the natural gas low price scenario achieving the globally optimal solution. The optimisation procedure achieved 98.9 (electricity low), 98.7 (electricity high), 100 (natural gas low), and

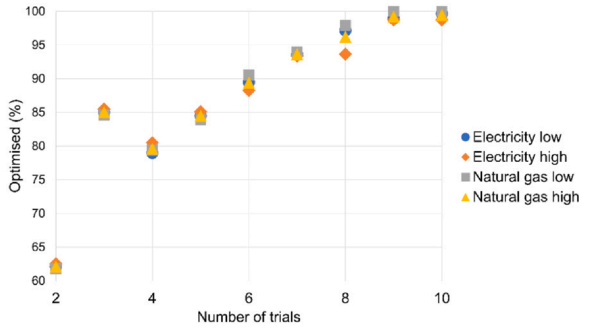

Fig. 8 – The results from the Bayesian optimisation procedure for the four scenarios of energy source and cost. The values represent the percentage optimised compared with the global optimum (100% optimised). The results from the first parameter combination trials are omitted as these represent the unoptimised system and therefore are located at 0% optimised.

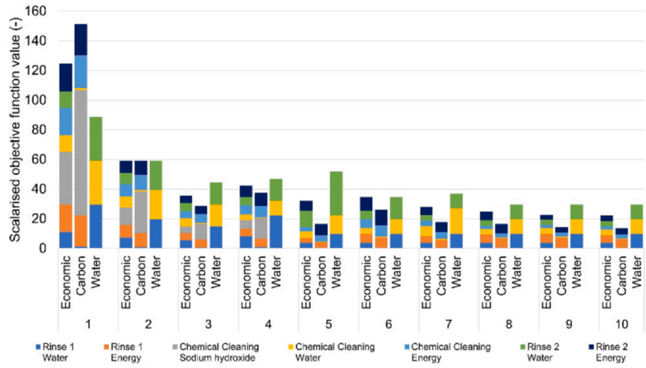

Fig. 9 – The contribution of each cleaning parameter to the scalarised economic, carbon footprint, and water use objective functions during the 10 trials of the Bayesian optimisation procedure for the low electricity price scenario.

99.2 (natural gas high) % compared with the global optima after nine trials. In a manufacturing environment, using experimental trials in place of the surrogate model, the global optima would be unknown. Therefore, the stopping criteria where no further trials were required would be determined by observing a plateau in the reduction of the objective function or when a pre-determined reduction target had been achieved.

Interestingly, the global optima for all scenarios were identical (Table 5) and consisted of a Rinse 1 stage with a water volume of 1 litre and temperature of 27.5 °C; a Chemical Cleaning stage with a sodium hydroxide solution concentration of 0%, water volume of 1 litre, and temperature of 25 °C; and a Rinse 2 stage with a water volume of 1 litre and temperature of 45 °C. This suggests that the lower cost of natural gas counteracted the lower carbon footprint of electricity (Tables 3 and 4). However, with increasing decarbonisation of the electricity grid, heating of the cleaning fluids with electricity may be more greatly favoured. Despite increases in costs of 58% and 63% for electricity and natural gas, respectively, between the low and high prices, the same global optima were predicted. This suggests, that for the process investigated, the optimisation procedure would not need to be repeated at times of high energy costs.

The globally optimal cleaning parameters determined using the surrogate model are similar to those identified in the feature importance results displayed in Fig. 7 where the temperature of the Rinse 2 stage was the most significant cleaning parameter. Contrastingly, the optima determined through the Bayesian optimisation procedure selected the highest fluid temperature for the Rinse 1 stage and the second highest temperature for the Rinse 2 stage (Table 5). This indicates that larger weighting could have been assigned to the exploration component of the acquisition function, facilitating the trialling of parameter combinations further away from previous trials. Notably, all optima determined that fluid volumes of 1 litre in all cleaning stages and no sodium hydroxide were required to minimise the scalarised multi-objective function for the fouling investigated. The contribution of each cleaning parameter to the three scalarised objective functions (economic cost, carbon footprint, and water use) is presented in Fig. 9 for the low electricity price scenario. Notably, sodium hydroxide was eliminated from the optimal cleaning parameters after four parameter combination trials, most likely due to its large carbon footprint. Water use was the largest contributor to the scalarised multi-objective function for trials 7–10 contributing to its limitation to 1 litre for each cleaning stage. Moreover, the volume of the cleaning fluid was determined to be the least important parameters to conduct cleaning (Fig. 7). Despite the differences in the selected cleaning fluid temperatures between the globally determined optima and the Bayesian optimisation identified cleaning parameters,

Table 5 – The global and local optima determined for the four energy source and cost scenarios. The global optimum was the same for all scenarios. The results displayed for the Bayesian optimisation procedure are following ten parameter trials. For comparison to the Bayesian optimisation procedure, the Design of Experiments (DoE) method used a 2^{7-4} fractional factorial design in addition to the centre point (Table 6). This is a total of nine parameter combinations.

