



MULTI-OBJECTIVE OPTIMIZATION OF HEAT-INTEGRATED REACTIVE
DISTILLATION ALTERNATIVES FOR FURFURAL AND ELECTRICITY CO-
PRODUCTION BY MACHINE LEARNING-BASED SURROGATE MODEL



By
Mr. Patcharapuek PATTARAMANON

A Thesis Submitted in Partial Fulfillment of the Requirements
for Master of Engineering CHEMICAL ENGINEERING
Department of CHEMICAL ENGINEERING
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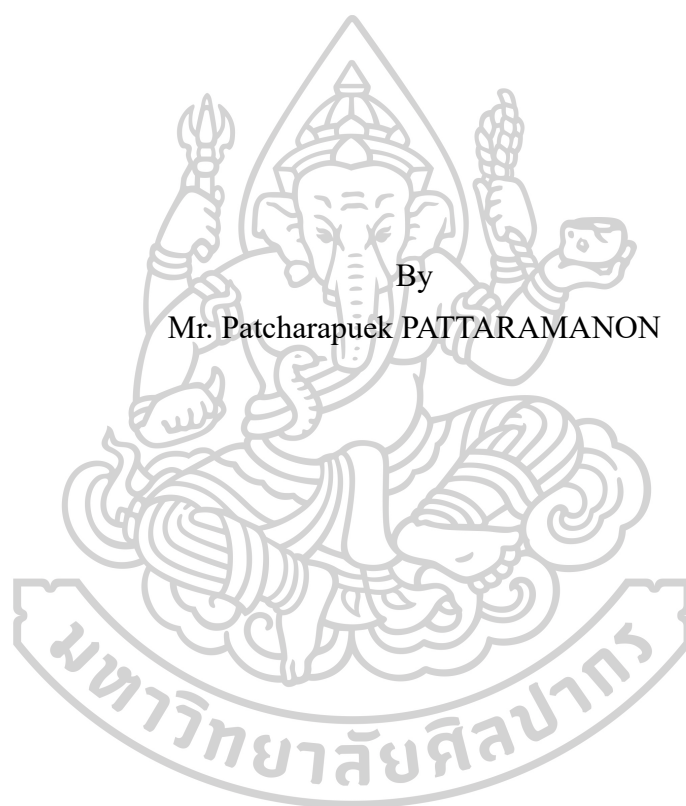
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Title	Multi-objective optimization of heat-integrated reactive distillation alternatives for furfural and electricity co-production by machine learning-based surrogate model
By	Mr. Patcharapuek PATTARAMANON
Field of Study	CHEMICAL ENGINEERING
Advisor	Assistant Professor Nutchapon Chotigkrai
Co Advisor	Assistant Professor Choowong Chaisuk

Faculty of Engineering and Industrial Technology, Silpakorn University in
Partial Fulfillment of the Requirements for the Master of Engineering

..... (Assistant Professor Arunsri Leejeerajumnean)	Dean of Faculty of Engineering and Industrial Technology
--	--

Approved by

..... (Assistant Professor Veerayut Lersbamrungsuk)	Chairperson
--	-------------

..... (Assistant Professor Nutchapon Chotigkrai)	Advisor
---	---------

..... (Assistant Professor Choowong Chaisuk)	Co Advisor
---	------------

..... (Associate Professor Worapon Kiatkittipong)	Committee
--	-----------

..... (Associate Professor Amornchai Arpornwichanop)	External Examiner
---	-------------------

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For efficient biomass utilization, the furfural and electricity co-production are investigated. In this study, the process of furfural production via heat-integrated reactive distillation (HIRD) consist heat pump-assisted reactive distillation (HPA-RD) and different pressure thermally coupled reactive distillation (DPTC-RD) were applied to furfural production. Multi-objective optimization (MOO) was performed to identify suitable process configuration. Moreover, Adaptive Latin hypercube sampling was selected to develop machine learning (ML) model. Multi-layer perceptron (MLP) models were developed to predict each objective functions separately consist total annual cost (TAC), total revenues, and CO₂ emissions. For MOO, non-dominated sorting genetic algorithm II (NSGA-II) and technique for order preference by similarity to ideal solution (TOPSIS) were employed to find Pareto front and optimal solutions. The MLP models demonstrated high predictive performance, with 10-folds cross validation of all models exceed 0.98 for R² and MAPE lower than 5%. DPTC-RD consistently outperforms HPA-RD across single- and MOO, offering better trade-offs among TAC, revenue, and CO₂ emissions. While HPA-RD benefits from energy integration, DPTC-RD shows greater flexibility and is identified by TOPSIS as the superior overall configuration. Biomass feed size is the most influential factor affecting TAC, revenues, and CO₂ emissions, while acetic acid concentration and biomass split also significantly effect on economic and environmental outcomes. Column design variables such as diameter and reactive stages have greater impact than operating conditions for increase revenues. DPTC-RD consistently achieves stronger economic performance than HPA-RD across all optimization objectives, reaching the highest revenues of \$35,004,229 per year. Under the maximum revenues scenario, both systems achieve a 6-year discounted payback period (DPP), although DPTC-RD attains a higher NPV of \$251,588,568, while HPA-RD reaches \$248,397,143. In multi-criteria decision-making, DPTC-RD performs especially well, achieving a 16.74% IRR, an 8-year DPP. Key cost contributors include biomass feed and the CHP unit, which represents the largest portion of total cost. As a result, DPTC-RD provides a more favorable balance among investment cost, profitability, and emissions, confirming it as the more resilient and economically advantageous configuration for furfural production.

