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Optimizing ethylene plant utilities *via* hybrid artificial neural network and first-principles modeling

ALEKSA MILADINOVIĆ[1]*, MIRJANA KIJEVČANIN[2], JOVAN JOVANOVIĆ[2], SABLA ALNOURI[3], VLADIMIR STIJEPOVIĆ[1] and MIRKO STIJEPOVIĆ[2]

[1]Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia and [3]Gas Processing Center, College of Engineering, Qatar University, Doha, Qatar

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Abstract: In this study, a hybrid modeling approach combining first-principles equations with an artificial neural network was developed to reduce operating costs and carbon emissions in process utility systems of an ethylene plant. The artificial neural network accurately predicted turbine power outputs under various operating conditions, with low maximum absolute percentage errors across all three turbines, demonstrating its ability to effectively capture nonlinear system behavior. The economic analysis showed that natural gas prices have a greater cumulative impact on operating expenses than the carbon tax due to their greater variability. Although the carbon tax has a higher local sensitivity, the steady increase in natural gas prices represents a persistent economic burden. This demonstrates the importance of managing fuel costs and monitoring changes in carbon policy to mitigate sudden increases in operating costs. With increasing output, the operating costs of the propylene and cracked gas turbines rose almost linearly, with the costs per megawatt rising more sharply for the propylene turbine. The ethylene turbine significantly impacted operating expenses despite lower output, showing that small output changes can affect costs. Overall, the proposed methodology provides a reliable framework for optimizing energy performance, predicting fuel consumption and supporting operational decision-making in large-scale processes.

Keywords utility system; modeling; artificial neural network; energy efficiency.

INTRODUCTION

Utility systems are fundamental components in a wide range of industrial applications, from power generation and chemical processing to manufacturing

* Corresponding author. E-mail: aleksa.miladinovic@ihtm.bg.ac.rs
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and district heating. These systems typically involve complex thermodynamic processes, including heat exchange, phase transformation, and mechanical work, often facilitated through steam turbines, boilers, heat exchangers and multi-stage compressors. They represent a notable example where optimizing operating parameters can yield significant benefits, owing to their inherent susceptibility to energy efficiency losses. Consequently, the optimization of operating parameters in utility systems can lead to substantial energy savings and enhanced overall system performance. To overcome the limitations of purely physical or purely data-driven approaches, hybrid modeling has emerged as a promising framework. Hybrid models integrate deterministic and stochastic elements to leverage the strengths of both domains, achieving the precision and structure of rule-based systems while incorporating the flexibility and uncertainty modeling of probabilistic approaches, ultimately enhancing predictive accuracy, robustness and adaptability in complex environments. In this context, stochastic elements refer to data-driven approaches such as artificial neural networks, which, although deterministic at inference, incorporate stochasticity during training and can effectively capture complex, nonlinear relationships under uncertainty. When applied to utility systems, hybrid modeling can enhance fault detection, predictive maintenance, performance optimization and real-time control.

Equipment like steam turbines and multi-stage compressors, after extended periods of use, lose efficiency and are prone to mechanical wear, performance degradation, and increased maintenance requirements. By leveraging data-driven models, it is possible to monitor the performance of such equipment in real time and implement optimization strategies that extend equipment life and maintain energy efficiency.

