Machine Learning-assisted Prediction and Optimization of Exergy Efficiency and Destruction of Cumene Plant under Uncertainty

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ABSTRACT

Machine Learning (ML)'s growing role in process industries during the digitalization era is notable. This study combines Artificial Neural Networks (ANNs) and Aspen Plus to predict exergy efficiency, exergy destruction, and potential improvements in a cumene plant under uncertain process conditions. An optimization framework, using Particle Swarm Optimization (PSO) and Genetic Algorithm (GA), was developed to enhance exergy efficiency amid uncertainty. Initially, a steady-state Aspen model evaluates exergy efficiency, irreversibility, and potential improvements. The proposed model is transitioned to a dynamic mode, introducing artificial uncertainties into key variables. An ANN model predicts exergy efficiency and exergy destruction under uncertainty. The PSO and GA-based optimization methods improve exergy efficiency and reduce exergy destruction. This work demonstrates the potential real-time application of intelligent methods in plant analysis.

Keywords-exergy analysis; digitalization; industry 4.0; machine learning; process uncertainties

I. INTRODUCTION

Cumene, a key chemical reagent, finds extensive applications in phenol and acetone production, forming the basis for about 98% of acetone and phenol manufacturing [1]. The world's 80% plastic demand is met by phenol and acetone-derived polymers, while about 98% of acetone and phenol production is based on cumene [2-4]. Forecasts indicate a substantial rise in global cumene demand, expected to reach USD 17.63 billion by 2025. To address this demand and enhance product quality while optimizing resource utilization, efforts are focused on exploring efficient cumene production processes. Computational methods play a crucial role in this endeavor, enabling the investigation of various aspects, including design enhancements, yield improvements, process control, and environmental impact [1]. Notable changes in design optimization have led to a 47% reduction in Total Annualized Cost (TAC) through the replacement of conventional distillation columns with reactive distillation and topological changes [5, 6]. Single dividing wall columns have replaced traditional ones, saving up to 18.75% in TAC [5]. Process parameter optimization, utilizing Response Surface Methodology (RSM) and Genetic Algorithm (GA), has achieved higher net present values and yield improvements [5-7]. Plant-wide control structures ensure production stability, with two advanced approaches offering superior performance [8, 9]. Multi-Objective Optimization (MOO) addresses environmental, safety, and economic aspects, optimizing material losses and process safety [14, 15]. Dynamic simulations identify key factors in cumene conversion and downstream distillation column overpressure [16]. The comparative study in [17] highlights intensified processes' economic attractiveness and environmental friendliness.

Exergy analysis is emerging as a prominent approach to enhance energy efficiency in cumene production, with potential applications from other industries [18-23]. Exergy analysis was performed on a cumene production plant utilizing Aspen Plus and MATLAB in [24]. The plant was divided into preheating, reaction, and separation segments, and physical and chemical exergy computations were conducted. The overall plant exergy efficiency achieved an impressive 84.93%.

The integration of machine learning into AI for exergy analysis has been explored in the literature. In [25], a Machine Learning (ML) model was devised to predict the exergy efficiency of a blast furnace. Subsequently, an Artificial Neural Network (ANN) model was developed to forecast exergy efficiency, relying on 11 uncertain process variables. In [26], a combination of Straight Run (SR), GA, and ANN models was employed to evaluate the impact of uncertainty in process conditions and crude composition on furnace exergy efficiency. Similarly, a study involved the development and comparison of Bootstrap Aggregating (bagging) and Random Forest (RF) models for predicting VDU exergy efficiency under uncertain process parameters [24]. Another study delved into the repercussions of process condition uncertainty on the overall exergy efficiency of naphtha reforming, employing an RF model with a Bootstrap Filter (BF) [27]. The present study builds upon the foundation laid in [24], introducing ML-based prediction and optimization concepts to enhance exergy efficiency and minimize exergy destruction. The major contributions of this study are:

- Development of dynamic modeling of the cumene production process through incorporation of uncertainty in a steady state process model and calculation of variations in exergy efficiency and exergy destruction.
- Development of an ANN-based model for the estimation of the process exergy efficiency and destruction.
- Development of an optimization framework based on GA and PSO to achieve higher exergy efficiency of the process.