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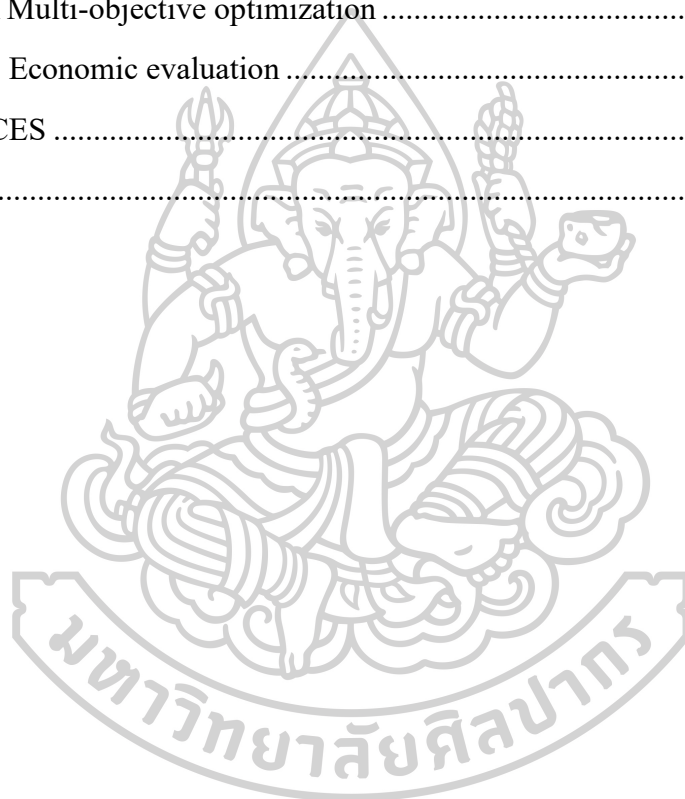
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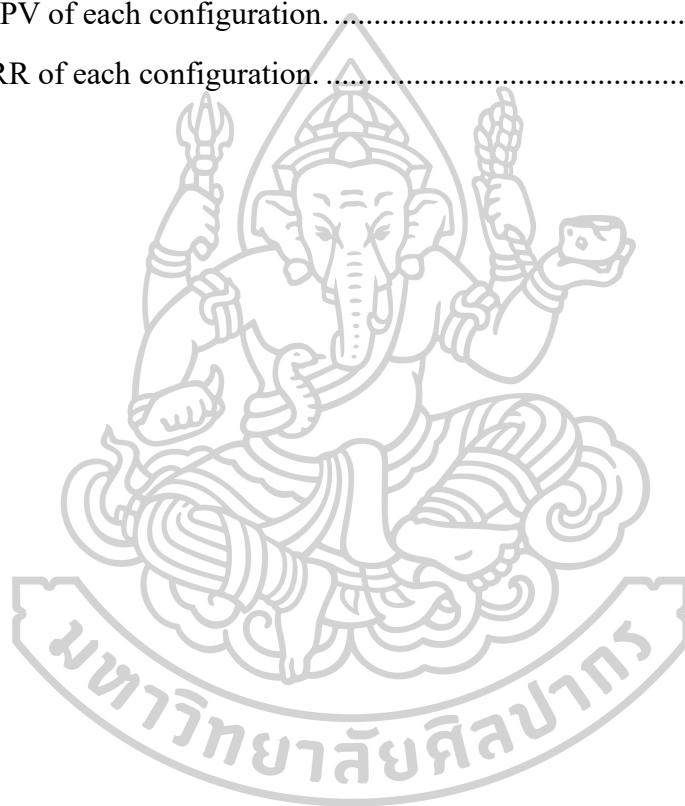
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LIST OF ABBREVIATIONS

5-HMF	5-hydroxymethylfurfural
CHP	Combined heat and power
CS	Corn stover
CV	Cross validation
DPP	Discounted payback period
DPTC-RD	Different pressure thermally coupled reactive distillation
FPM	First-principles modeling
HIRD	Heat-integrated reactive distillation
HPA-RD	Heat pump-assisted reactive distillation
HPC	High pressure column
IRR	Internal rate of return
LHS	Latin hypercube sampling
LPC	Low pressure column
MAPE	Mean absolute percentage error
ML	Machine learning
MLP	Multi-layer perceptron
MOO	Multi-objective optimization
NPV	Net present value
NRTL	Non-random two liquid
NSGA-II	Non-dominated sorting genetic algorithm II
ORC	Organic Rankine cycle
PI	Process intensification
R123	2,2-Dichloro-1,1,1-trifluoroethane
R ²	Coefficient of determination
RD	Reactive distillation
SB	Sugarcane bagasse
SD	Standard deviation

SHAP	SHapley Additive exPlanations
TAC	Total annual cost
TCI	Total capital investment
TOPSIS	Technique for order of preference by similarity to ideal solution
WS	Wheat straw



Chapter 1 Introduction

1.1 Motivation

In 2019, fossil fuels such as natural gas, coal, and oil accounted for approximately 66.3% of the world's total energy consumption [1]. The combustion of these non-renewable fuels releases substantial amounts of greenhouse gases, thereby exacerbating global climate change [2]. Transitioning toward renewable and sustainable energy systems is therefore essential to mitigate environmental impacts. Consequently, biomass has emerged as a promising renewable energy source due to its carbon-neutral nature and versatility. Biomass can be transformed into a variety of energy carriers such as biogas, bio-oil, and hydrogen through thermochemical and biochemical conversion processes [3, 4].

Furfural stands out as one of the top 30 value-added chemicals derived from lignocellulosic biomass [5]. It serves as a platform chemical for the synthesis of a wide range of industrial products, including resins, solvents, biofuel additives, and pharmaceuticals [6]. However, conventional furfural production is highly energy-intensive due to the azeotropic behavior of the furfural-water mixture, which requires a complex separation process [7]. Therefore, a crucial step in improving the sustainability of biomass-based chemical manufacture is decreasing the energy intensity of furfural production, such as through process intensification (PI) and heat integration.