Numerous studies have optimized the performance of utility systems using various modeling approaches. Mavromatis and Kokossis[1] developed a turbine hardware model based on Willan's line, while Zhu *et al.*[2] and Li *et al.*[3] used mixed-integer nonlinear programming (MINLP) models to optimize multi-turbine utility systems, achieving cost and coal reductions. Recent work[4–8] has integrated artificial intelligence (AI) techniques, such as artificial neural networks (ANN) and machine learning, to predict performance and improve the operational efficiency of steam turbines and related systems. Various machine learning approaches have been applied to energy systems, including data envelopment analysis with artificial neural networks for petrochemical energy optimization,[4] steam methane reforming control,[5] extreme learning for steam turbine monitoring[6] and regression models for boiler and turbine performance.[7] Despite these advances, few studies[9–11] have combined deterministic models with ANNs to simultaneously increase steam production efficiency and reduce costs. A reduction of 1.4 % in steam production costs was achieved by using a hybrid ANN model to optimize turbine operating parameters, as demonstrated by Li *et al.*[9] A hybrid ANN-mechanistic model was developed to accurately characterize the performance of multistage compressors, as shown by Chu *et al.*[10] Another study[11] modeled and optimized a steam turbine power plant with fifteen design variables, resulting in up to a 3.76 % increase in thermal efficiency and a 3.84 % reduction in total cost rate compared to actual plant data. This highlights the potential for hybrid models that utilize both physical principles and data-driven methods for better adaptability and accuracy.

Most existing approaches tend to rely heavily on deterministic models, which may lack flexibility especially when experimental measurement of all required operating parameters is not available. As a result, there is significant potential for further exploration and development of hybrid modeling approaches that combine the strengths of both physical principles and data-driven techniques. Such integrated models may offer higher predictive power and adaptability of neural networks while maintaining the transparency and robustness of first-principles equations.

In this study, a hybrid modeling approach was developed to minimize the operational expenditure of the utility system by integrating deterministic optimization techniques with artificial neural networks, thereby enhancing the system's efficiency, reliability and cost-effectiveness under varying operational conditions.

PROBLEM STATEMENT AND MODEL FORMULATION

The utility system analyzed in this study is illustrated in Fig. 1. Steam is initially generated in a boiler and routed to a high-pressure (HP) steam header, which serves as the central distribution point for steam delivery across the plant. From the HP header, steam is directed to three steam turbines, designated as RT-1, RT-2 and RT-3, each serving distinct process units associated with cracked gas, propylene, and ethylene production, respectively. Additionally, a portion of the HP steam is diverted through a pressure reducing valve (RV-1), which lowers the pressure before routing it into the medium-pressure (MP) steam header and ultimately to the condensate system.

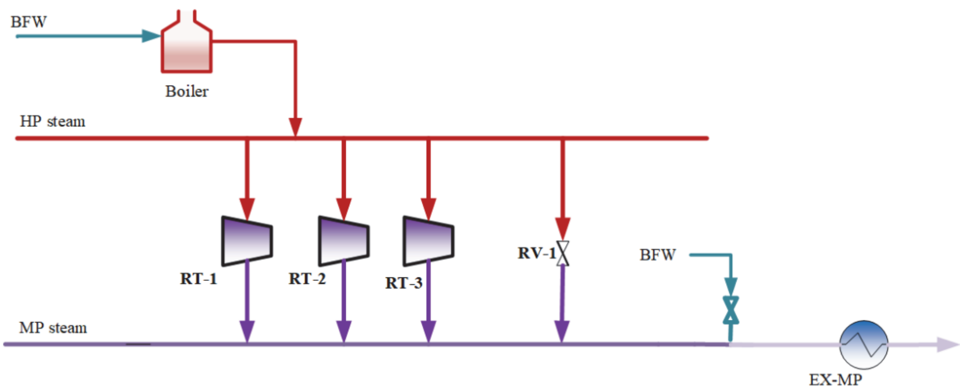

Fig. 1. Utility system.

Within the MP header, the medium-pressure steam is mixed with boiler feed water (BFW) to adjust its thermal state. This mixing reduces the steam temperature to the corresponding saturation temperature at the designated pressure level, thereby ensuring that the steam entering downstream units is saturated rather than superheated. Maintaining saturated steam conditions is essential to protect equipment and ensure optimal performance, particularly for components designed to operate specifically under such conditions.

Although a deterministic model of the boiler is available and can be reliably used to simulate steam generation across a range of operating conditions, modeling the rest of the utility system poses significant challenges.