II. THEORETICAL FUNDAMENTALS

A. Process Description

This study considers the process that involves feed preheating, reactor reactions, and component separation in the depropanizer and benzene columns, as shown in Figure 1. In the Preheating and Reactive segment, the process involves warming propene, benzene feeds, and recycled benzene from the separation section using heat from the reactor's outlet stream (Reac-Out). Propene is heated by the heat exchanger (E-2), while benzene feeds and recycled benzene are warmed by a separate heat exchanger (E-1). After preheating, the streams are blended to reach the required reaction temperature. Then, a furnace (H-1) further raises the temperature before introducing the stream into the reactor (R-1) for alkylation and transalkylation reactions. The reactor effluent's heat is exchanged with incoming feeds in heat exchangers (E-3 and E-2) for energy efficiency. Effluent temperature is reduced to the propene column temperature via a Waste Heat Boiler (WHB). Moving to the Separation phase, the reactor effluent enters the depropanizer column for component separation based on boiling points. The upper output provides unreacted propylene and inert propane, while the lateral output supplies fuel gas. The lower stream (Sep-1 Bottom) from the depropanizer column containing benzene, cumene, and DIPB (diisopropylbenzene), exchanges heat with other process streams using the heat exchanger (E-1) before entering the benzene column. The unreacted benzene is the upper output in the benzene column, while cumene and DIPB comprise the lower output. DIPB-containing lower stream is treated as waste, and cumene is collected from the upper part of the cumene recovery column.

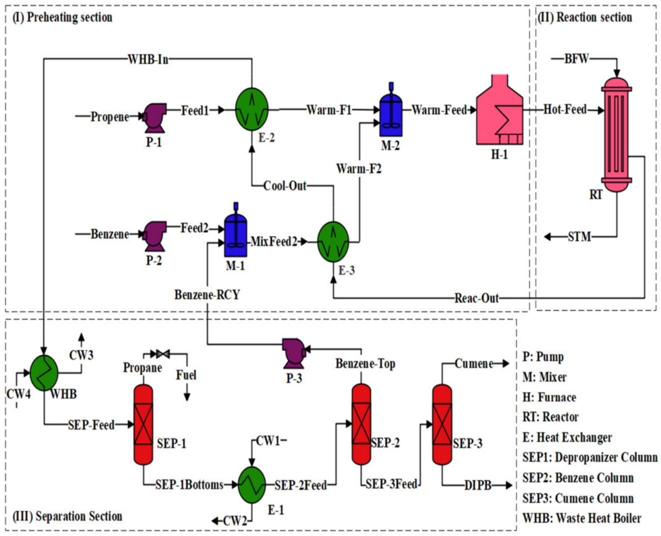

Fig. 1. Cumene process flow diagram.

B. Exergy Performance Indicators

Exergy analysis is a fundamental tool utilized in assessing the thermodynamic performance of a system. It encompasses the evaluation of system exergy efficiency and exergy destruction. Irreversibility serves as a quantification of the exergy destroyed within a processing unit, measured by the disparity between exergy inflows and outflows from the unit streams, as defined by:

$$I = \dot{Ex}_{destroyed} = \sum \dot{Ex}_{in} - \sum \dot{Ex}_{out} \quad (1)$$

The irreversibility of a distillation column, on the other hand, is determined by (2) which considers the heat duty of the reboiler and condenser (Q_r and Q_c) as well as the respective temperatures (T_r and T_c).

$$I = \dot{Ex}_{destroyed} = \sum \left(\dot{Ex}_{feed} + \left(1 - \frac{T_o}{T_r}\right) Q_r\right) - \sum \left(\dot{Ex}_{Product} + \left(1 - \frac{T_o}{T_c}\right) Q_c\right) \quad (2)$$

The concept of exergy efficiency, on the other hand, gauges the degree of system proximity to an ideal state. In reversible conditions, exergy efficiency denotes the system's effectiveness relative to optimal performance. While various exergy efficiency formulas exist in the literature, the widely adopted and straightforward approach is the universal exergy efficiency, which represents the ratio of useful exergy output to input, as expressed in (3):

$$\varphi_{universal} = \frac{E_{out}}{E_{in}} \quad (3)$$

This metric provides a concise measure of system performance and aids in assessing the effectiveness of energy utilization within the analyzed process.

C. Artificial Neural Networks

ANNs encompass a suite of algorithms that replicate human brain operations, enabling quantitative data interpretation through training/learning procedures. Comprising three layer types -input, hidden, and output- an ANN incorporates interconnected neurons to model intricate and nonlinear functions. The input layer receives external environmental information or features, while neurons within the hidden layers extract system-related data. Neurons process inputs via predetermined activation functions, employing associated weights for calculations. For each input variable, the neuron's output is determined through a nonlinear amalgamation of inputs (x_1, x_2, ..., x_n) and corresponding weights (w_1, w_2, ..., w_n). Conclusively, the output neuron layer generates and showcases the network's ultimate outputs, derived from prior-layer neuron processing activities.