However, the chemical process model often occurs with some error due to the limitation of the model. The machine learning (ML) model was a powerful tool for capturing complex chemical processes and effective for exploration in infeasible domains for optimization frameworks [8]. Moreover, ML models enable rapid evaluation of process alternatives, significantly reducing computational time while maintaining predictive accuracy [9].

1.2 Objective

Machine learning-based multi-objective optimization framework for the co-production of furfural and electricity from lignocellulosic biomass through heat-integrated reactive distillation to enhance both economic feasibility and environmental sustainability by minimizing total annual cost and CO₂ emission while maximizing product yield.

1.3 Scope

1. Process simulation for furfural and electricity production consists of four sections: biomass pretreatment, combined heat and power (CHP), organic Rankine cycle (ORC), and furfural production via heat-integrated reactive distillation (HIRD) by Aspen Plus V14.
2. Multi-objective optimization (MOO) using ML as a surrogate model to predict objective functions.
 - 2.1. Training the ML models by adaptive Latin hypercube sampling (LHS).
 - 2.2. Objective functions of this MOO comprise minimizing total annual cost (TAC) and CO₂ emissions and maximizing total revenues.
 - 2.3. Non-dominated sorting genetic algorithm II (NSGA-II) and technique for order of preference by similarity to ideal solution (TOPSIS) were selected to find the Pareto front and select the optimal solution, respectively.

3. ML models interpretation by the SHapley Additive exPlanations (SHAP) library for analysis of the impact of features on objective functions.
4. Economic evaluation by using net present value (NPV), internal rate of return (IRR), and discounted payback period (DPP) as indicators for comparison of each configuration.

1.4 Contribution

This research contributes to reducing energy consumption in furfural production and enhancing biomass valorization for renewable energy generation, thereby improving overall process profitability. Furthermore, it aims to decrease computational time within complex MOO frameworks by employing ML techniques integrated with adaptive LHS.



Chapter 2 Literature Review

2.1 Furfural production

The conventional furfural production process, first developed by the Quaker Oats Company in 1922, generally involves the acid-catalyzed hydrolysis of hemicellulose-rich lignocellulosic biomass into pentosans, followed by their dehydration to furfural in an aqueous medium [7]. This reaction is typically catalyzed by mineral acids such as sulfuric acid and carried out at temperatures between 153°C and 240°C [6]. The process, which can operate in either batch or continuous mode, often results in relatively low furfural yields (approximately 50%) due to undesirable side reactions [7]. The furfural is recovered and purified commonly through energy-intensive distillation processes, which are complicated by the presence of large amounts of water and the formation of a furfural-water azeotrope [10]. Consequently, the conventional process is operated with low conversion efficiency, high energy consumption during purification, and the generation of acidic waste streams [10].

PI offers a promising approach to overcoming the inherent limitations of conventional furfural production, which is typically associated with high energy consumption and low product yields [10-12]. Reactive distillation (RD), which integrates the reaction and separation steps within a single unit, can significantly reduce both capital and operating costs [11, 12]. Furthermore, RD enhances product yield by continuously separating furfural from the reaction medium, thereby minimizing side reactions [13]. However, RD requires substantial heating energy and high-pressure steam in the reboiler, as it typically operates at around 10 bar to achieve the desired reaction temperature [11].

2.2 Heat integrated reactive distillation

The implementation of heat-integrated distillation columns is motivated by the necessity to address the substantial energy consumption inherent to conventional distillation—the primary separation operation in the chemical industry, responsible for an estimated 3% of world energy usage [14, 15]. Conventional distillation suffers from thermodynamic inefficiency because heat is typically supplied at the reboiler (high temperature) and rejected at the condenser (low temperature), where the recovered thermal energy is often too low to be reused within the unit, leading to energy degradation [14]. Therefore, the core rationale for heat integration is to significantly enhance energy efficiency, reduce reliance on external energy inputs, and facilitate the transition from fossil fuel-based thermal energy to mechanical work (electrification) in alignment with decarbonization goals [15, 16]. Among the critical energy-efficient advancements are heat pump-assisted distillation technologies, which use mechanical compression to recover and reuse heat [14]. For example, in a vapor recompression column, overhead vapor is compressed to a higher temperature so it can provide the heat required by the reboiler [16]. This technique offers large energy savings, particularly beneficial for separating close-boiling mixtures. The different pressure thermally coupled column further intensifies energy recovery [14, 16]. This arrangement operates the stripping and rectifying sections at different pressures—the stripping section at a lower pressure and the rectifying section at a higher pressure to create a temperature differential [14]. Vapor from the low-pressure stripping section is compressed before entering the high-pressure rectifying section, allowing heat exchange between the hot rectifying vapor and the cold stripping liquid throughout

the column length. A major advantage of different pressure thermally coupled over heat pump-assisted is the requirement for a lower compression ratio because the compressor only operates across the internal temperature difference, not the entire column range, potentially reducing the compressor duty [16]. Consequently, heat integration structures are essential for achieving significant reductions in energy consumption, leading to potentially over a 50% reduction in total annualized costs and increasing the substitution of thermal energy with electrical power [15, 16].

For instance, Wiranarongkorn et al. [17] study conducts an energy analysis and life cycle assessment comparing three integrated biorefinery process scenarios for the co-production of furfural and 5-hydroxymethylfurfural (5-HMF) from sugarcane bagasse: conventional RD and heat pump-assisted reactive distillation (HPA-RD). The heat pump significantly enhanced thermodynamic performance, increasing the overall energy efficiency of the proposed process to a maximum of 35.5%. Li et al. [18] proposed a novel different pressure thermally coupled reactive distillation (DPTC-RD) process for the synthesis of isoamyl acetate via esterification, utilizing a steady-state model developed in Aspen Plus. Economic optimization demonstrated that the DPTC-RD design offers significant efficiency gains, achieving a 39.65% saving on operating cost and a 1.25-19.05% reduction in TAC when the payback period ranges from five to ten years, compared to conventional methods.