Stage	Parameters	Global optimum (for all scenarios)	Bayesian optimisation				DoE method (for all scenarios)
			Electricity		Natural gas		
			Low	High	Low	High	
Rinse 1	Water volume (L)	1	1	1	1	1	1
	Temperature (°C)	27.5	42.5	45	40	42.5	35
Chemical Cleaning	Sodium hydroxide concentration (% wt)	0	0	0	0	0	0
	Water volume (L)	1	1	1	1	1	1
Rinse 2	Temperature (°C)	25	25	25	25	25	35
	Water volume (L)	1	1	1	1	1	1
	Temperature (°C)	45	32.5	35	32.5	32.5	35

Table 6 – The nine parameter combinations used for the Design of Experiments (DoE) method. The DoE method used a 2^{7-4} fractional factorial design in addition to the centre point of the parameter ranges.

Stage	Parameters	1	2	3	4	5	6	7	8	9
Rinse 1	Water volume (L)	1	3	1	3	1	3	1	3	2
	Temperature (°C)	25	25	45	45	25	25	45	45	35
Chemical Cleaning	Sodium hydroxide concentration (% wt)	0	0	0	0	2	2	2	2	1
	Water volume (L)	3	1	1	3	3	1	1	3	2
Rinse 2	Temperature (°C)	45	25	45	25	25	45	25	45	35
	Water volume (L)	3	3	1	1	1	1	3	3	2
	Temperature (°C)	25	45	45	25	45	25	25	45	35

the Bayesian optimisation procedure achieved the same objective function value as the global minimum for the low price natural gas scenario. This is because both methods selected that 1 litre of cleaning fluid and no sodium hydroxide be used whilst using the same amount of energy to heat the cleaning fluid, only that different cleaning stages should have higher temperatures. This difference likely due to the different datasets used to train the surrogate and Bayesian optimisation models leading to each favouring higher temperatures for different cleaning stages.

The results from the Bayesian optimisation procedure were compared with a DoE method (Table 5) similar to those used in Palabiyika et al. (2015), Piepiórka-Stepuk et al. (2016), Piepiórka-Stepuk et al. (2021), Brooks and Roy (2022), and Deponte et al. (2020). DoE methods are used to efficiently explore the effects of multiple factors and their interactions on a response variable. However, DoE methods are not designed to minimise the number of trials by selecting those that are the most informative to the optimisation procedure unlike Bayesian optimisation. To compare with Bayesian optimisation, the DoE method used a 2^{7-4} fractional factorial design in addition to the centre point to produce nine parameter combinations owing to Bayesian optimisation finding optimal solutions after trialling nine parameter combinations (Gunst and Mason, 2009). The parameter combinations used for the DoE method are provided in Table 6. The surrogate model was used to determine whether these nine parameter combinations would clean the metal plate. These results were used to train ten neural networks that were used to determine the optimal solution identified by the DoE method. The same methodology as used for the Bayesian optimisation procedure (Section 2.2.3.1 Bayesian optimisation) was used for training and evaluating the models.

For all energy source and price scenarios, the DoE method selected a Rinse 1 stage with a water volume of 1 litre and temperature of 35 °C; a Chemical Cleaning stage with a sodium hydroxide solution concentration of 0%, water volume of 1 litre, and temperature of 35 °C; and a Rinse 2 stage with a water volume of 1 litre and temperature of 35 °C. In comparison, the Bayesian optimisation displayed a small improvement (0–4.7% improvement in the objective function depending on the energy source and cost evaluated) compared with the DoE method. The reason that this improvement is only small is likely due to the parameter values for the global optima being located at the extremes of the ranges examined, enabling the DoE method to identify that the minimum volume of cleaning fluid and sodium hydroxide content were required. However, the DoE had diminished resolution closer to the centre of the parameter ranges evidenced by the selection of 35 °C for all cleaning fluid temperatures. The advantage of using the Bayesian optimisation procedure compared with the DoE method may be more prominent in other cleaning instances where the optimal solution is not close to the parameter extremes explored. These results display the benefit of the Bayesian optimisation approach that is able to select the most valuable parameter combinations to trial.