In particular, the absence of sufficient real-time measurements and detailed operating data for key components – including the steam turbines (RT-1, RT-2 and RT-3), the pressure reducing valve (RV-1), and the downstream steam network – limits the ability to construct a fully deterministic model for the entire system. These components exhibit complex, nonlinear behavior that cannot be accurately captured without comprehensive instrumentation and historical performance data.

To address this limitation, a hybrid modeling approach has been employed. The boiler is modeled using a deterministic, first-principles framework grounded in thermodynamic laws, ensuring accurate representation of steam generation processes. For the remaining components of the utility system, an artificial neural network (ANN) is developed using available historical operational data. The ANN is trained to capture the nonlinear relationships and dynamic behavior of these units, effectively compensating for the lack of detailed physical models and real-time measurements.

This hybrid approach combines the strengths of both modeling paradigms – physical accuracy from the deterministic model and adaptive predictive capability from the ANN. As a result, it enables a more comprehensive and practical representation of the entire utility system, supporting improved performance analysis, operational optimization, and informed decision-making under variable plant conditions. Therefore, the primary goal of this work is to optimize the utility system with respect to steam generation, aiming to reduce operating expenses (OPEX) and simultaneously lower CO_2 emissions. By minimizing the amount of steam generated (and consequently the natural gas consumption required in the boiler) both economic and environmental benefits can be achieved.

The boiler hardware model (BHM) was taken from the study of Shang and Kokossis,[12] which considers the relationship between fuel input, heat loss, and the resulting steam output. The fuel requirement (Q_{fuel}) is calculated based on the heat added to the steam (Q_{steam}) and the heat losses (Q_{loss}):

$$Q_{\text{fuel}} = Q_{\text{steam}} + Q_{\text{loss}} \tag{1}$$

The heat, Q_{steam}, can be estimated from the following relation:

$$Q_{\text{steam}} = M_{\text{HP}}(C_p T_{\text{sat}} + q) \tag{2}$$

where C_p represents the specific heat of saturated steam (kJ kg^{-1} K^{-1}), T_{sat} is the temperature of the saturated steam (K), q denotes the specific heat load of fuel (kJ kg^{-1}) and M_{HP} is the mass flow rate of high-pressure steam (t·h^{-1}); the heat losses are estimated from:

$$Q_{\text{loss}} = (aM_{\text{HPmax}} + bM_{\text{HP}})(C_p T_{\text{sat}} + q) \tag{3}$$

where a and b represent regression parameters adjusted on the basis of the experimental data and M_{HPmax} is the maximum steam mass flow rate through the boiler (t h^{-1}).

By combining Eqs. (2) and (3), the total energy input from fuel combustion, Q_{fuel}, can be calculated using the following equation:

$$Q_{\text{fuel}} = (aM_{\text{HPmax}} + (1+b)M_{\text{HP}})(C_p T_{\text{sat}} + q) \tag{4}$$

The BHM is a deterministic model for predicting the fuel demand of a boiler based on its size, load and operating conditions. It takes into account heat losses and thermodynamic properties, making the model more realistic compared to constant efficiency assumptions.

Due to the lack of measurement data for key operating parameters- in particular for the outlets of the three turbines feeding into the MP header, their efficiencies, and the outlet conditions of RV-1 – the remaining utility system cannot be accurately modeled using conventional deterministic methods. Therefore, an artificial neural network (ANN), presented in Fig. 2, is used to capture the system behavior under these conditions.

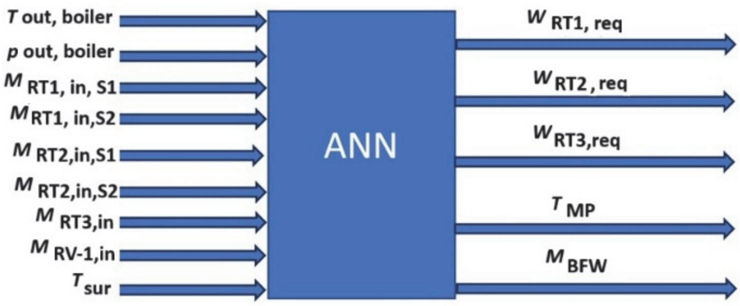

Fig. 2. The implemented artificial neural network.