2.3 Integrated biorefinery processes

Integrated biorefinery processes offer significant advantages in improving energy efficiency and optimizing resource utilization. By coupling various biorefinery subsystems such as furfural and 5-HMF production with heat and power generation, waste energy can be effectively recovered and reused [19]. Furthermore, integrated approaches facilitate comprehensive biomass valorization by converting key components, including hemicellulose and cellulose, into high-value products, thereby minimizing waste generation and enhancing overall process efficiency [20, 21].

Integrated biorefineries also demonstrate enhanced economic and environmental performance [22]. Techno-economic analyses have shown that co-production of multiple value-added products such as furfural, 5-HMF, ethanol, and lignin can diversify revenue streams and enhance the overall economic feasibility of biorefinery operations. This approach frequently results in a higher IRR when compared to single-product facilities [19, 20]. Furthermore, the decrease in external energy requirements, particularly those derived from fossil fuels, leads to notable environmental advantages, including a lower global warming potential and a reduction in other negative environmental impacts [17]. Consequently, this integrated biorefinery approach not only optimizes resource utilization and energy efficiency but also promotes a more sustainable and economically viable pathway for the production of bio-based chemicals and fuels.

2.4 Integration of Machine Learning with first-principles modeling

The integration of ML with first-principles modeling (FPM) offers significant potential for addressing complex processes. While FPM offers a mechanistic understanding, it can be limited by the difficulty in characterizing thermodynamics, reaction kinetics, and mass transfer, often resulting in computationally expensive models [8]. ML model offers a powerful alternative or supplement by extracting patterns and correlations directly from data, without needing explicit underlying

mechanisms [9]. These models offer several advantages, including faster computation, enhanced robustness in predicting system performance, and the ability to generate accurate predictions with fewer inputs and limited system knowledge [9, 23]. This integration can help to overcome the computational intensity associated with combining simulators and solvers for optimization, as ML-based surrogate models can significantly reduce computational complexity [9].

The integration of ML with FPM is proving to be a valuable approach for process optimization across various energy and chemical processes. By combining FPM to generate data in design spaces with the learning capabilities of ML algorithms like eXtreme Gradient Boosting and Artificial Neural Networks, it becomes possible to search for optimal solutions, even in infeasible domains that are difficult to explore with FPM alone [8, 24]. ML techniques have been successfully applied to optimize complex processes like biomass gasification and pyrolysis, syngas production, and hydrogen production from various feedstocks [9, 25]. For example, ML-based surrogate models have been employed for MOO, targeting the minimization of economic cost, exergy destruction, and CO₂ emission, while maximizing hydrogen yield and other valuable products. These ML-based optimization frameworks show strong potential in low-carbon hydrogen production system design, particularly in cases involving highly coupled variables and strict process constraints, often outperforming traditional FPM-based optimization within extended or infeasible design domains [8]. Consequently, the application of ML-based surrogate models can substantially accelerate optimization procedures and effective exploration in infeasible domains compared with the direct use of complex thermodynamic models integrated with metaheuristic algorithms.

The construction of robust global surrogate models, essential for facilitating the analysis and optimization of complex systems, is fundamentally constrained by the high computational cost of obtaining sufficient high-quality data [26]. Rigorous mathematical models, particularly those based on detailed first principles (such as equations of state like PC-SAFT), demand computationally expensive evaluations to map the functional behavior across the entire design space [26-28]. Consequently, traditional one-shot sampling approaches, which often require a large number of sample points to represent the entire problem space, become computationally prohibitive due to the resultant high costs and time consumption [26, 29]. Compounding this challenge, the attainment of requisite predictive accuracy in the surrogate model depends critically on the dataset's ability to capture complex functional characteristics [27, 28]. Specifically, the underlying systems often exhibit crucial features such as strong nonlinearities, sharp curvatures, or discontinuities. Specifically, the underlying systems often exhibit crucial features such as strong nonlinearities. These complex structures are frequently insufficiently resolved by purely space-filling sampling designs, as such methods often fail to place enough samples in the critical regions where the model behavior is most difficult to approximate [26, 29]. Therefore, efficient surrogate model generation necessitates the use of adaptive sequential sampling procedures, which are specifically designed to minimize the required number of function evaluations while strategically exploiting complex regions to enhance global model accuracy [26, 29].

In this work, all results were computed on a laptop. Laptop specification is shown in Table 1. Moreover, the chemical process model was simulated in Aspen Plus V14. Machine learning and multi-objective optimization frameworks were developed in Visual Studio Code.

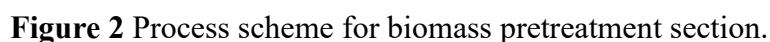
Processor	Intel(R) Core(TM) Ultra 7 155H 3.80 GHz
RAM	16GB (2x8GB) DDR5
Windows	Windows 11 Home Single Language (64 bit)
Display adapter	NVIDIA GeForce RTX 4050 Laptop
Storage	512GB NVMe PCIe 4.0 x4

3.2.1 Aspen Plus model development



The furfural and power co-production process comprises several sections: biomass pretreatment (S100), CHP (S200), furfural production (S300), and ORC (S400), as shown in Figure 1. The non-random two liquid (NRTL), SYSOP0, and REFPROP property methods were selected as predicted thermodynamic properties. Whereas, NRTL was used for biomass pretreatment and furfural production. Moreover, SYSOP0 and REFPROP were selected for CHP and waste heat recovery, respectively. The chemical composition of each feedstock, including sugarcane bagasse (SB), corn stover (CS), and wheat straw (WS), was shown in Table 2. Assume moisture content for all biomass feedstock was 50%.

