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AutoML-based predictive framework for predictive analysis in adsorption cooling and desalination systems

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Abstract

Adsorption cooling and desalination systems have a distinct advantage over other systems that use low-grade waste heat near ambient temperature. Since improving their performance, including reliability and failure prediction, is challenging, developing an efficient diagnostic system is of great practical significance. The paper introduces artificial intelligence (AI) and an automated machine learning approach (AutoML) in a real-life application for a computational diagnostic system of existing adsorption cooling and desalination facilities. A total of 1769 simulated data points containing data indicating a failure status are applied to develop a comprehensive AI-based Diagnostic (AID) system covering a wide range of 42 input parameters. The paper introduces a conditional monitoring system for adsorption cooling and desalination systems. The novelty of the presented study mainly consists of two aspects. First, the intelligent system predicts the health or failure states of various components in a complex three-bed adsorption chiller installation using the extensive input data sets of 42 different operating parameters. The developed AID expert tool, based on selecting the best from 42 models generated by the DataRobot platform, was validated on the complex, existing three-bed adsorption chiller. The AID system correctly identified healthy and failure states in various installation components. The developed expert system is very efficient (AUC = 0.988, RMSE = 0.20, LogLoss = 0.14) in predicting emergency states. The proposed method constitutes a quick and easy technique for failure prediction and represents a complementary tool compared to the other condition monitoring methods.

KEYWORDS

automated machine learning, condition monitoring, DataRobot, net-zero emissions, predictive maintenance, waste heat utilization

1 | INTRODUCTION

1.1 | Adsorption cooling and desalination systems

The progressing effects of global warming have led to the development of eco-friendly adsorption cooling and desalination systems. They can already compete with compressor-based equipment, as they allow more efficient conversion and management of low-grade waste heat at near-ambient temperatures,^{1–3} taking part in implementing the net zero emissions strategy. Moreover, the adsorption refrigeration-desalination technologies fit into the ecologically sustainable development concepts.^{4–9} They utilize low-temperature thermal energy sources, including heat produced in cogeneration, waste heat, and solar and geothermal energy.^{8,10,11}

An adsorption chiller typically comprises critical components such as an evaporator, a condenser, and a minimum of two beds housed in separate reactors. These beds are filled with adsorbents and adsorbates, functioning as a working pair. The solid, porous sorbent within these beds exhibits a notable affinity for the refrigerant, characterized by a high sorption capacity. Heat transfer within the system, specifically between the hot and cold water and the sorbent, is facilitated through submerged coils within the beds.

The working principle of a typical adsorption chiller is as follows. The refrigerant's vapor (e.g., water) flows from the evaporator to the adsorption bed, generating the cooling effect in the evaporator. The adsorption process is sustained until the pressure within the bed approximates the saturation pressure of water. Cooling water flows through heat exchanger pipes inside the adsorption beds to increase the sorption capacity.

Subsequently, to initiate the regeneration phase of the adsorption bed, hot water is introduced into the coil of the heat exchanger, triggering the release of vapor from the bed.

Adsorption cooling and desalination systems represent a cutting-edge, thermally driven technology garnering increasing attention for its efficiency and sustainability. This technology stands out in the competitive landscape of cooling and desalination methods due to its dual-functionality. It can concurrently produce desalinated water and cooling effects within an adsorption chiller. This system leverages renewable energy sources such as solar, geothermal, and waste heat, making it a versatile solution.

Particularly noteworthy is the technology's ability to process feed water with high salinity levels, yielding low-salinity, potable water with minimal operational costs and a reduced environmental footprint. It harnesses

low-grade heat sources, which can be derived from various origins, including waste heat from industrial processes, marine engines, and solar energy. The significance of sorption-based thermal energy management becomes evident, considering over 90% of the world's primary energy consumption is heat. Moreover, using water as a refrigerant in sorbent–water working pairs offers numerous advantages. Water is environmentally benign, nonflammable, abundantly available, and has a high latent heat of evaporation, making it an ideal choice. For instance, conventional adsorption materials like silica gels are eco-friendly, inexpensive, and highly effective, capitalizing on water's significant phase change enthalpy.

Considering the above, adsorption chillers contribute to reducing fossil fuel consumption, promoting the efficient use of renewable and waste energy, and assisting in mitigating global climate change. Thus, they are emerging alternatives in the context of Net-Zero Emissions strategies, demonstrating their potential to contribute to sustainable energy solutions.

The efficiency of cooling-desalination systems depends on several parameters, mainly on the sorption processes in the adsorbent bed^{12–14} and the operating conditions, that is, the temperature and mass flow rates of cooling, hot and chilled water.^{15–17}

The evaporation of the refrigerant in the evaporator is the main stage of the adsorption chiller's operating cycle. The harnessing of heat from the water flowing through the heat exchanger enables the production of so-called chilled water. Due to the low operating pressures in the 760–2340 Pa range, the evaporator of the adsorption chillers is essential to the adsorption cooling-desalination (ACD) facility.^{18–20}

The condensation phase occurs under certain physical circumstances as it proceeds in the entire volume of saturated vapor and starts due to the vapor subcooling below the saturation temperature at a given pressure. As the vapor condenses, a rapid volume reduction occurs in the pipe wall's direct vicinity, resulting in unidirectional adsorbate flow toward the wall. Many condensers' variants always work by effectively removing heat from the gas stream using cooling media.²¹

The possibility of improving the chiller performance using a multistage cycle was numerically shown in Ali et al.²² Artificial intelligence (AI) methods were employed to optimize adsorption processes.^{16,17} The Adaptive Neuro-Fuzzy Inference System (ANFIS) was used to study the effect of the evaporator's thermal conductivity and adsorption bed on the AC performance. Simulations in ANSYS Fluent software confirmed the possibility of improving the heat transport conditions in the bonded sorbent bed.^{23,24} Performance analyses of adsorbate–adsorbent systems at

different bed configurations and cycle conditions can be found in several papers.^{25–27}

The computational tools developed allow engineers and scientists to suggest how to improve the efficiency of adsorption cooling-desalination systems. However, nothing was mentioned in the literature about conditioning monitoring as an effective way to increase ACDS performance. To fill the gap in the literature, we developed an Artificial Intelligence-based Diagnostic (AID) model via an automated machine learning (AutoML) approach, allowing accurate identification of the failure conditions of the adsorption cooling and desalination systems. Both the developed model and the whole methodology of the AutoML platform applications are the primary outcomes of the paper.

1.2 | Review of previous studies on fault diagnostics with AI approach

Advances in computing capacity and algorithms have increased interest in numerical modeling and AI methods to diagnose operating states.^{28–31}

The need for higher energy conversion efficiency and reliability of industrial systems has been growing in many sectors of the economy.³² Predictive analytics are becoming essential tools for forecasting these critical variables. Condition monitoring of an energy system's health may reduce downtime and enhance its performance. Since the overall investment costs decrease when technology becomes smarter (IEA report on intelligent grid analysis), disturbance forecasting and diagnosis are crucial for the equipment and associated energy management systems' sustainable and reliable operation.