The input data for the ANN – including the outlet temperature and pressure of the boiler stream, the inlet steam mass flow rates to the two sections of turbine RT-1, to the two sections of turbine RT-2, to turbine RT-3, to the pressure reduction valve RV-1 and the ambient temperature – are obtained directly from the plant measurement system.

By combining the above-mentioned BHM and the artificial neural network (details are given in the Supplementary material to this paper), a new hybrid model was developed using Python, specifically the Keras library.[13] Conventional linear and nonlinear models typically require larger datasets and often struggle to capture complex system interactions. In contrast, our hybrid model is more efficient and achieves comparable or improved performance with substantially less data. Although it demonstrates improved prediction accuracy over the deterministic model, its applicability is subject to certain constraints. The hybrid framework is valid only within the operational range covered by the training data and underlying assumptions, which include steady-state and dynamic conditions corresponding to boiler loads. Additionally, the neural network component of this hybrid model cannot account for unmeasured disturbances. The primary purpose of this model is to reduce operating costs and simultaneously lower CO_2 emissions, as quantified using the following equations:

$$M_{\text{HP}} = M_{\text{RT1,in}} + M_{\text{RT2,in}} + M_{\text{RT3,in}} + M_{\text{RV-1,in}} \tag{5}$$

$$M_{\text{MP}} = M_{\text{RT1,out}} + M_{\text{RT2,out}} + M_{\text{RT3,out}} + M_{\text{RV-1,out}} + M_{\text{BFW,MP,NN}} \tag{6}$$

All the following mass flow rates, M_i, are given in tons per hour (t h^{-1}) and are defined as: M_{HP} – required for the high-pressure steam; $M_{\text{RT1,in}}$ – required inlet for the cracked gas turbine;

$M_{RT2,in}$ – required inlet for the propylene turbine; $M_{RT3,in}$ – required inlet for the ethylene turbine; M_{MP} – of the medium-pressure steam header; $M_{RT1,out}$ – of the cracked gas turbine outlet; $M_{RT2,out}$ – of the propylene turbine outlet; $M_{BFW,MP,NN}$ – boiler feed water stream entering the MP header, which is estimated using the ANN.

Eq. (5) defines the steam mass flow in the high-pressure steam header (HP) as the cumulative sum of the inlet mass flows to the three steam turbines and the RV-1(MRV-1,in). Eq. (6) defines the steam mass flow rate in the medium-pressure (MP) steam header as the cumulative sum of the outlet mass flows from the three steam turbines, the outlet of RV-1(MRV-1,out) and the boiler feed water stream entering the MP header. The boiler feed water stream is estimated using the artificial neural network. The total heat output and natural gas (NG) flow rate, are given by the following relations:

$$Q = M_{BFW}(h_L - h_{BFW}) + M_{HP}(h_{SH} - h_L) \tag{7}$$

$$M_{NG} = \frac{Q}{0.85LHV} \tag{8}$$

where Q is the total heat output (MW), M_{BFW} is the mass flow rate of the boiler feed water (t h^{-1}), h_L is the specific enthalpy of the liquid water at operating pressure (kJ kg^{-1}), h_{BFW} is the specific enthalpy of the boiler feed water (kJ kg^{-1}), h_{SH} is the specific enthalpy of the superheated steam leaving the boiler (kJ kg^{-1}), M_{NG} is the mass flow rate of natural gas (kg s^{-1}) and LHV is the lower calorific value of natural gas (MJ kg^{-1}).