The first section is biomass pretreatment, as shown in Figure 2. In this section, biomass was soaked with sulfuric acid and hot water to increase water content and then fed into a hydrolysis reactor. Hemicellulose was hydrolyzed into xylose, while cellulose was degraded into acetic acid, which functioned as a catalyst for furfural production. Subsequently, hydrolysate from the reactor was sent into the blowdown tank (D-101) to separate steam and fed into the condenser to recover waste heat for ORC. In the blowdown tank, the NRTL-HOC was selected to prevent overestimation of acetic acid in vapor [30]. The hydrolysate from blowdown tank was separated into solid residue by a solid-liquid separator (SL) and washing column (SW-101). The solid residue, primarily comprising cellulose and lignin, was fed into the CHP section for use as fuel. Moreover, the hydrolysate, primarily comprising xylose, was neutralized by lime to remove sulfuric acid and then fed into furfural production. The key parameters for the biomass pretreatment section are shown in Table 3. Moreover, the liquid load to solid outlet of all solid-liquid separators was assumed to be 50%.



The electricity and high-pressure steam were generated in the CHP section as shown in Figure 3. The biomass and solid residue were combusted with air to produce steam at 63 bar for driving a multi-stage turbine (TG-201). The boiler feed water was fed at 176°C and 63 bar. The combustor (B-201) was operated at 870°C and 1 bar. In the combustor, combustion conversion was assumed to be 98% [30]. The outlet pressure of each turbine was 13.17, 9.5, and 0.1 bar [30]. The high-pressure steam (13.17 bar) was extracted to utilize in the other process. Heat and work losses of this section were assumed to be 5%. Isentropic and mechanical efficiencies were 85% and 96%, respectively [32].

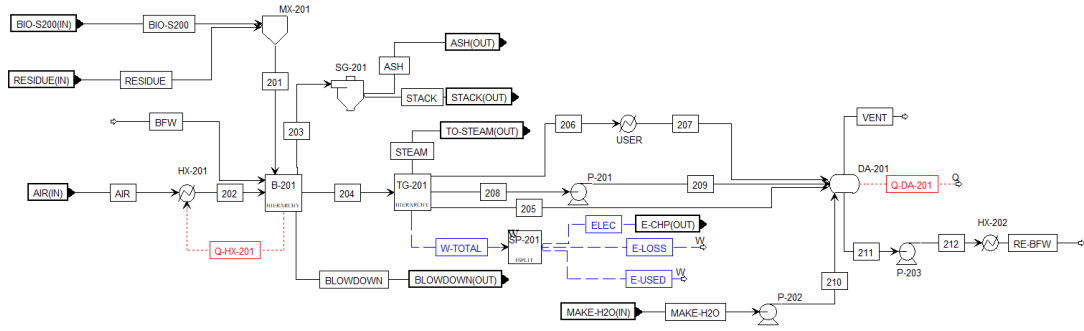


Figure 3 Process scheme for CHP section.

The furfural production was developed in 2 configurations comprising HPA-RD and DPTC-RD. Hydrolysate from S100 was mixed with water and acetic acid to adjust acetic acid concentration and then fed into S300.

The first configuration is HPA-RD, as shown in Figure 4. Hydrolysate was pressurized and preheated before sent to the RD column (DC-301). Within the DC-301 column, xylose was dehydrated to produce furfural using acetic acid as a catalyst, although a portion of the furfural degraded into humins, as indicated in reactions (1)-(3). Kinetic models for these reactions are presented in reactions (4)-(6). Where $[A]$, $[C_X]$, and $[C_F]$ are acetic acid concentration in mol/l, xylose concentration in mol/l, and furfural concentration in mol/l, respectively. This kinetic model was reported by Chen et al. [33]. The overhead vapor was fed into a compressor (M-301) to increase pressure and temperature for exchange in the reboiler. After that, overhead vapor was reducing pressure and condensation before splitting into reflux and distillate. The distillate of the DC-301 column mainly contained furfural and water at near azeotropic composition, and the bottom was mainly comprised of water and acetic acid. The distillate product was cooled to 60°C and fed into a decanter. From the nature of furfural and water, it was separated into two phases. The organic phase was fed into a distillation column (DC-302) to increase the purity of furfural. DC-302 separated furfural at the bottom product and recycled the distillate product back to the decanter to recover furfural. The aqueous phase from the decanter was increased in pressure and sent to DC-301 for furfural recovery.

The second configuration is DPTC-RD, as shown in Figure 5. The pressurized and preheated hydrolysate was fed into a high-pressure column (HPC) to produce furfural from reactions (1)-(3). The bottom product of HPC was fed into a low-pressure column (LPC) to recover furfural as a vapor product. Subsequently, the vapor product of the LPC was fed into the compressor and then fed to the HPC. The vapor product of HPC was exchanged in the reboiler of the LPC for condensation and split into reflux and distillate. After that, the distillate product was fed into a decanter and distillation column to increase the purity of furfural.

In furfural production, the DC-302 of all configurations had varied reboiler duty to obtain a specific purity of furfural of about 99.95 wt% by design spec. Moreover, all columns were simulated using the RadFrac model. The reactive column was simulated by the rate-based model. The other column was simulated by the equilibrium model. The sieve tray column was applied to the reactive column. The flooding approach for sizing diameter of distillation column was assumed to be 80%. In addition, HX-302 was used as a heat source for the ORC section.