As disturbance prediction and diagnosis are crucial for the equipment and associated energy management systems' sustainable and reliable operation, several works dealing with this issue can be found in the literature.^{33–35} The transient analysis of residual patterns in diagnosing faults in heating, ventilating, and air conditioning systems (HVAC) was presented in Cho et al.³⁵ The authors underlined that a fault detection technology is necessary for efficient energy management to detect performance deterioration properly and respond quickly to faults, improving reliability and system safety.

AI methods show the potential to supervise changes in the equipment's operating conditions, detect the location of faults, and predict or prevent potential failures that may generate significant financial losses.²⁹ The authors proposed, for example, intelligent data analytics for fault diagnosis in photovoltaic technology using deep convolutional neural networks (CNNs). They noted that the developed ConvNet algorithm allowed for covering all possible failure cases. A graphical and

unified analysis of the unsymmetrical shunt faults was depicted in Chen.³⁶ A review of the main trends, challenges, and prospects for applying artificial neural networks (ANN) for fault detection and diagnosis in photovoltaic technology is depicted in Li et al.³⁷ The authors underlined the difficulty in adequately configuring the model and reaching an open database on photovoltaic system failures.

More extensive literature concerning wind turbines can be found.^{38,39} The possibility of conducting surveillance and fault diagnosis in wind turbines using automatic machine-learning techniques was confirmed by Vives et al.⁴⁰ Several machine-learning methodologies were evaluated through simulations to predict and detect electrical and mechanical failures. An integrated monitoring and diagnosis system using machine learning algorithms tailored to different wind turbine components was also proposed in the studies. A review of failure modes, condition monitoring, and fault diagnosis techniques, including AI methods, can be found in large-scale wind turbine bearings.³⁸ The authors concluded that monitoring wind turbine bearings is necessary to improve the electric energy output and reduce operation and maintenance costs. A new idea for the design and integration of energy harvesters and damage detection methods of wind turbine blades, where the devices are self-powered and wireless, was proposed by Du et al.³⁹ Fault feature extraction of low-speed roller bearing based on the teager energy operator and complementary ensemble empirical mode decomposition (CEEMD) was presented in Han et al.⁴¹ Saari et al. used the support vector machine (SVM) technique to identify windmill-bearing faults.⁴² The proposed approach was able to detect improper behavior earlier than using traditional methods without any false alarms. A frequency-shift multiscale noise tuning stochastic resonance method for fault diagnosis of generator bearing in wind turbine was shown in Li et al.⁴³ Optimal parameters were selected through modified signal-to-noise ratio and genetic algorithms (GAs).

A supervisory control and data acquisition (SCADA) system was used to monitor wind turbines' performance, allowing the acquisition of measurement data from wind turbines, which can then be processed using AI methods.⁴⁴ Chandrasekhar et al.⁴⁵ presented an approach based on machine learning to predict the damage to wind turbine blades. The proposed Gaussian Processes methodology indicated a blade's edge frequencies, considering the second blade state. These relationships between the pairs of blades have been learned when the blades are in healthy conditions. The proposed approach was able to identify when the blades start behaving differently from one another over time. The system identified the early

onset of damage 6 months before it was identified and remedied.

A novel virtual sample generation method for predictive maintenance within combined heat and power plants was proposed by Olesen and Shaker.⁴⁶ The approach relies on random walks and particle swarm optimization (PSO) methods. According to the results, applying the technique to a public data set found that having just 10 run-to-failure incidents combined with generated virtual samples could compete with the accuracy of having 50 run-to-failure incidents for training.

The adaptive neuro-fuzzy inference system (ANFIS) method, consisting of backpropagation and least-squares learning algorithms, was implemented in Yalçın et al.⁴⁷ Leakage locations in a water distribution system were estimated. The hybrid algorithm was trained with variables measured during regular system operation, that is, acceleration, pressure, and flow rate.

Practical predictive analysis for energy efficiency and fault detection using AI was conducted in Crespo Márquez et al.⁴⁸ The authors proposed an ANN-based tool adapted to the existing operating conditions and dynamically triggers preventive maintenance activities. Comparative analysis between a machine learning algorithm implementation and an ANN in detecting minor faults of induction motor bearings was discussed in Esakimuthu Pandarakone et al.⁴⁹ SVM, naive Bayes classifier algorithm, k-nearest neighbour algorithm, decision tree (DT), random forest (RF), and deep learning with a CNN architecture were selected and discussed. The study helped understand the difference between the diagnostic approaches and their effectiveness in detecting bearing faults in an induction motor.

1.3 | Motivation and scope of research

Intelligent and efficient waste energy use belongs to the urgent actions to address environmental and energy management challenges.^{50–55} Moreover, improving energy efficiency and reducing energy demand and greenhouse gas emissions constitute significant tasks.^{3,56,57} The capability to exploit heat waste and renewable and recycled heat from low-temperature sources is part of the 4th Generation District Heating (4GDH) concept.^{58–60}

The reduction of energy consumption for air-conditioning purposes and the possibility of using low-temperature, waste thermal energy sources motivates the use of advanced computational methods such as the computational fluid dynamics and AI approach.^{61–65}

The analysis of the applied diagnostic solutions in the industry indicates that AI methods allow for the early

detection of possible failures. The service period and reliability of the facility reduce capital costs and enhance system utilization. It enables it to meet the power demands and maintains the system's performance, safety, and stability, improving the energy conversion and management processes.²⁹ This issue is of great interest in the energy sector since the system's malfunction constitutes an economic loss, and downtimes are punished by significant market opportunity costs.⁴⁶ The discussed issues on reducing service periods and improving reliability align with the other initiatives concerning investigating novel adsorbents and operational strategies.^{66–72}

Thus, effectively predicting potential failures will significantly improve low-grade waste thermal energy conversion efficiency and reliability, so it should be considered in management and operational strategy scenarios.

Therefore, the major objectives and contributions of the research are to perform a unique computational AI-based diagnostic model to identify a three-bed adsorption cooling-desalination system's health and failure operation states. The paper fills gaps in the literature and introduces a novel and comprehensive AID system for adsorption cooling and desalination installations. This comprehensive AI-based approach covers a wide range of 42 input parameters. The AID model was successfully validated on a complex, three-bed adsorption chiller under chilled and freshwater production modes.

The novelty of the presented study mainly consists of two aspects. First, the prediction of healthy and failure states of various components in a complex three-bed adsorption chiller installation using the extensive input data sets of 42 different operating parameters acquired from the system. Second, the efficient AutoML approach with the DataRobot application was used in the study. The tool allowed the selection of the most effective model, which turned out to be the Gradient Boosted Trees Classifier. The developed AID model was successfully validated on the complex, three-bed adsorption chiller. The AID model correctly identified healthy and failure states in various installation components under a wide range of operating parameters.

To the best of our knowledge, this is the first framework for predictive analysis in adsorption cooling and desalination systems. Monitoring the diagnostic function of a four-bed two, two-evaporator adsorption chiller was described by Chen et al.⁷³ However, the digital twin approach was applied in this case.