Eqs. (7) and (8) quantify the required fuel input for boiler heating and determine the corresponding amount of natural gas needed to provide this thermal energy. In Eq. (8), 0.85 means that 85 % of the energy from the combustion of natural gas is actually transferred to the boiler as useful heat. Eq. (9) defines the operational expenditure, *OPEX*, as the sum of the cost of the required natural gas and the carbon tax associated with the corresponding CO_2 emissions resulting from its combustion:

$$OPEX = M_{NG}\times Pr(\mathrm{NG}) + M_{NG}\times EF(\mathrm{CO_2})\times CTX \tag{9}$$

where Pr(NG) is the price of natural gas (\$·kg^{-1}), $EF(CO_2)$ is the emission factor for CO_2 (kg CO_2·kg^{-1} NG) and CTX is the carbon tax (\$·kg^{-1}).

OPEX is minimized based on the following constraints:

$$|W_{RTi,req} - W_{RTi,NN}| \le 0.01,\ \text{for } i = 1,2,3 \tag{10}$$

$$M_{MP} \ge M_{MP,req} \tag{11}$$

where $W_{RTi,req}$ is the required (or actual) power output of turbine i (MW), $W_{RTi,NN}$ is the predicted power output of turbine i, obtained from the artificial neural network (MW) and $M_{MP,req}$ is the required mass flow rate in the medium-pressure steam header (t h^{-1}).

Eq. (10) states that the discrepancy between the required output of the three turbines and the values predicted by the neural network must be minimized, while Eq. (11) enforces the mass balance condition for the medium-pressure steam line, which states that the incoming steam mass flow must be equal to the medium-pressure steam demand.

The proposed hybrid model integrates a deterministic BHM, which is used to compute the required fuel input based on thermodynamic principles, with an artificial neural network (ANN) module that supplements the system by providing additional data necessary for imposing model constraints.

Parameter estimation

The parameters for this hybrid model of the boiler and the utility system given in Table I, were estimated based on historical operating data from the utility system.

TABLE I. Parameters of the boiler and the utility system

Boiler		Utility system	
M_{HP} / t h^{-1}	169	$T_{out,boiler}$ / °C	465
M_{BFW} / t h^{-1}	178	$p_{out,boiler}$ (bar)	102
h_{BFW} / kJ kg^{-1}	502.4	$M_{RT1,in,S1}$ / t h^{-1}	86.0
h_L / kJ kg^{-1}	1416.4	$M_{RT1,in,S2}$ / t h^{-1}	45.4
h_{SH} / kJ kg^{-1}	3280.1	$M_{RT2,in,S1}$ / t h^{-1}	60.0
Q / MW	132.6	$M_{RT2,in,S2}$ / t h^{-1}	46.3
LHV / MJ kg^{-1}	52.5	$M_{RT3,in}$ / t h^{-1}	22.9
M_{NG} / kg s^{-1}	3	$M_{RV-1,in}$ / t h^{-1}	0.06
M_{HPmax} / t h^{-1}	260	T_{sur} / °C	15
a	0.0126		
b	0.2156		

In addition, in estimating the ANN parameters, the optimization framework was used to identify the optimal operating conditions of the utility system for input into the neural network. These parameters were rescaled by normalizing the input parameters to a dimensionless range between –1 and 1. For each variable, the normalized (optimized) values were computed according to:

$$x_{opt} = 2\frac{x_{in} - x_{min}}{x_{max} - x_{min}} - 1 \tag{12}$$

where x_{in} is the actual input value, and x_{min} and x_{max} represent the lower and upper bounds of the corresponding parameter. This transformation ensures that all parameters are optimized consistently within their feasible range.

After constructing the neural network, the weight matrices were initialized for each layer. Specifically, W_1 and W_2, corresponding to the first and second hidden layers, were generated with dimensions [12×9], while the output layer matrix W_3 was generated with dimensions [5×12]. In addition, bias vectors were created for each layer: c_1 and c_2 for the hidden layers (each containing 12 elements) and c_3 for the output layer (containing 5 elements). Thus, both hidden layers consisted of 12 neurons, whereas the output layer comprised 5 neurons.