3.4. *Real-time optimisation using US sensors*

Ten variations of fouling conditions were used to evaluate the real-time optimisation using US sensor data. To simulate this variability, the starting US feature values input into the surrogate model were randomised between the ranges encountered during the experimental data collection. This alters the trajectory of the US features simulated by the surrogate model owing to natural variation of the fouling condition, adhesion, and volume encountered within the experimental data used to train the surrogate model. Only the low electricity price scenario was used for this procedure as similar global and local optima were determined for all scenarios. Table 7 displays results from using real-time optimisation models trained using data from the ten parameter combinations from the Bayesian optimisation procedure. It is shown that the selection of the cleaning fluid temperature for the Rinse 2 stage displays the greatest variability, ranging between 25 and 35 °C. This is because it is the most important cleaning parameter for the cleanliness of the equipment (Fig. 7), it is at end of the CIP process and therefore responsible for completing the cleaning, and its selection being decided during both real-time optimisation procedures (optimisation of the Chemical Cleaning stage and subsequently optimisation of the Rinse 2 stage). The real-time optimisation results presented in Table 7 improved the CIP process for three out of ten of the fouling variations tested, were equal for five out of ten variations, and performed worse for two out of ten variations. Furthermore, the real-time optimisation selected to increase the Chemical Cleaning fluid volume to 1.25 litres for two fouling variations and the temperature to 30 °C for a single variation. This indicates that further data is required to develop real-time optimisation models representative of the cleaning process given the local and global minima determined during the Bayesian optimisation procedure selected the cleaning fluid volume of the Chemical Cleaning stage to be 1 litre and the temperature as 25 °C for all scenarios investigated (Table 5). This is most likely due to the greater number of inputs to the real-time optimisation models (15) compared with the Bayesian optimisation models (7) producing a more complex network for the same number of datapoints and therefore diminished accuracy in regions of the cleaning parameter space.

Table 7 – The cleaning parameters selected during real-time optimisation. The real-time optimisation models were trained using data from the ten parameter combinations trialled during the Bayesian optimisation procedure. Ten variations in fouling conditions were evaluated.

Fouling variation	Chemical Cleaning			Rinse 2		Comparison to Bayesian optimisation local minima
	Sodium hydroxide (% wt)	Water volume (L)	Temperature (°C)	Water volume (L)	Temperature (°C)	Change in objective function (%)
1	0	1	25	1	35	+ 0.0
2	0	1	25	1	35	+ 0.0
3	0	1.25	25	1	25	+ 0.6
4	0	1	25	1	35	+ 0.0
5	0	1	30	1	27.5	- 1.6
6	0	1.25	25	1	25	+ 0.6
7	0	1	25	1	32.5	- 1.6
8	0	1	25	1	35	+ 0.0
9	0	1	25	1	30	- 3.3
10	0	1	25	1	35	+ 0.0

Table 8 – The cleaning parameters selected during real-time optimisation. The real-time optimisation models were trained using data from the ten parameter combinations trialled during the Bayesian optimisation procedure and five additional cleaning processes conducted under normal operation using the local minimum obtained from the Bayesian optimisation process. Ten variations in fouling conditions were evaluated.

Fouling variation	Chemical Cleaning			Rinse 2		Comparison to Bayesian optimisation local minima
	Sodium hydroxide (% wt)	Water volume (L)	Temperature (°C)	Water volume (L)	Temperature (°C)	Change in objective function (%)
1	0	1	25	1	35	+ 0.0
2	0	1	25	1	35	+ 0.0
3	0	1	25	1	32.5	- 1.6
4	0	1	25	1	30	- 3.3
5	0	1	30	1	27.5	- 1.6
6	0	1	25	1	30	- 3.3
7	0	1	25	1	30	- 3.3
8	0	1	25	1	27.5	- 4.8
9	0	1	25	1	30	- 3.3
10	0	1	25	1	27.5	- 4.8