No reports are dedicated to applying AI algorithms for failure state prediction of such devices, and the lack of such studies results from the high complexity of the systems considered. Moreover, the novel idea of automating the

entire machine learning pipeline (AutoML) approach was introduced in the paper as a hot topic in industry and academia nowadays.^{74,75}

The three-bed adsorption chiller system considered in the study is a complex low-pressure cooling and desalination equipment. Due to low operating pressures and temperatures, these devices cannot be easily used. Moreover, selecting, acquiring, and preparing adequate signals to develop the presented expert system requires many techniques, including experts' knowledge. This justifies using an effective AutoML-based approach using state-of-the-art meta-learning methods.^{76–78} Thus, this paper's innovation is also a condition monitoring methodology in cooling and desalination systems.

The DataRobot application used in the paper is one of the best AutoML platforms. It has more models, auto preprocessing and feature engineering, and many validation methods than other tools, thus allowing the implementation of the state-of-the-art meta-learning approach. Moreover, this platform can run various state-of-the-art open-source algorithms parallel to different versions, testing thousands of possible data preprocessing and parameter settings combinations and deploying the best models in real-time. Considering the above, the work constitutes a research and development elaboration built in the modern Industry 4.0 domain and provides novel achievements in enhancing the state-of-the-art mathematical models performed via meta-learning techniques for measurement-oriented purposes.

Moreover, since overall investment is decreasing while its technology has become smarter due to harnessing helpful information about the installation, allowing accurate energy management, the developed AID system provides for improving the energy efficiency of cooling and desalination systems.

2 | OBJECTS AND METHODS

The diagnostic system of the adsorption cooling-desalination facility is built by utilizing machine learning methods. According to the literature review presented above, several AI methods allow for predicting failure states. They differ in the approach to the problem, the selection of hyperparameters, and computing times. This causes considerable work to compare and select the most appropriate AI method. Therefore, in this article, we chose the AutoML platform, which makes this process much easier, faster, and more accurate.

DataRobot platform (<https://www.datarobot.com/>) that includes AutoML can run multiple predictive models simultaneously, providing time-consuming model development and selection automation. This approach enables

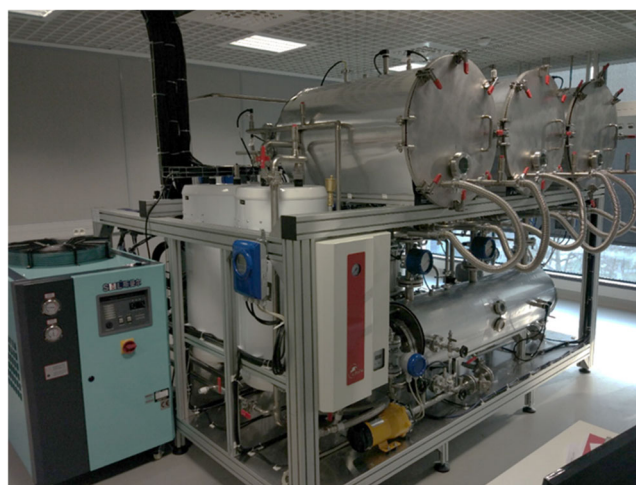


FIGURE 1 The three-bed adsorption chiller.

obtaining high-quality models characterized by high-level scalability.⁷⁹ It also allows for various learning techniques based on the supplied data, including supervised and unsupervised learning. The two main approaches implemented by the DataRobot are classification and regression. The classification task was employed in this paper for condition monitoring in an adsorption cooling-desalination system equipped with a three-bed adsorption chiller (Figure 1).

The system is at the AGH University of Science and Technology Energy Center in Krakow, Poland. The unit produces up to 40 dm³ of fresh water daily in desalination mode or delivers 1.5 kW of cooling power in cooling mode.^{20,80} The unit's sections have acquisition and control systems that monitor all critical operating parameters. The evaporator was supplied with a refrigerant (water) distributor and a tubular heat exchanger system. The sorption section consists of three beds in a horizontal arrangement, and thyristor controllers maintained the proper temperature in the hot and cooling water circuits. The individual beds are connected to the evaporator and the condenser. Steam pipelines are closed using electromechanical valves. The basic parameters of the adsorption beds are given in Table 1.

Additionally, because the sorbent mass is 12 kg,⁸¹ the specific cooling power SCP equals 241.7 W/kg.

The acquired data were split into learning and test data, unknown to the model during the model learning process, to evaluate its performance. The 90/10 split ratio of the learning/test data was employed, meaning that 90% (1769) points are learning data, and 10% (197) points are test data. The input variables (features) include pressures, temperatures, and the working medium's mass flow rates at various installation points.

TABLE 1 Nominal parameters of adsorption beds.

Parameter	Value
Cooling capacity (CC), kW	2.9
Required heating power (HP), kW	2.9
Cooling water inlet temperature, °C	max. 34
Hot water inlet temperature, °C	max. 85
Cooling water mass flow rate, kg/s	0.25
Hot water mass flow rate, kg/s	0.25

The output variable (target) is the valid/invalid indicator taking the values from the set (yes, no) informing of the occurrence of a failure state (“yes”) or failure-free operation of the installation (“no”).

Even though the failure states were simulated, the similarity to real-world situations is kept. Since the system is set to detect failures and abnormal operating conditions, more failure cases were collected during the measurement campaigns. Thus, such a distribution corresponds to situations where a system is somewhat unreliable and works improperly, which justifies the applicability of the acquired data.

The information on a situation corresponding to the installation's failure was identified based on the input values. Exceeding the acceptable ranges, defined in the provided data set, of at least one of all inputs indicated the existence of a failure condition of the whole system, which may lead to damage and eventually to the emergency stopping of the installation. The developed comprehensive AID system considers various input parameters. It covers the 42 inputs listed and is described with acceptable change limits in Table 2. The measurement points described in Table 2 are located in the complex installation shown in Appendix S1.

3 | RESULTS AND DISCUSSION

Binary classification models were explored in the study. The DataRobot system runs several algorithms of different versions and tests thousands of possible combinations of data preprocessing and parameter settings.⁷⁹ The modeling blueprint is given in Figure 2.

The AutoML platform developed a total of 42 various models in the final project. A leaderboard, which is a rank-order list of models according to performance metrics and constraints, including the prediction speed, is shown in Figure 3.

Several metrics were used for the evaluation of the developed models. For this research, we selected the three best models for further consideration. The result of

testing is provided in the Blueprints tab, where a blueprint represents the high-level end-to-end procedure for fitting the model, including any preprocessing steps, algorithms, and postprocessing.⁷⁹ DataRobot system provides a sophisticated automated preprocessing feature engineering that optimizes true signal and controls for model overfitting and different optimization metrics, depending on the project type (regression, binary classification, multiclass). Since the considered case belongs to the binary classification tasks, 10 optimization metrics in Table 3 are available in the AID.

The Gradient Boosted Trees Classifier algorithm is the “best” model of all 42 generated models and is chosen in the project, and its performance is summarized in Table 3. For the comparison of the proposed method, implemented by the Gradient Boosted Trees Classifier and the next two applied by AVG Blender and ENET Blender are also included in Table 3.