For clarity and reproducibility, the complete numerical values of the generated weight matrices (W_1, W_2, W_3) and bias vectors (c_1, c_2, c_3) can be provided upon request.

After the weight and bias matrices were generated, the pre-activation values Z and activation values A were estimated (see Supplementary material, Eqs. (S1) and (S2), respectively). The input values, as previously mentioned, were normalized prior to the calculations.

RESULTS AND DISCUSSION

The results obtained from the hybrid modeling framework demonstrate its capability to accurately simulate the dynamic behavior of the utility system under diverse operating conditions. Fig. 3 illustrates the relationship between operating expenditure (*OPEX*) and two important economic factors: natural gas price (on the left *y*-axis) and carbon tax (on the right *y*-axis). Each variable is shown as a function of its own OPEX range, reflecting its individual impact on system costs.

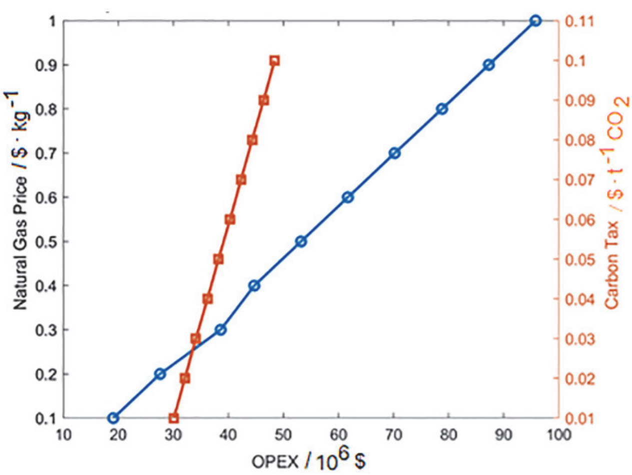

Fig. 3. Correlation between operational expenditure, natural gas price and carbon tax.

Fig. 3 shows that the price of natural gas has a much greater impact on operating expenses than the carbon tax. The trends show a positive linear correlation between *OPEX* and both variables. While the carbon tax curve has a steeper local slope, the natural gas price varies over a much wider range of operating expenditures, implying that natural gas price exerts a greater cumulative influence on *OPEX* over the entire operating window. The natural gas price exhibits a consistent and gradual increase across a wide range of operating expenses, suggesting a stable but cumulative economic burden. In contrast, the carbon tax exhibits higher local sensitivity, suggesting that even small increases in carbon cost policies within certain thresholds can lead to noticeable *OPEX* fluctuations.

In Fig. 4 the effects of cracked gas turbine power output, propylene turbine power output and ethylene turbine power output, on operational expenditure are presented. Fig. 4a shows that increasing the cracked gas turbine output from 7 to 14 MW leads to an almost linear increase in operating costs, from about $ 32.8 million to $ 38.9 million. This indicates that the cracked gas turbine has a significant and direct impact on operating costs, likely because it provides most of the mechanical power in the system. The steady increase indicates a cost-dependent relationship, possibly related to fuel consumption, load conditions, or efficiency degradation at higher loads.

Moreover, Fig. 4b demonstrates a similar trend for the propylene turbine, where operating costs rise from about $ 41.3 million to $ 48.6 million as output increases from 7 to 12 MW. The steeper increase compared to Fig. 4a suggests that the propylene turbine has an even greater marginal cost per MW, possibly due to the particular operating conditions or energy conversion efficiency. This result underlines the importance of carefully managing the output of this turbine to minimize cost impact. Similarly, Fig. 4c demonstrates the relationship between the output of the ethylene turbine and *OPEX*, where the output range is smaller (1.25 to 2.4 MW). *OPEX* increases slightly from around \$ 38.5 million to \$ 39.6 million. While the absolute increase is smaller than in the previous cases, the relatively large increase over a narrow range indicates that even small increases in ethylene turbine output can affect system costs.