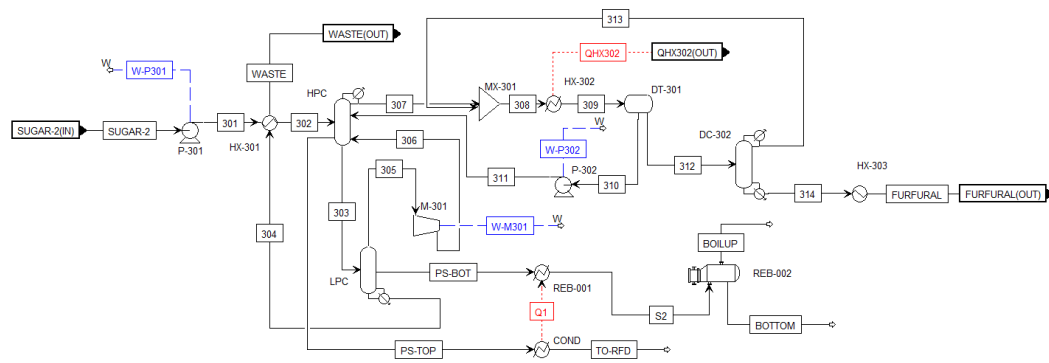


Figure 5 Process scheme for furfural production via DPTC-RD.

In the ORC section, electricity was generated from waste heat in other sections. The scheme of this section was shown in Figure 6. 2,2-Dichloro-1,1,1-trifluoroethane (R123) was selected for working fluid due to lower global warming potential, ozone depletion potential, atmospheric life, and suitable low-temperature waste heat [36]. R123 was vaporized at a pressure of 7 bar by using heat from HX-102 and HX-302 and then fed into a turbine to produce electricity. The outlet pressure of this turbine was 1.4 bar due to the requirement of using cooling water to condense working fluid into saturated liquid.

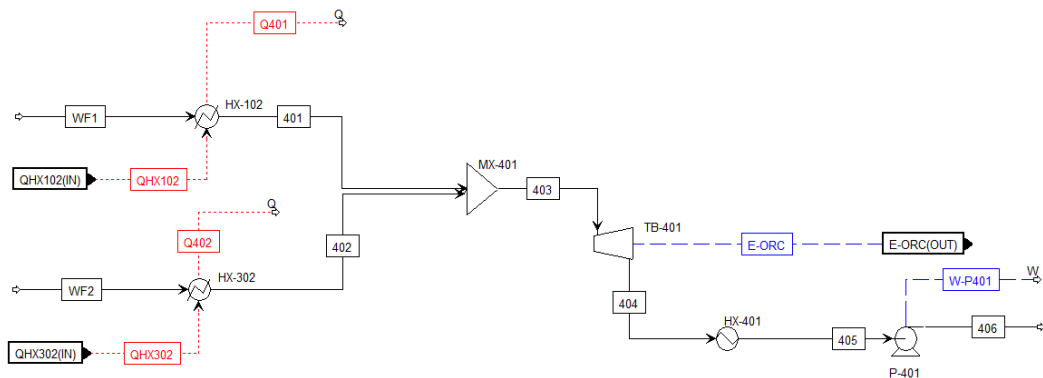


Figure 6 Process scheme for ORC section.

3.2.2 Machine learning model development and multi-objective optimization

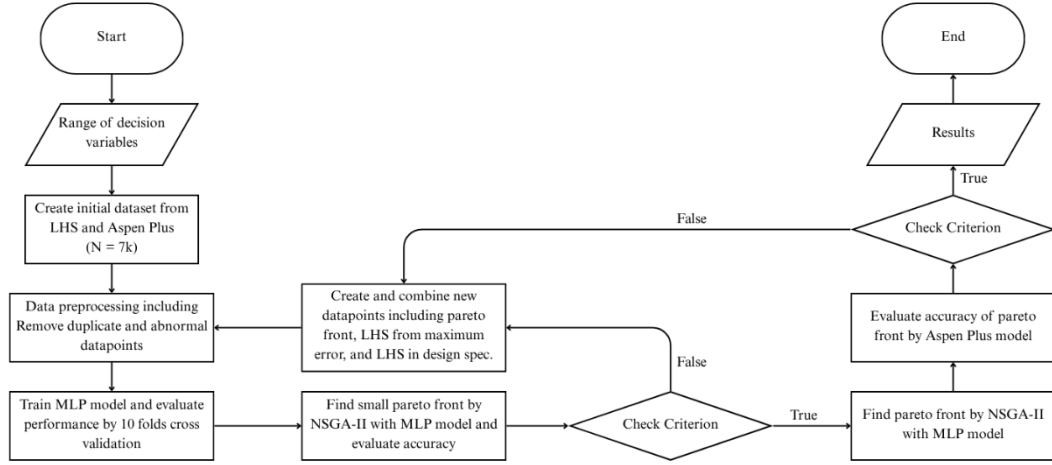


Figure 7 Flow chart of adaptive LHS for ML model development and multi-objective optimization.

The adaptive LHS method was selected to train the ML model and MOO. A flowchart of adaptive LHS was shown in Figure 7. This proposed method was adjusted from existing work done by Borisut et al. [29]. The boundary of the decision variable was shown in Table 4. The adaptive LHS method starts at creating an initial dataset from LHS, where the number of datapoints was equal to 7 times the number of features. Subsequently, the initial dataset was computed objective functions from the Aspen Plus model. The dataset for training the ML model was removed abnormal and duplicate datapoints. After that, the multi-layer perceptron (MLP) model was trained and evaluated. The structure of the MLP model was a single hidden layer and 30 nodes, which used the ReLU activation function. Moreover, the limited-memory Broyden–Fletcher–Goldfarb–Shanno algorithm was selected for weight optimization, effective for small datasets. 10-fold cross-validation (CV) method was selected for MLP model evaluation, for which the coefficient of determination (R^2) and mean absolute percentage error (MAPE) were applied to indicators to evaluate performance as shown in equations (7)-(8). Where y_i is the real value, $\hat{y}_i$ is the predicted value, and $\bar{y}$ is the average of the real values. The trained MLP models are then employed within the NSGA-II to identify a small Pareto front. To enhance prediction accuracy and ensure coverage of critical regions in the design space, additional data points are generated by combining LHS sampling around high-error regions (3 data points for each objective, which total 9 data points), the previously obtained small Pareto front (20 data points), and LHS in design spec (11 data points). These new data are merged with the existing dataset to retrain the MLP model, and the optimization cycle repeats until the convergence criterion. The criteria for this step are R^2 higher than 0.95, MAPE lower than 5%, and a percentage error of a small Pareto front lower than 5% for 3 consecutive iterations. If the criteria are true, the full Pareto front was computed, and then the accuracy of the Pareto front was evaluated. The criterion of this step is a percentage error of the full Pareto front lower than 5%. 20 and 200 populations with 100 generations are used in NSGA-II to find small and full Pareto fronts, respectively.