High metrics were also obtained by the other algorithms implemented in the following two top models. Even though modified particle swarm optimization (modified PSO), modified genetic algorithm (modified GA) and modified grey wolf optimization (modified GWO)^{82–88} can be found as the latest optimization algorithms for minimizing errors in desalination systems, the high accuracy and precision of the developed in the paper AID system is also reported. According to Table 3, the best turned out to be the Gradient Boosted Tree Classifier.

This model blueprint is utilized as the core of the developed AID model (Figure 4). The blueprint includes automated data pre-processing and feature engineering.

Gradient Boosted Trees Classifier (Gradient Boosting Classifier or Generalized Boosted Models [GBM]) is a cutting-edge algorithm for fitting highly accurate predictive models. GBMs are considered the most versatile and valuable modeling algorithm, requiring little preprocessing, efficiently handling missing data, striking the right balance between bias and variance, and finding complicated interaction terms. GBMs are a generalization of Freund and Schapire's AdaBoost algorithm to handle arbitrary loss functions. In concept, they are very similar to RFs, as they fit individual DTs to random resamples of the input data, where each tree sees a bootstrap sample of the rows of the data set and the N arbitrarily chosen columns where N is a configurable parameter of the model.⁷⁹ GBMs differ from RFs in a single significant aspect. The GBM fits each successive tree to the residual errors from all the previous trees combined rather than fitting the trees in parallel. This is advantageous, as the model focuses each iteration on the most challenging examples to predict and, therefore, most beneficial to get correct. The algorithm's two critical parameters are the

TABLE 2 Input parameters of the AID system.

ID	Parameter	Acceptable limits of changes
1	TT01—Evaporator top steam temperature, °C	2–6
2	TT02—Cooling outlet water temperature from the condenser, °C	15–30
3	TT03—Cooling water inlet temperature to the condenser, °C	15–30
4	TT04—Temperature of hot water in the heating circuit of the bed after the hot water tank (after the pump), °C	77–80
5	TT05—Temperature of hot water in the heating circuit before the hot water tank, °C	75–78
6	TT06—Chilled water inlet temperature to the evaporator, °C	10–12
7	TT07—Chilled water outlet temperature from the evaporator, °C	8–11
8	TT08—Cooling water temperature after condensing unit, °C	15–30
9	TT09—Cooling water temperature before condensing unit, °C	15–30
10	TT10—Cooling water temperature after the cooling water tank (after the pump), °C	15–30
11	TT11—Temperature in bed volume 1, °C	35–45
12	TT12—Temperature in bed volume 2, °C	35–45
13	TT13—Temperature in bed volume 3, °C	35–45
14	TT14—Temperature of water in evaporator—bottom, °C	3–7
15	TT15—Temperature of adsorption bed 1, °C	40–50
16	TT16—Temperature of adsorption bed 2, °C	40–50
17	TT17—Temperature of adsorption bed 3, °C	40–50
18	TT18—Temperature in the condenser, °C	20–30
19	TT19—Temperature of water—outgoing from the condenser, °C	20–30
20	TT20—Temperature of removal from evaporator °C	3–7
21	TT21—Temperature of water circulating in the evaporator, °C	8–11
22	TT22—Evaporator feedwater temperature, °C	10–20
23	PT01—Pressure in feedwater tank, kPa	5–13
24	PT02—Pressure in the brine tank, kPa	5–13
25	PT03—Pressure in the desalted water tank, kPa	5–13
26	PT04—Pressure inside the evaporator, kPa	0.5–2.5
27	PT05—Pressure inside the bed 3, kPa	0.7–5
28	PT06—Pressure inside chamber 2, kPa	0.7–5
29	PT07—Pressure inside chamber 1, kPa	0.7–5
30	PT08—Pressure in hot water outlet system, kPa	22–150
31	PT09—Pressure in the cooling water supply system, kPa	22–150
32	PT10—Pressure inside the condenser, kPa	2–5
33	PT11—Pressure in the chilled water supply system, kPa	22–150
34	LT01—Water level indicator in feedwater tank, %	<10% filling the tank
35	LT02—Water level indicator in the brine tank, %	<10% filling the tank
36	LT03—Water level indicator in the desalinated water tank, %	<10% filling the tank

(Continues)

TABLE 2 (Continued)

ID	Parameter	Acceptable limits of changes
37	FT01—Hot water flow rate in the bed heating circuit after the hot water tank (after the pump), dm ³ /min	12–16
38	FT02—Cooling water flow rate—condenser outlet, dm ³ /min	15–17
39	FT03—Chilled water flow rate—evaporator outlet, dm ³ /min	2–4
40	FT07—Evaporator circulating water flow rate, m ³ /h	40–70
41	FT08—Cooling water flow—after the cooling water tank (after the pump),	30–45
42	FT10—Desalted water mass flow rate—condenser outlet, kg/h	0.3–3

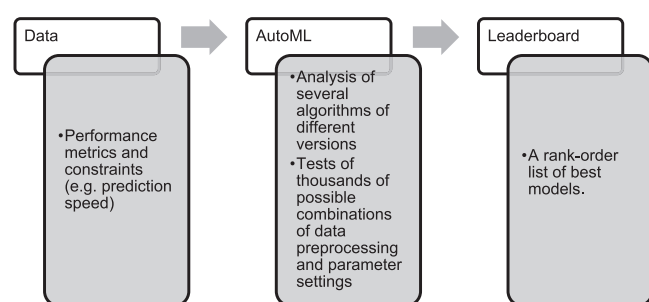


FIGURE 2 The modeling blueprint.

learning rate and the number of trees in the model. A correctly performed cross-validation of both parameters allows GBM to find the exact point in the training data where overfitting begins and stops iteration before that. GBMs can achieve the highest possible accuracy without overfitting.⁷⁹

Since identifying the essential drivers of a machine learning model's outcomes allows checking the quality of the data source, the Feature Impact, that is, a statistical measure of each feature's effect on the target variable, is a crucial step.⁷⁹ In other words, Feature Impact measures how important a feature is in the context of a model, that is, it estimates how much the accuracy of a model would decrease if that feature were removed. The Feature Impact is evaluated by altering input data and observing the effect on a model's score. The feature engineering procedure, provided by the [DataRobot platform](#), includes many tasks, such as identifying missing values and their imputation, measuring the correlation between features, and automatically creating the feature list according to their importance based on the complex relationships in the data and permutation importance⁷⁹ (Figure 5).