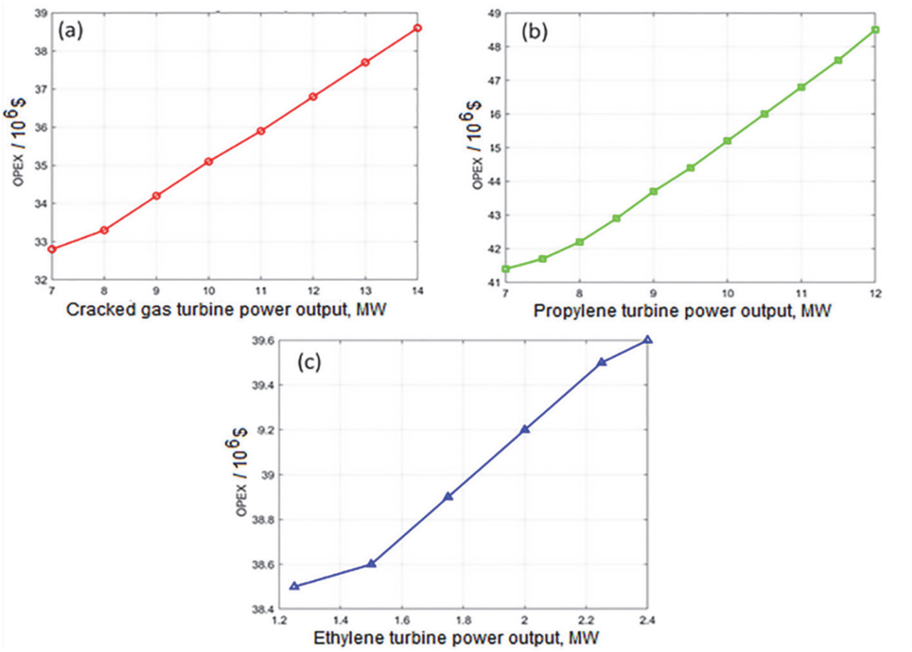

Fig. 4. Effect of: a) cracked gas turbine power output, b) propylene turbine power output and c) ethylene turbine power output, on operational expenditure

CONCLUSION

In this study, a hybrid modeling approach was developed that combines first-principles equations with artificial neural network models to reduce operating costs and lower carbon emissions. The ANN model was trained to predict the required turbine power outputs under different operating conditions. The deviation between the predicted and actual turbine performance served as an important performance measure to evaluate the accuracy of the model. The results show a high agreement between the ANN predictions and the measured data, with low maximum absolute percentage error values for all three turbines. These results confirm the ability of the ANN to effectively capture the nonlinear behavior of steam-driven systems under variable loads. The results also show that the natural gas price has a much larger cumulative impact on operating costs than the carbon tax, primarily due to its broader range of variation within the operating window. While the carbon tax demonstrates a steeper local slope, indicating high sensitivity to incremental changes, the natural gas price trend is more gradual but sustained, suggesting a consistent and growing economic burden. This difference highlights the importance of fuel cost management and diversification strategies, as well as the need to monitor evolving carbon policy thresholds that could trigger sudden increases in operating costs. The cracked gas and propylene turbines show a sharp, near-linear increase in operating costs as output increases, with the propylene turbine showing a greater increase in cost per MW. The ethylene turbine, while operating in a lower range, also has a noticeable impact on OPEX, indicating that even small changes in output can affect system costs. The proposed methodology provides a reliable and efficient framework for optimizing energy performance, predicting fuel consumption and supporting decision-making in large thermal process systems.