To investigate this further, Table 8 displays results using models trained using the Bayesian optimisation trials plus five additional cleaning trials conducted under normal operation using the local optimum obtained from the Bayesian optimisation process. As these five additional trials represent normal operation, inclusion of this data represents no further disruption to a manufacturing process beyond the trials conducted during the Bayesian optimisation procedure. Using this additional data, the real-time optimisation procedure produced improvements for eight out of ten fouling variations investigated, producing a decrease in the objective function value by up to 4.8%. This shows that the collection of additional data under normal cleaning operation provides improvements to the optimisation models with no further disruption to the manufacturing process. During deployment of these optimisation procedures to a manufacturing site, minimal process disruption would be required for the initial Bayesian optimisation, with further accuracy available for the real-time optimisation using US sensors through the collection of data during normal operation.

4. Discussion

Industry is often risk averse and may be reluctant to alter parameter combinations that could result in cleaning failures. Consequently, the Bayesian optimisation methodology presented in this work could utilise existing cleaning parameters as initial reference points. For instance, the acquisition function could incorporate a distance metric to favour cleaning parameter combinations closer to the company's current ones. Alternatively, a confidence threshold could be applied to select parameter combinations with a high probability of effectively cleaning the equipment for testing. These methods could facilitate the identification of the most important cleaning parameters while minimising the occurrence of cleaning failures. Furthermore, in the multi-objective optimisation, greater priority can be given to objectives that align with the company's preferences. For instance, greater weighting can be applied to reduce economic costs that may be achieved by minimising energy consumption or the use of sodium hydroxide.

Since this work uses a laboratory-based methodology and was not based on an industrial application, economic considerations beyond the cleaning process, such as the loss of production time during cleaning, were not factored into the multi-objective optimisation. However, in practical settings, the cost of time to the manufacturer should be taken into account to select parameters that also minimise cleaning time. Moreover, this information may be used to quantify the costs associated with implementing the proposed optimisation approaches. For instance, failed trials result in wasted time and additional expenses incurred through re-cleaning the equipment. Additionally, the optimisation methods necessitate testing the cleanliness of the equipment after each trial to determine whether the parameters have successfully completed the cleaning process, which may be unnecessary during regular production. Furthermore, the development and application of these methods consume engineering time, further contributing to the overall cost. By quantifying these cost factors, it becomes possible to calculate the payback time of the implemented optimisation method, which determines when the benefits derived from the optimised cleaning parameters outweigh the costs incurred during development and implementation.

While the current research concentrates on optimising cleaning parameters for simple soiling, the same methodologies can be extended to optimise cleaning process for fouling that has been subjected to heating or scenarios involving microbial growth.

5. Conclusions

CIP procedures often over-clean process equipment leading to unnecessary use of energy, water, and chemicals. This work optimised a CIP process using Bayesian optimisation followed by real-time optimisation using US sensor data. Bayesian optimisation was used to determine optimal cleaning parameters for the average fouling instance whilst minimising the number of parameter combinations that were required to be trialled and thereby reduce disruption to a manufacturing process. US sensors were used to monitor the cleaning process and enable real-time optimisation of the cleaning parameters to adapt to variations in the condition of fouling. A surrogate model was produced from experimental data to conduct both optimisation tasks. Multi-objective optimisation was used to simultaneously minimise the economic cost, carbon emissions, and water usage of the CIP process. Bayesian optimisation was able to optimise the process after trialling only nine cleaning parameter combinations (achieving between 98.7% and 100% optimisation of the objective function compared with the global optimum). Bayesian optimisation displayed a small advantage (0.0–4.7% decrease in the objective function) compared with a DoE method. Real-time optimisation of the cleaning parameters using ultrasonic sensor measurements improved the optimisation objective function by 0.0 – 4.8% for all fouling instances tested when utilising results from ten trials conducted during the Bayesian optimisation procedure along with five additional cleaning repeats under normal operation.

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CRediT authorship contribution statement

Alexander L. Bowler: Conceptualization, Methodology, Software, Formal analysis, Investigation, Data curation, Writing – original draft, Visualization. **Sarah Rodgers:** Methodology, Writing – original draft, Writing – review & editing, Visualization. **David J. Cook:** Writing – review & editing, Supervision, Project administration, Funding acquisition. **Nicholas J. Watson:** Resources, Writing – review & editing, Supervision, Project administration, Funding acquisition.

Data Availability

Data will be made available on request.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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