The relative importance of each input feature ranked from the most important (scaled to 100%) to the least important (with importance close to 0%), is shown by

blue bars. All importance values are relative to the top-ranked input feature.⁷⁹

The following eight parameters are of the utmost crucial in the data sets used to develop the AID model: the evaporator top steam temperature (TT01), hot water flow rate in the bed heating circuit after the hot water tank, after the pump (FT01), the pressure inside condenser (PT10), the temperature of hot water in the heating circuit before the hot water tank (TT05), chilled water outlet temperature from the evaporator (TT07), evaporator return water temperature (TT21), the temperature in the condenser (TT18), the temperature of water in evaporator—bottom (TT14). The above-listed features are the most important to the predictive power of a trained model. In other words, the TT01, FT01, PT10, TT05, TT07, TT21, TT18, and TT14 have significantly stronger predictive power than the rest of the input features.⁷⁹

The Lift Chart demonstrates how close, in general, model predictions are to the actual target values of the training data. In other words, it compares the average model predictions and the average actual target values, sorted by the predicted values in ascending order, split into up to 60 bins.⁷⁹ The Lift Chart for the developed AID model is given in Figure 6.

Since the orange and blue lines are close to each other, and they cross over many times, indicating that the model does not consistently overestimate or underestimate and both the blue and orange lines gradually slope upwards, the developed AID model achieved a good trend and accuracy in its predictions.⁷⁹

The receiver operating characteristic curve (ROC curve), that is, a graphical plot that illustrates a binary classifier system's performance, is depicted^{79,89} in Figure 7.

Since the ROC curve is created by plotting the true positive rate (hits) against the false positive rate (false alarms) at various threshold settings, good performance was achieved by the AID model.

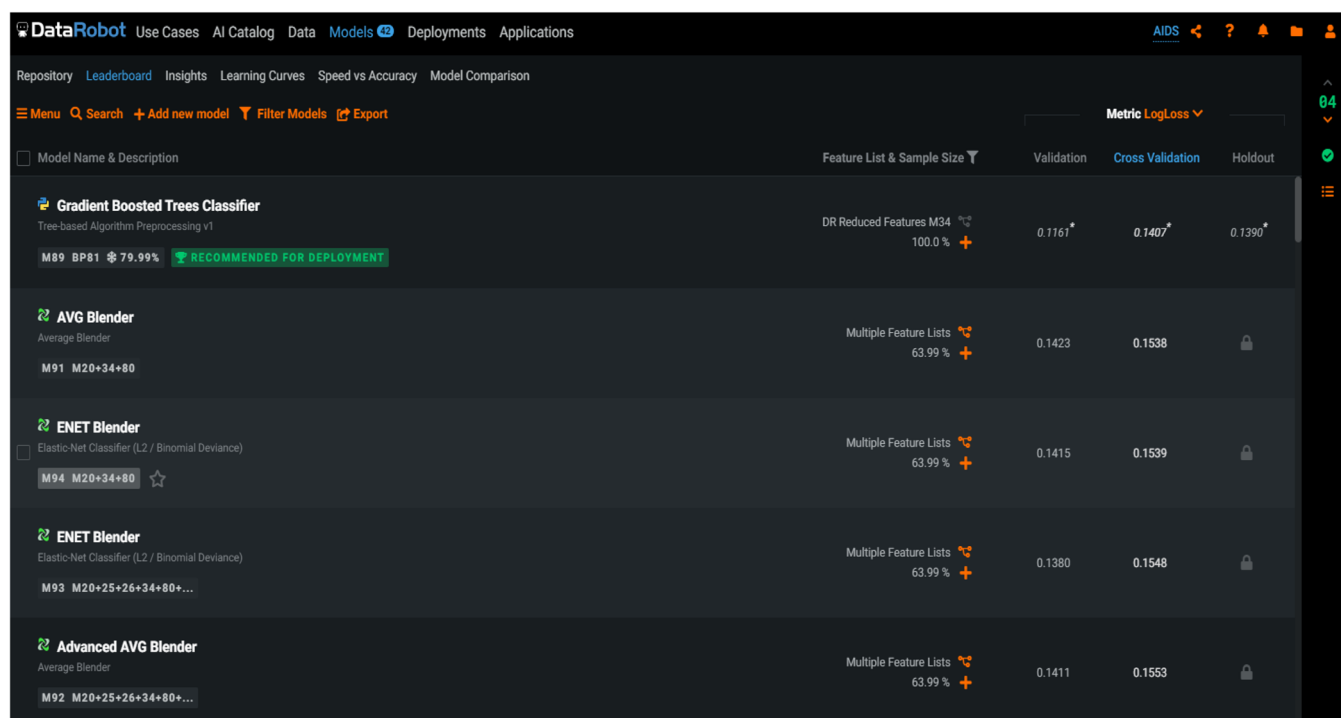


FIGURE 3 The leaderboard of the DataRobot system.

The cumulative lift chart, that is, a visual aid for measuring model performance, is depicted in Figure 8.

Using about 60% of model predictions, we will get more than 1.5 more positive class responses than random selection.

Due to the AID model's complexity, Feature Effects functionality shows the impact of changes in each feature's value on the model's predictions. It depicts how a model "understands" the relationship between each feature and the target.⁷⁹

Feature Effects plots prepared for the highest Feature Impact, that is, the feature TT01 most related to the target, are shown in Figure 9.

As expected, the best accuracy is observed for the training data. However, some areas in the inputs' domain corresponding to the more deficient model's performance can be located for validation and holdout data sets. Additional data sets in these areas could improve the model's accuracy.

Since the developed system should make a yes or no decision when detecting a failure state in the considered fault diagnosis problem, the AID model needs to turn the predicted probability correctly into a decision. It is crucial for the model's functionality, and the prediction distribution plot allows for assessing the performance of the considered AID model based on the Gradient Boosted Trees Classifier (Figure 10).

According to Figure 10, the model can separate yes decisions from no decisions. However, a region of

decision uncertainty, where the purple and green areas overlap, and neither part dominates, is quite broad. It indicates that predicted probabilities in this range will not accurately choose yes or no outcomes and may be the result related to the data sets used in the study.⁷⁹ Since the data applied for training were acquired during the artificial induction of emergency states, they may be burdened by the poor understanding of the theoretical mechanisms which rule the failure process in such a complex system.⁹⁰ Thus, additional conditions should be considered during the model's development based on the operating parameters to increase the model's accuracy. More training data sets may also be beneficial.

To review the distribution of the quantitative indicator of the effect of the variable on the predictions and, therefore, to discover what drives the model, the prediction explanations functionality is necessary to apply (Figure 11).

Qualitative indicators of the explanation's strength: strong (+++), medium (++) , or weak (+) positive or negative (−) influence depict the impacts of features (the "reasons") for each outcome the model generates. Suppose an explanation's score is trivial and has little or no qualitative effect. In that case, the output displays three grayed-out symbols (+++ or − − −), indicating that both the impact and its directionality are minor.⁷⁹ The top influential inputs are included in the Prediction Explanations plot from Figure 11.

TABLE 3 Optimization metrics of the AID system.