III. METHODOLOGY

This study employed an integrated environment consisting of Aspen Plus and MATLAB to conduct an exergy analysis of a cumene producing plant. The following steps were followed:

1. The EXERGYFL property set of Aspen Plus was utilized to calculate the physical energy of the system.
2. MATLAB was integrated with Aspen Plus through their interface to determine the chemical exergy of the process.
3. The cumene production process was divided into sections treated as control volumes. The exergy entering each section was computed by considering the streams entering the control volume, while the energy leaving the section was considered as the outlet energy of the streams.
4. Irreversibility equations were utilized to calculate the values of irreversibility for each section.
5. The exergy efficiency, which represents the potential for exergetic improvement, was calculated based on the obtained exergy analysis results.
6. Data sets for ANN training and testing were generated by introducing artificial uncertainties of ± 10% in the steady state values by integrating MATLAB and Aspen PLUS. The 80% of the data were used for training the ANN and 20% for testing.
7. Finally, an optimization framework based on GA and PSO was developed for achieving higher exergy efficiency and lower exergy destruction of the process.

IV. RESULTS AND DISCUSSIONS

This section presents the results and discussion of the prediction of exergy destruction and exergy efficiency in the cumene production process using an ANN. The ANN model was trained and validated using a comprehensive dataset. The trained model was then utilized to predict the exergy efficiency and destruction of the process for various operating conditions. The results obtained from the ANN predictions are analyzed and compared with the actual exergy analysis data to assess the accuracy and reliability of the model. The implications and significance of the findings are discussed, along with potential areas for process optimization and improvements based on the predicted exergy values.

In this study, the initial step involves performing a steady-state exergy analysis of a cumene production plant, achieved through an integrated framework of Aspen Plus and MATLAB. Subsequently, an uncertainty analysis of the cumene production plant is conducted within an integrated setting encompassing Aspen Plus, MATLAB, and Microsoft Excel's Aspen Simulation Workbook. The physical exergy is calculated with the use of MATLAB and Aspen Plus interface.

A. Exergy Efficiency

The overall plant exergy efficiency was calculated with (4) and its value is 84.89. In (4), E_{out} is the overall total exergy out from the system and E_{in} is the overall total exergy entering the system.

$$\eta = \frac{E_{out}}{E_{in}} \quad (4)$$

For the analysis of a cumene production plant, 9 input variables which are affecting the production and the efficiency of the cumene plant are selected. In these 9 input variables, an uncertainty of ± 10% is introduced for the analysis (Table I). These input variables include the entering flow rates of propylene and benzene, the outlet pressures of Pump-1 and Pump-2, the heater outlet temperature, the mole fractions of propylene and propane, and the outlet pressure and temperature of the Heat Exchanger-1. The data distribution of all the input variables is shown in Figures 2-10.

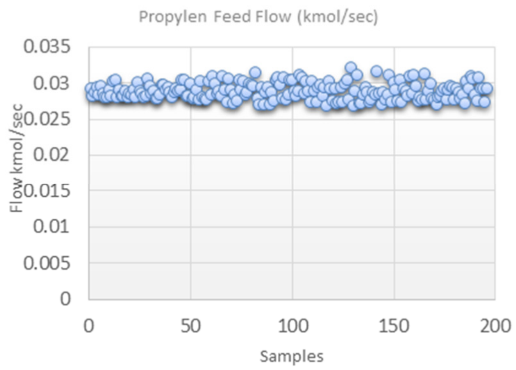

Fig. 2. Propylene feed flow vs number of samples.

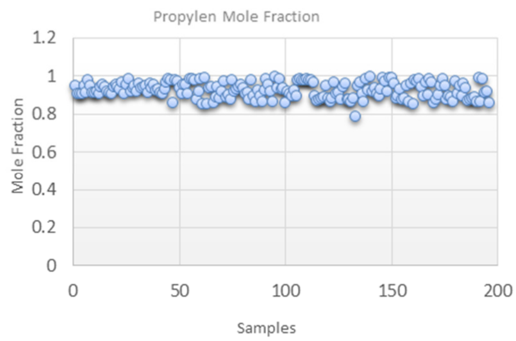

Fig. 3. Propylene µole fraction vs number of samples.