NOMENCLATURE

ANN – Artificial neural network
a – Regression parameter adjusted on the basis of the experimental data
BFW – Boiler feed water
BHM – Boiler hardware model
b – Regression parameter adjusted on the basis of the experimental data
C_p – Specific heat of saturated steam (kJ kg^{-1} K^{-1})
CTX – Carbon tax (\$ kg^{-1})
c_i – i = 1,2,3, bias vector
EF(CO_2) – Emission factor for CO_2 (kg CO_2 kg^{-1} NG)
HP – High pressure
h_{BFW} – Specific enthalpy of the boiler feed water (kJ kg^{-1})
h_L – Specific enthalpy of the liquid water at operating pressure (kJ kg^{-1})
h_{SH} – Specific enthalpy of the superheated steam leaving the boiler (kJ kg^{-1})
LHV – Lower calorific value of natural gas (MJ kg^{-1})
M – Steam mass flow rate (t h^{-1})
MINLP – Mixed integer nonlinear programming
MP – medium pressure
M_{BFW} – Mass flow rate of the boiler feed water (t h^{-1})
$M_{BFW,MP,NN}$ – Boiler feed water steam entering the MP header estimated by ANN (t h^{-1})
M_{HP} – Mass flow rate of HP steam (t h^{-1})
M_{HPmax} – Max. steam mass flow rate through the boiler (t h^{-1})
M_{MP} – Mass flow rate of MP steam (t h^{-1})
$M_{MP,req}$ – Required mass flow rate of MP steam (t h^{-1})
M_{NG} – Natural gas mass flow rate (kg s^{-1})

SUPPLEMENTARY MATERIAL

Additional data and information are available electronically at the pages of journal website: https://www.shd-pub.org.rs/index.php/JSCS/article/view/13552, or from the corresponding author on request.

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ИЗВОД

ОПТИМИЗАЦИЈА РАДА СИСТЕМА ПАРЕ У ФАБРИЦИ ЕТИЛЕНА ПОМОЋУ ХИБРИДНОГ МОДЕЛА ВЕШТАЧКЕ НЕУРОНСКЕ МРЕЖЕ И МОДЕЛА ЗАСНОВАНОГ НА ФУНДАМЕНТАЛНИМ ПРИНЦИПИМА

АЛЕКСА МИЛАДИНОВИЋ[1], МИРЈАНА КИЈЕВЧАНИН[2], ЈОВАН ЈОВАНОВИЋ[2], SABLA ALNOURI[3], ВЛАДИМИР СТИЈЕПОВИЋ[1] и МИРКО СТИЈЕПОВИЋ[2]

[1]*Институт за хемију, технологију и металургију, Институт од националног значаја за Републику Србију, Универзитет у Београду, Његошева 12, 11000 Београд,* [2]*Технолошко–металуршки факултет, Универзитет у Београду, Карнегијева 4, 11000 Београд и* [3] *Gas Processing Center, College of Engineering, Qatar University, Doha, Qatar*

У овом раду је развијен модел који комбинује фундаменталне једначине и вештачку неуронску мрежу у циљу смањења оперативних трошкова и емисије CO_2 у оперативним системима фабрике етилена. Вештачка неуронска мрежа може да прецизно предвиди снагу три турбине под различитим оперативним условима са ниском максималном апсолутном грешком, што демонстрира способност мреже да прецизно прикаже нелинеарно понашање система. Економска анализа система је показала да цене природног гаса имају већи, кумулативни утицај на оперативне трошкове од пореза на CO_2 због њихове веће варијабилности. Иако порез на CO_2 има већи непосредан утицај, стални раст цена природног гаса представља дугорочно, економско оптерећење. Ово указује на значај управљања трошковима горива и праћење промена у политици заштите од утицаја CO_2 како би се ублажила нагла повећања оперативних трошкова. Са порастом снаге, оперативни трошкови пропиленске и крек-гас турбине расту готово линеарно, при чему је уочен израженији раст трошкова по мегавату код пропиленске турбине. Етиленска турбина је имала значајан утицај на оперативне трошкове упркос нижем производном капацитету, што указује да чак и мале промене у снази имају утицај на трошкове. Предложена методологија пружа поуздан оквир за енергетску оптимизацију, предвиђање потрошње горива и подршку у доношењу одлука у великим, индустријским процесима.

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