ID	Optimization metric (GBM algorithm)	Validation	Cross-validation	Holdout
Gradient Boosted Trees Classifier				
1	AUC	0.9923	0.9868	0.9887
2	Area under PR curve	0.9952	0.9921	0.9932
3	FVE binomial	0.8258	0.7889	0.7913
4	Gini norm	0.9846	0.9737	0.9774
5	Kolmogorov–Smirnov	0.9139	0.9029	0.9008
6	LogLoss	0.1161	0.1407	0.1390
7	Max MCC	0.9109	0.9017	0.9104
8	RMSE	0.1873	0.1998	0.2037
AVG blender				
1	AUC	0.9866	0.9850	0.9835
2	Area under PR curve	0.9928	0.9910	0.9902
3	FVE binomial	0.7864	0.7686	0.75820
4	Gini norm	0.9731	0.9701	0.9671
5	Kolmogorov–Smirnov	0.8909	0.8855	0.8806
6	LogLoss	0.1423	0.1538	0.2152
7	Max MCC	0.8952	0.8807	0.8873
8	RMSE	0.2021	0.2139	0.2152
ENET blender				
1	AUC	0.9862	0.9849	0.9832
2	Area under PR curve	0.9926	0.9909	0.9900
3	FVE binomial	0.7869	0.7684	0.7576
4	Gini norm	0.9724	0.9697	0.9663
5	Kolmogorov–Smirnov	0.8990	0.8820	0.8916
6	LogLoss	0.1415	0.1539	0.2152
7	Max MCC	0.8960	0.8794	0.8982
8	RMSE	0.2010	0.2140	0.2152

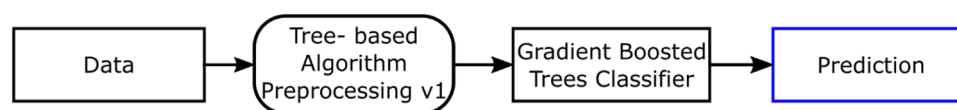


FIGURE 4 The blueprint for the AID model.

The prediction runtime is a vital parameter for an efficient diagnostic system. In other words, it is crucial to determine how long a real-time prediction will take. To score as this measurement is of interest for the system's reliability and helps to choose the best model with the lowest overhead.⁷⁹ The tradeoff between runtime and predictive accuracy is shown in Figure 12. The currently selected metric, that is, LogLoss, is listed on the Y-axis,

while the X-axis displays the estimated time in milliseconds to make 1000 predictions.⁷⁹ Although total prediction time includes a mixture of factors and varies based on the final implementation and, most importantly, it does not include the time for the round-trip API call, that is, network latency (it ought to be tested in the actual system), the selected Gradient Boosted Trees Classifier for the developed AID model is the best choice.

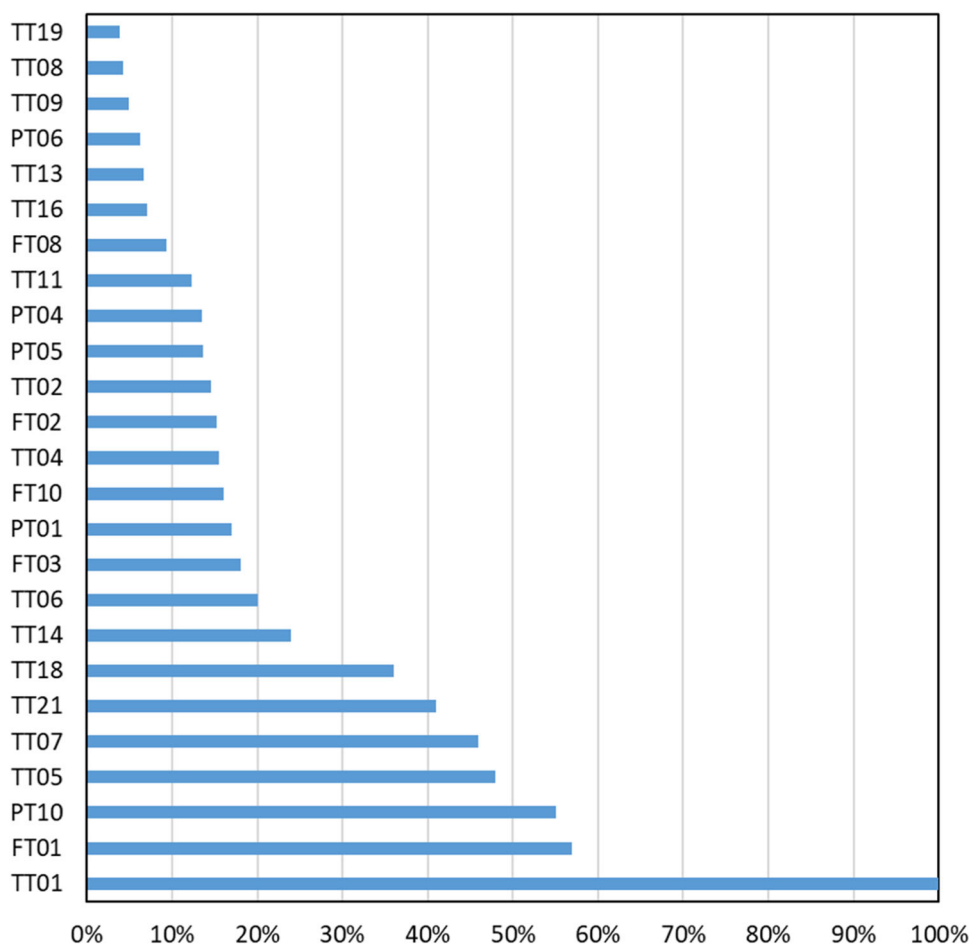


FIGURE 5 The Feature Impact graph of the AID model.

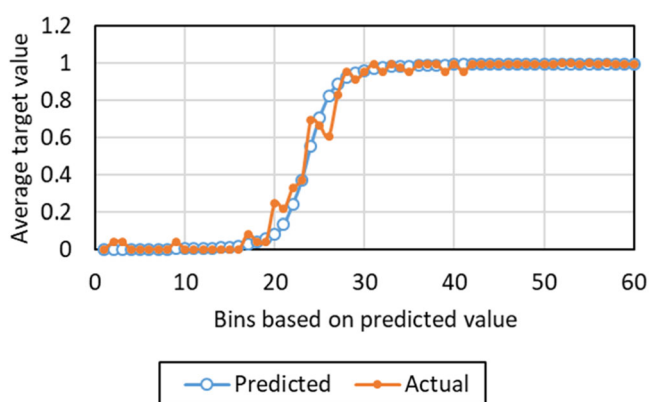


FIGURE 6 The lift chart for predicted and actual target values.

According to Figure 12, the developed AID model has a lower error and the highest prediction speed.

Comparing the results obtained from experiments and the AID model for the training and test data is depicted in Appendix S2 and Appendix S3, respectively. Columns AQ (“Exp. Label”) and AR (“Predict. Label”) correspond to labels from the actual and predicted by the AID model. A

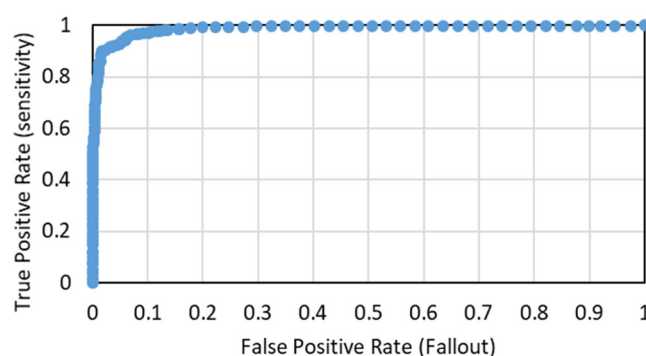


FIGURE 7 The receiver operating characteristic curve for the AID model.

marked red cell inside a sheet indicates failure conditions, and if it appears, the whole set is counted as a set with a detected failure by “1” in the AQ (“Exp. Label”) column. Data in column AS (“Err [–]”) indicate the prediction errors (Appendix S2 and Appendix S3).