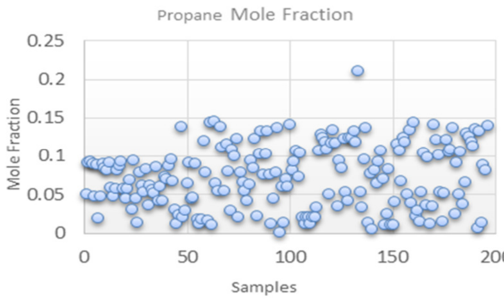

Fig. 4. Propane mole fraction vs number of samples.

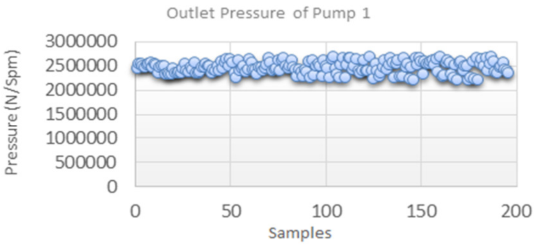

Fig. 5. Outlet pressure of Pump-1.

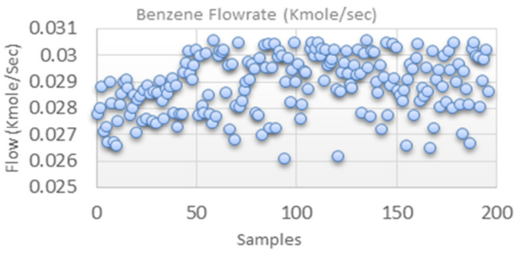

Fig. 6. Benzene flow rate vs number of samples.

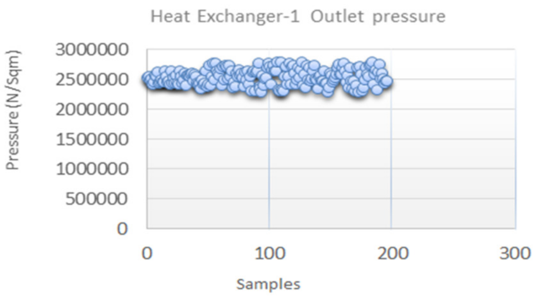

Fig. 7. Heat Exchanger-1 outlet pressure vs number of samples.

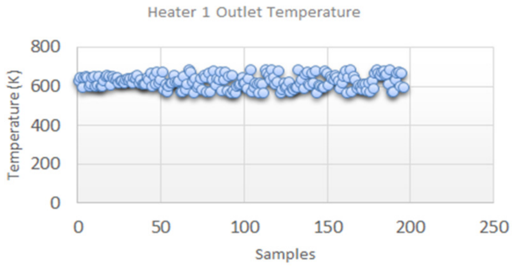

Fig. 8. Heater-1 outlet temperature vs number of samples.

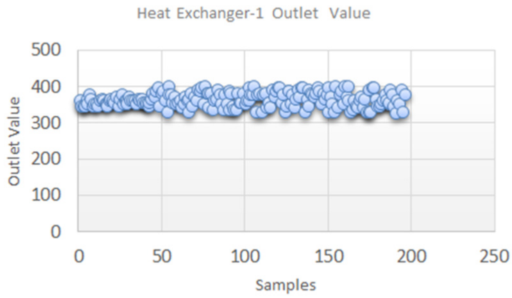

Fig. 9. Heat Exchanger-1 outlet values vs number of samples.

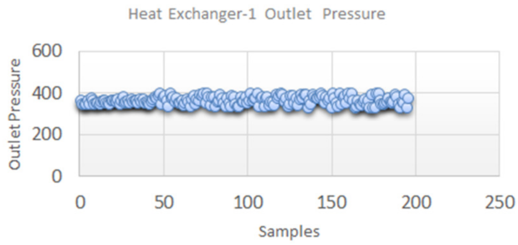

Fig. 10. Heat Exchanger-1 outlet pressure vs number of samples.

Table I shows the original values of the process conditions and their corresponding modified values by inserting uncertainty. From Table I we can see the effect of the uncertainty on the overall exergy efficiency of the cumene plant. For instance, in case of the heater outlet temperature at steady state and after introducing the uncertainty, there is a significant difference between the reported values. For instance, the steady state heater outlet temperature is 623.15 K and in case 1 and case 2 it is 640.79 K and 592.61 K, respectively.