The objective of this optimization consists of TAC, total revenues, and CO_2 emission. The equation for calculating TAC was shown in equation (9). TAC is an

economic measure used to evaluate the cost-effectiveness of a process by combining the annualized capital cost and the annual operating cost. The capital cost includes expenses for equipment and installation, while the operating cost includes raw materials, chemicals, utilities, and waste treatment. The total revenues comprise revenue from furfural and electricity. CO₂ emission was obtained from flue gas in the CHP section.

For MOO, NSGA-II and TOPSIS were selected. NSGA-II is a widely used MOO algorithm designed to efficiently solve problems involving conflicting objectives by generating a diverse set of optimal solutions, known as the Pareto front. It achieves this by employing a fast non-dominated sorting approach to rank solutions, along with a crowding distance metric that maintains diversity among the solutions, and an elitism strategy that ensures the best solutions are carried over to subsequent generations. This balance of convergence and diversity makes NSGA-II a popular choice in fields such as engineering, economics, and operations research for optimizing complex systems with multiple criteria. TOPSIS is a multi-criteria decision-making method that ranks alternatives based on their geometric distance from an ideal solution and a negative ideal solution. The method first constructs these ideal and negative ideal benchmarks by considering the best and worst values for each criterion, respectively. Then, for each alternative, it computes the Euclidean distance to these benchmarks and calculates a relative closeness score, which is used to rank the alternatives.

$$R^2 = 1 - \frac{\sum (\hat{y}_i - y_i)^2}{\sum (y_i - \bar{y})^2} \quad (7)$$

$$MAPE = \frac{100}{\text{Number of observations}} \sum \frac{|y_i - \hat{y}_i|}{|y_i|} \quad (8)$$

$$TAC = \frac{\text{Capital cost}}{\text{Payback Period}} + \text{Total operating cost} \quad (9)$$

3.2.3 SHAP analysis

SHAP is a model interpretability technique that explains individual predictions by assigning each feature an importance value based on Shapley values from cooperative game theory. It quantifies how much each feature contributes to the difference between the actual prediction and the average prediction by considering all possible combinations of features, ensuring a fair distribution of credit among them. This approach not only helps in understanding the decision-making process of complex models but also supports global and local interpretability, enabling users to diagnose, trust, and improve ML models.

Table 4 Decision variable and boundary for Adaptive LHS.

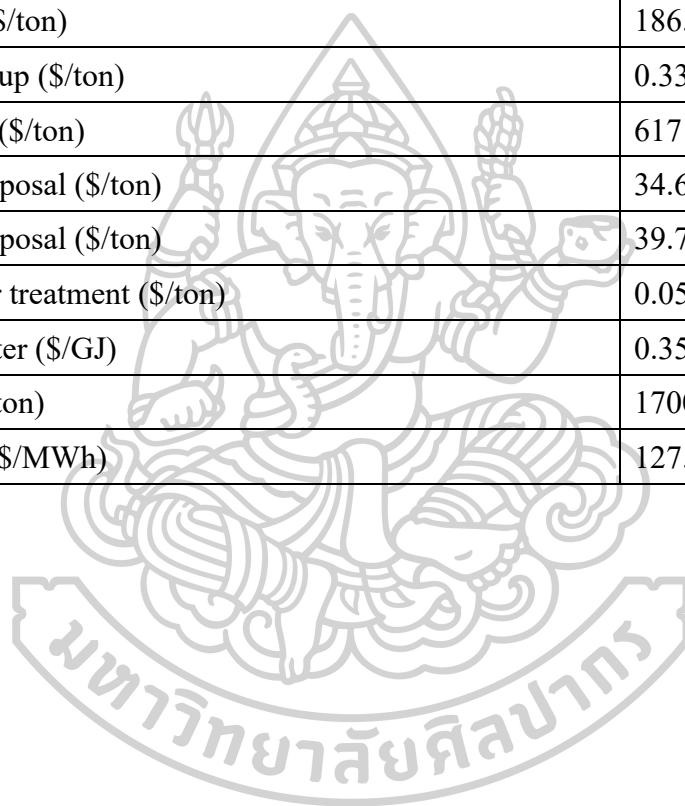
Variable	Min	Max	Unit
Type of Biomass	0	2	
Feed flow rate of biomass	0.5	1.5	
Ratio of feed into CHP	0.25	1	
Acetic acid concentration	0.1	0.5	mol/L
Mole reflux ratio of RD or HPC	1	10	
Mole reflux ratio of DC	0.01	5	
Reboiler duty of RD or LPC	5	30	MW
Pressure ratio of compressor	1.2	1.6	
Pressure of RD or LPC	8	12	bar
Diameter of RD or HPC	2	4	m
Number of reactive stage (RD and HPC)	5	20	
Number of stripping stage (RD and LPC)	5	10	
Number of rectifying stage (RD and HPC)	5	10	

3.2.4 Economic evaluation

NPV is a financial metric used to evaluate the profitability of an investment or project. It represents the difference between the present value of cash inflows and the present value of cash outflows over a given period. NPV is widely used in capital budgeting and investment decision-making to determine whether a project or investment is financially viable. A positive NPV indicates that the investment is expected to generate more value than its cost, while a negative NPV suggests a loss. The IRR is a financial metric used to evaluate the profitability of an investment or project. It represents the discount rate that makes the NPV equal to zero. The discounted payback period is an indicator for evaluating when a project can pay back the investment cost. The total capital investment (TCI) was calculated by a factor obtained from an NREL report [30]. Moreover, the economic assumption was shown in Table 5.