The results obtained reveal that all the states of operation given in the sheet with training data, corresponding to the real situations of failure (value “1”) and healthy (value “0”)

conditions, were correctly predicted by the developed AID. The achieved accuracy for the set of data, containing 1769 sets of cases, is equal to 100%.

The model's accuracy is slightly worse but still high, equal to 97.5%, for the test data sets containing cases not

seen before by the model during the development stage. The presented data shows that the number of incorrect system interpretations for the analyzed new 197 cases was 5. According to the previous findings, a possible reason for the detected errors might be an imperfect

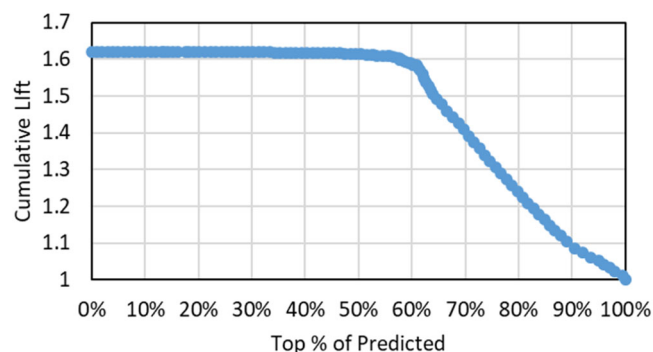


FIGURE 8 The cumulative lift for the AID model.

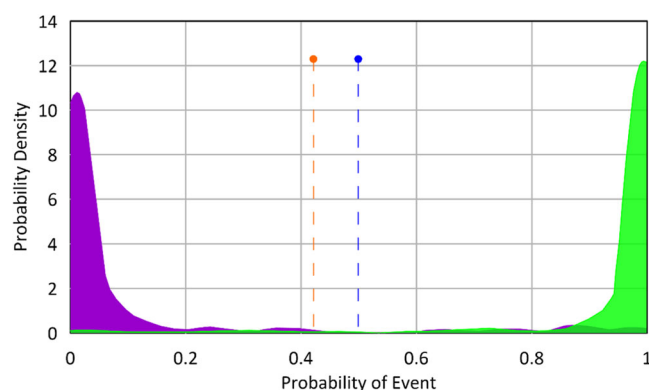


FIGURE 10 The prediction distribution plot for the AID model.

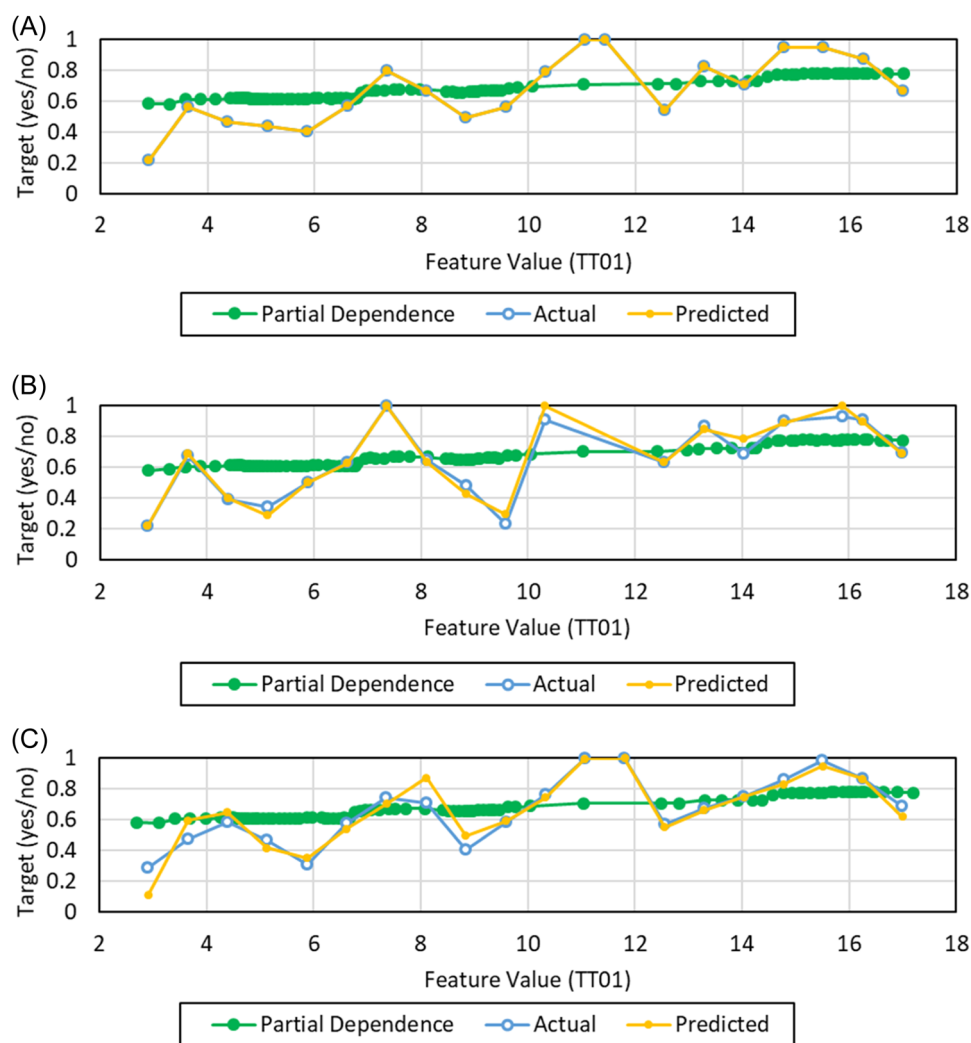


FIGURE 9 Feature effects plots for TT01, (A) training, (B) validation, and (C) holdout.