TABLE I. ORIGINAL AND MODIFIED (WITH UNCERTAINTY) INPUT AND OUTPUT PROCESS VARIABLES

	Variable	**Values**	**Case 1**	**Case 2**	**Case 3**	**Case 4**	**Case 5**
Input	Propylene flowrate	0.029	0.028251	0.028686	0.029324	0.028262	0.029537
	Propylene mole fraction	0.95	0.9082	0.90649	0.909245	0.95209	0.911715
	Propane mole fraction	0.05	0.0918	0.09351	0.090755	0.04791	0.088285
	Outlet pressure of Pump-1	2451662.5	2537716	2557084	2499960	2472011	2528890
	Benzene flowrate	0.027	0.028006	0.028806	0.027125	0.027272	0.026719
	Outlet pressure of Pump-2	2533125	2548070	2494622	2519446	2420148	2451305
	Heater-1 outlet temperature	623.15	640.7851	592.6157	644.524	649.4469	640.0374
	Heat Exchanger-1 outlet temperature	363.15	347.1714	346.5177	347.5709	363.9489	348.5151
	Heat Exchanger-1 outlet pressure	245166	246612.5	241439.5	243842.1	234231.6	237247.1
Output	Overall plant exergy efficiency	84.888	84.79163	84.95358	84.78349	84.80763	84.806

To carry out the analysis of cumene production plant we developed a data set consisting of 200 samples, with changes in the selected 9 input variables. From physical and chemical exergy we found the total exergy of each piece of equipment and then with these values we found the overall plant exergy efficiency. After calculating all the respective values, MATLAB environment was used to develop the ANN model. The model has 5 hidden layers with 18, 13, 11, 13, and 18 neurons, respectively. The utilized model training method was Levenberg-Marquardt. The values of RMSE, MSE, and R^2 of the model are 0.115, 0.0133, and 0.1466, respectively. Figure 11 shows the training state of the model. The training R^2 value is 0.996. After training the ANN model, for testing we gave the input data to the ANN for predicting the output against those values. Figure 12 shows the result. Figure 13 is a regression graph of the ANN model predicted versus the targeted values of exergy efficiency. The testing R value is 0.923. Figure 14 shows the performance of the ANN model in the prediction of the targeted Aspen model values.

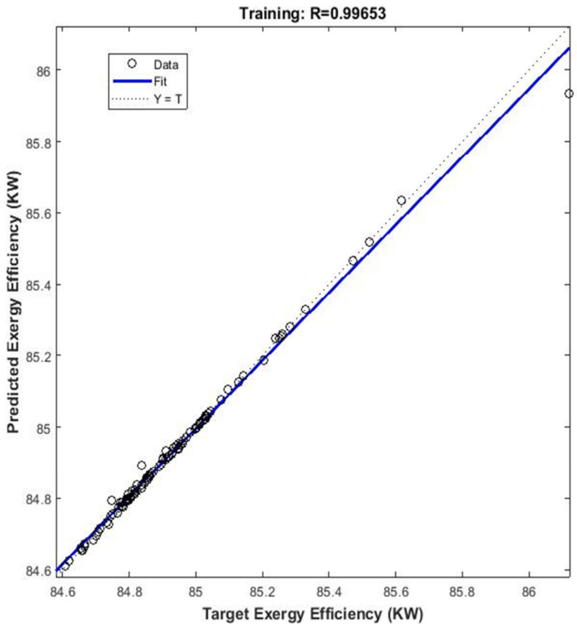

Fig. 11. Performance of the ANN model on the training data for the prediction of exergy efficiency.

To boost the exergy efficiency of the cumene production process, PSO and GA algorithms are employed, utilizing a trained ANN model for optimization under uncertainty. The exergy efficiency comparison is detailed in Table II, encompassing the SA, GA, and PSO models. Figures 14 and 15 illustrate the exergy efficiency disparities among the models. The SA model, an unoptimized Aspen first-principle model under uncertainty, exhibits lower exergy efficiency compared to GA and PSO models. For example, in data sample 1, the SA model achieves 84.89% exergy efficiency, while the GA and PSO optimizations result in 89.46% and 89.54%, respectively. Similar trends are observed in data sample 2, with the SA model at 85.47% and the GA and PSO optimizations reaching 86.09% and 88.20%, respectively.