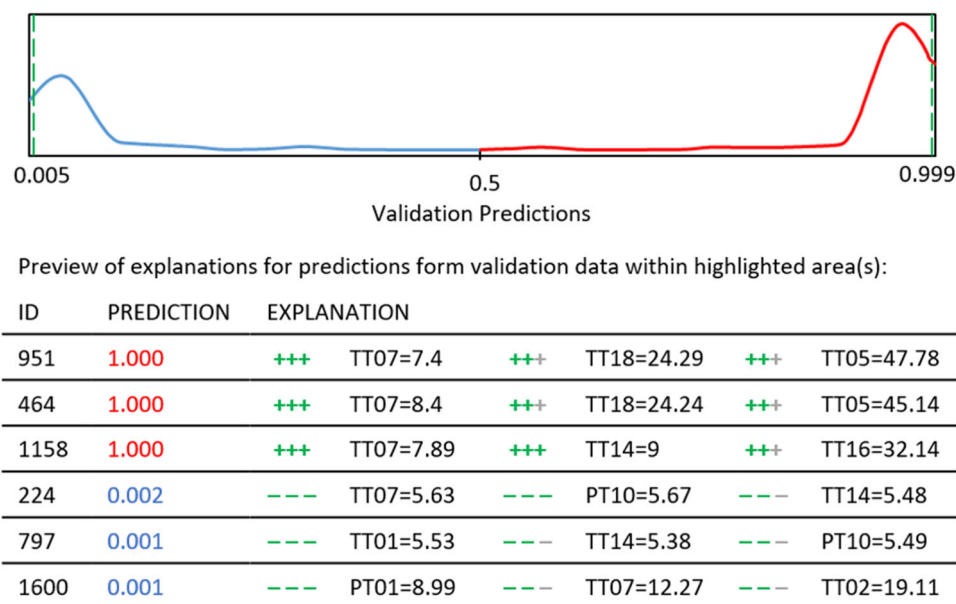


FIGURE 11 The prediction explanations plot for the AID model.



FIGURE 12 Seed versus accuracy for the developed models.

theoretical understanding of failure patterns and associated missing features.⁹⁰ Additional data would improve the developed comprehensive AID model.

A similar comparison was made between the two other AutoML methods provided by BigML and R².ai. The accuracy of predictions was worse, equal to 93.91% for BigML on the new, independent data and 99.15% for R².ai on training data.

Thus, the approach provided by DataRobot was the best of all compared methods.

The developed AID model enhances the utilization of the adsorption-desalination system. It also helps meet power demands, maintain the system's performance and stability, and improve energy conversion and management. Thus, the work constitutes a research and development elaboration built in the modern Industry 4.0 domain and provides novel achievements in enhancing the state-of-the-art mathematical models for measurement-oriented purposes.

The practical significance of the study's findings is multifaceted.

1. The introduction of the AID system fault prediction in cooling and desalination systems marks allows for early detection of potential failures, reducing downtime and associated costs.
2. Considering 42 diverse input operational parameters, the AID system can optimize the performance of the adsorption chiller, leading to better management of waste energy, lowering operating costs and improving the overall efficiency of the entire installation,
3. The AutoML application enables handling large and complex data sets, which is crucial for data-driven decision-making in advanced systems like adsorption cooling and desalination facilities.
4. The methodology introduced in the paper accelerates experimentation and offers new insights, which could be pivotal in driving innovation in adsorption technology and lead to the developing of more advanced and efficient systems.

4 | CONCLUSIONS AND PERSPECTIVES FOR FURTHER RESEARCH

The paper deals with one of the most effective ways of chilled and freshwater production via adsorption technology, utilizing multigeneration heat. The work introduces a novel methodology for condition monitoring of cooling and desalination systems.

Fault diagnosis in cooling and desalination systems is one of the most essential parts of the condition

monitoring area. Since the system's malfunction constitutes an economic loss and downtimes result in significant market costs, failure prediction is challenging to enhance the facilities' energy conversion and management strategies. Thus, it is an issue of great interest in the energy sector.

A three-bed adsorption chiller is considered in the study. The AutoML approach with the DataRobot application as an efficient tool and one of the best AutoML platforms in the market is introduced in the paper.

A specific aspect of the AutoML approach is facilitating the calculation process. However, proper and appropriate selection of the inputs and the extensive data acquisition from the presented complex system is not easy, considering that adsorption cooling and desalination systems are low-pressure facilities. That is why there are no such applications in the literature. To our knowledge, it is the first paper dealing with failure prediction in such complex systems, constituting the paper's novelty.

We managed to develop a comprehensive and innovative AID expert diagnostic system based on a total of 42 wide-range input parameters and providing diagnoses for different fault types of the entire facility. The AID model achieved high efficiency in predicting failure conditions and constitutes a powerful diagnostic tool for complex adsorption cooling and desalination systems.

The accuracy of the developed AID model, using 42 various input parameters defining the installations' state, was as high as 99.23%. The obtained findings result in recommendations for selecting hot, cooling, and chilled water temperatures and other operating parameters to intensify sorption processes in the bed.

The novelty of the AutoML application enables researchers to analyze large and complex datasets efficiently, automate model selection and optimization, and discover previously unseen patterns and relationships within the considered data. The methodology of condition monitoring in cooling and desalination systems based on the AutoML approach introduced in the paper enhances the scientific process by accelerating experimentation and providing novel insights and discoveries.

The results obtained in the article prove the validity of using the AutoML platform, especially for complex, extensive systems and installations, such as adsorption cooling and desalination systems.

Future research may concern a next-generation AI-based model, prescribing the safe exploitation of cooling and desalination systems.

NOMENCLATURE

AI	Artificial Intelligence
AC	Adsorption Chiller modified PSO
ACDS	Adsorption Cooling and Desalination System
AID	Artificial Intelligence-based Diagnostic system
ANFIS	Adaptive-Network-Based Fuzzy Inference
ANN	Artificial Neural Networks
AutoML	Automated Machine Learning
CNN	Convolutional Neural Network
DT	Decision Tree
GBM	Gradient Boosting Machines (or Gradient Boosted Trees)
HVAC	Heating, Ventilation and Air Conditioning
IEA	International Energy Agency
RF	Random Forest
SCADA	Supervisory Control and Data Acquisition
SVM	Support Vector Machine,
4GDH	4th Generation District Heating

AUTHOR CONTRIBUTIONS

The contribution of co-authors in creating the article is conceptualization, Jaroslaw Krzywanski; methodology, Jaroslaw Krzywanski, Dorian Skrobek; software, Dorian Skrobek, Jaroslaw Krzywanski; validation, Karol Sztékler, Jaroslaw Krzywanski; formal analysis, Waqar Muhammad Ashraf, Wojciech Nowak, Lukasz Mika, Jaroslaw Krzywanski, Dorian Skrobek; investigation, Jaroslaw Krzywanski, Karolina Grabowska, Marcin Sosnowski, Dorian Skrobek; resources, Jaroslaw Krzywanski, Karol Sztékler, Marcin Sosnowski, Lukasz Mika, Wojciech Nowak; data curation, Jaroslaw Krzywanski, Karol Sztékler, Karolina Grabowska, Dorian Skrobek; writing—original draft preparation, Jaroslaw Krzywanski, Karolina Grabowska, Karol Sztékler, Dorian Skrobek; writing-review and editing, Dorian Skrobek, Jaroslaw Krzywanski, Marcin Sosnowski, Karol Sztékler, Wojciech Nowak; visualization, Jaroslaw Krzywanski, Karol Sztékler, Dorian Skrobek; supervision, Jaroslaw Krzywanski, Wojciech Nowak; project administration, Wojciech Nowak, Lukasz Mika, Karol Sztékler; funding acquisition, Wojciech Nowak, Lukasz Mika. All authors have read and agreed to the published version of the manuscript.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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