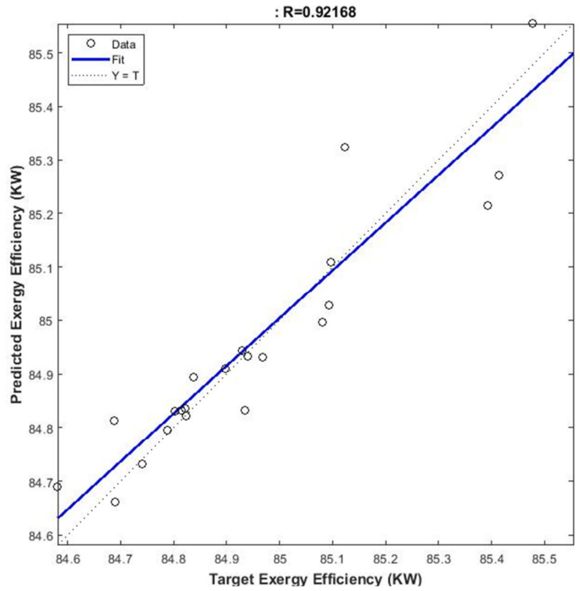

Fig. 12. Performance of the ANN model on the testing data for the prediction of exergy efficiency.

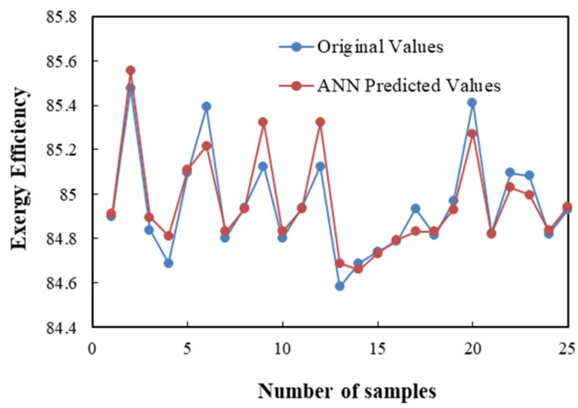

Fig. 13. Performance of the ANN model vs the number of samples.

TABLE II. EXERGY EFFICIENCY COMPARISON

Data sample	Exergy efficiency (%)		
	SA	GA-optimized	PSO-optimized
1	84.89	89.46	89.54
2	85.47	86.09	88.20
3	84.83	89.49	89.66
4	84.68	89.72	89.81
5	85.09	86.22	86.26
6	85.39	89.24	89.54
7	84.80	88.95	89.54
8	84.93	89.29	89.57
9	85.12	89.47	89.62
10	84.80	88.96	88.97

B. Exergy Destruction

Again, we created a dataset with 200 samples with changes in the selected 9 input variables. From physical and chemical exergy, we found the total exergy of each piece of equipment and with these values we find out the overall plant exergy destruction.

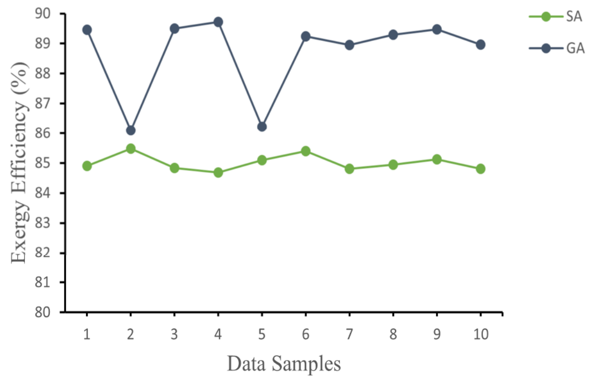

Fig. 14. Comparison of SA and GA exergy efficiency.

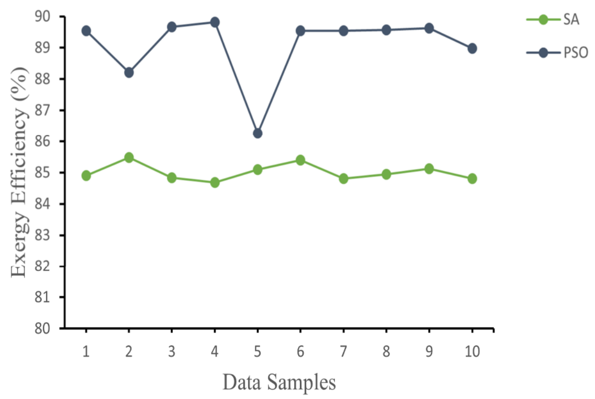

Fig. 15. Comparison of SA and PSO exergy efficiency.

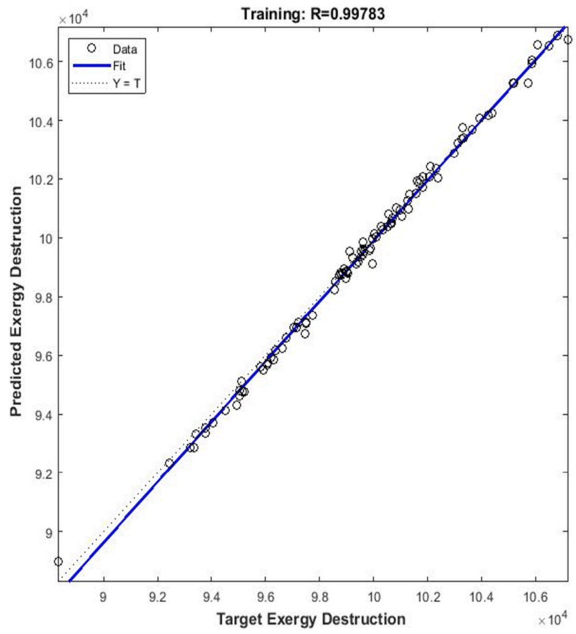

Fig. 16. Performance of the ANN model on the training data for the prediction of exergy destruction.

After calculating all the respective values, the ANN model was constructed in MATLAB. The model has 5 hidden layers with 18, 18, 12, 18, and 18 neurons. The Levenberg-Marquardt training method was utilized. The values of RMSE, MSE, and R^2 of the model are 1.4790e+03, 2.1875e+06, and 0.8930, respectively. Figure 17 shows the training state of the model. The training R value is 0.998.

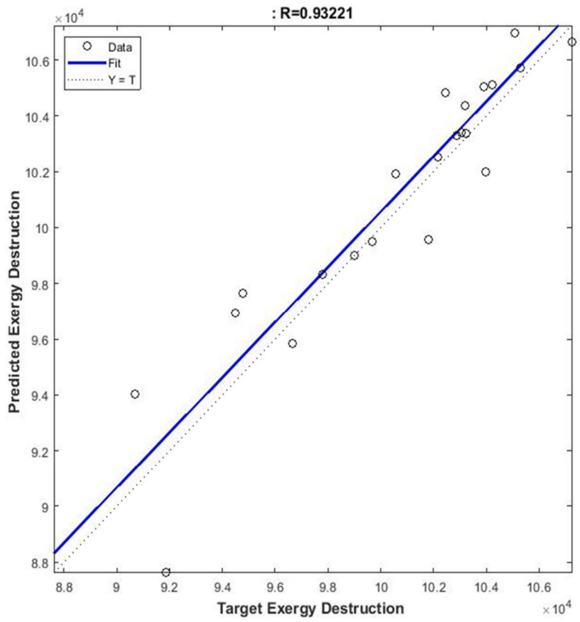

Fig. 17. Performance of the ANN model on the testing data for the prediction of exergy destruction.

Figure 18 shows a regression graph of the ANN model predicted exergy destruction values versus the targeted values. The testing R-value is 0.932. Figure 18 shows how efficient the ANN model is for the prediction of the targeted values.

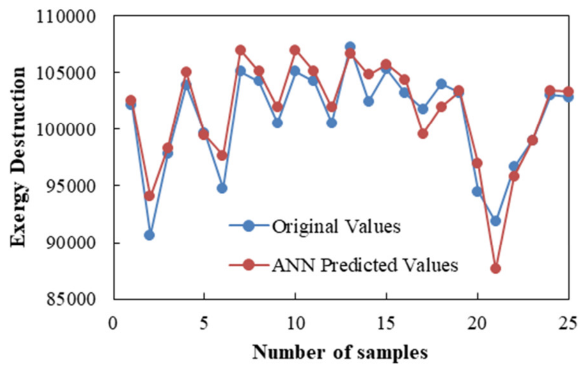

Fig. 18. Performance of the ANN model on the testing data for the prediction of exergy destruction.

To optimize the process of cumene production exergy destruction, PSO and GA algorithms were used with the trained ANN model for surrogate optimization under uncertainty. The comparative exergy destruction analysis is shown in Table III. Figures 19 and 20 show the exergy destruction differences between the SA, GA, and PSO models. It can be seen that the SA model, representing the initial unoptimized Aspen first-principle modeling under uncertainty, yields higher exergy destruction values than the GA and PSO models.

TABLE III. EXERGY DESTRUCTION COMPARISON

Data sample	Exergy destruction (%)		
	SA	GA-optimized	PSO-optimized
1	104236.21	94039.73	93917.13
2	100564.41	89896.23	89832.06
3	97807.401	77742.91	77374.90
4	103897.21	78950.98	78461.67
5	99689.17	92298.68	92159.99
6	94773.92	88431.85	88415.37
7	105077.15	81670.35	81332.63
8	104235.50	94178.04	93917.13
9	100564.37	90241.66	89832.06
10	105077.29	82050.40	81332.63

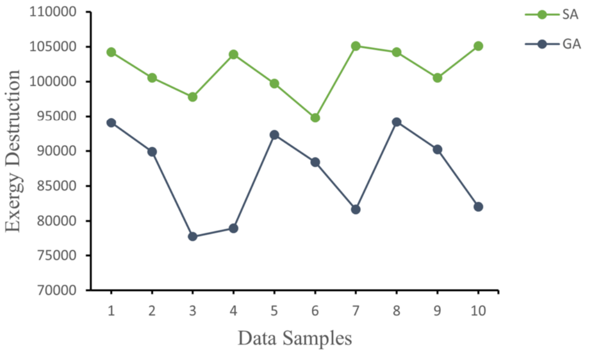

Fig. 19. Comparison of SA and GA exergy destruction.

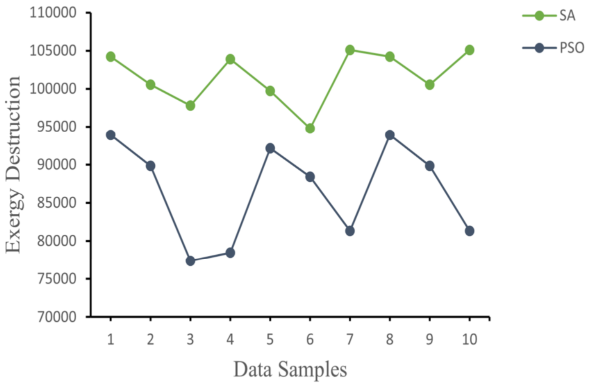

Fig. 20. Comparison of SA and PSO exergy destruction.

V. DISCUSSION

The current study assessed overall plant exergy efficiency in cumene production, achieving a value of 84.89%. With 9 key input variables under ± 10% uncertainty, visualized in Figures 2-10. The data distribution highlighted variable impact. A dataset of 200 samples was constructed. The 5-layer ANN model with Levenberg-Marquardt training in MATLAB, showed robust performance (RMSE: 0.115, MSE: 0.0133, R^2: 0.1466). PSO and GA optimizations enhanced exergy efficiency, surpassing the unoptimized Aspen model, as evidenced in Table II and Figures 14-15 across various data samples.

For the cumene production plant's uncertainty analysis, the MATLAB-built ANN efficiently predicted the exergy destruction. The training results, illustrated in Figure 16, showed a high correlation (R = 0.998), with the testing results displaying the effectiveness of the model (Figure 17, R-value: 0.932). PSO and GA optimizations, outlined in Table III and Figures 19-20, consistently outperformed the unoptimized Aspen model (SA), achieving reduced exergy destruction values across different data samples.

VI. CONCLUSION

In this study, steady-state exergy analysis of a cumene production plant was performed using Aspen Plus and MATLAB. Nine input variables influencing production and exergy destruction were selected for uncertainty analysis. An optimization framework with Genetic Algorithm (GA) and Particle Swarm Optimization (PSO) was developed to enhance exergy efficiency under ± 10% uncertainty. The analysis involved 200 data samples with variations in the 9 input variables. An ANN model with 5 hidden layers was created using Levenberg-Marquardt training. The model showed RMSE and MSE values of 0.115 and 0.0133, respectively, with a correlation coefficient of 0.92 for predicting exergy efficiency and 0.93 for exergy destruction. Both the GA and PSO-based frameworks outperformed the non-optimized model by increasing exergy efficiency and decreasing exergy destruction.

Utilizing the Artificial Neural Network (ANN), the research underscores the transformative potential of digital tools for real-time prediction of exergy efficiency and destruction, redefining process optimization and control. The current study introduces a sustainable optimization framework, employing GA and PSO for enhanced energy efficiency in manufacturing processes.

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