Table 5 Economic assumptions [10, 19].

Parameter	value
Annual operating hours (h/y)	8500
Plant lifetime	30
Bagasse cost (\$/ton)	25
Corn stover cost (\$/ton)	58.5
Wheat straw cost (\$/ton)	38.85
Sulfuric acid cost (\$/ton)	108.13
Lime cost (\$/ton)	186.83
Water makeup (\$/ton)	0.33
Acetic acid (\$/ton)	617
Gypsum disposal (\$/ton)	34.69
Gypsum disposal (\$/ton)	39.73
Waste water treatment (\$/ton)	0.056
Cooling water (\$/GJ)	0.354
Furfural (\$/ton)	1700
Electricity (\$/MWh)	127.2



Chapter 4 Results and Discussion

4.1 Aspen Plus model validation

The accuracy of the NRTL model in predicting the vapor–liquid equilibrium behavior of the furfural-water system was evaluated at different pressures ranging from 1.01 bar to 9.64 bar. Figure 8 presents the R^2 values obtained for each pressure condition. Across all cases, the R^2 values exceeded 0.90, indicating a strong correlation between the experimental and predicted equilibrium compositions.

Table 6 summarizes the validation results of the proposed kinetic model for predicting furfural yield during xylose dehydration. The model was tested under various operating conditions, including different temperatures (180-210 °C), initial xylose concentrations ($X_0 = 50$ -120 g/l), and initial furfural concentrations ($F_0 = 0$ -8 g/l). The performance was evaluated by comparing the predicted furfural yield against reference data over the reaction time range of 0-10 min, with the average percentage error and standard deviation (SD) serving as accuracy indicators. The model achieved an average error between 0.95% and 2.93% with a small SD, demonstrating high predictive reliability across all tested conditions. The model's accuracy across a wide range of conditions indicates robust parameter estimation and reliable reaction pathway representation.

The performance of the Aspen Plus simulation model for the combined heat and power section was validated against reference data from report of NREL [30]. Table 7 presents the comparison between the predicted and reference values for key parameters. The model exhibited strong agreement with reference values, with deviations ranging between 0.14% and 5.16%. The outlet temperatures at turbine stages 1-3 showed minimal error, lower than 3.2%, confirming accurate thermodynamic prediction across multiple expansion stages. Similarly, the vapor fraction of the vacuum steam was estimated with an error of only 1.35%, indicating precise phase equilibrium calculations. The total work output and condenser duty exhibited slightly higher deviations, about 5.16% and 1.52%, respectively, which remain within acceptable engineering tolerance for process simulations.

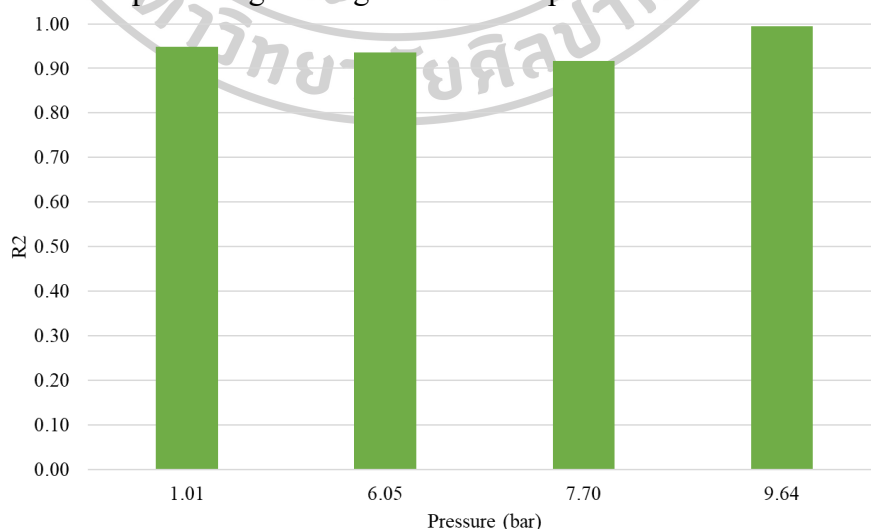


Figure 8 Performance of the NRTL model in estimating vapor-liquid equilibrium for the furfural-water system at different pressures.

Table 6 Parameters and performance metrics for the validation of the kinetic model of xylose dehydration to furfural.

Temperature (°C)	X ₀ (g/L)	F ₀ (g/L)	Average error (%)	SD
210	80	0	1.59	1.02
190	80	0	1.05	1.14
180	80	0	0.95	1.3
190	120	0	1.36	1.19
190	50	0	0.95	1.34
190	80	4	1.48	1.11
190	80	8	2.93	2.12

Table 7 Parameters and performance metrics for validation of the CHP section.

Parameter	This Work	Reference	Unit	Error (%)
Outlet turbine stage 1	273.31	266	°C	2.75
Outlet turbine stage 2	240.45	233	°C	3.20
Outlet turbine stage 3	46.06	46	°C	0.14
Vapor fraction (Vacuum steam)	0.89	0.9		1.35
Total Work	43454.33	41324	kW	5.16
Condenser duty	59.88	58.98	MW	1.52

Table 8 Parameters and performance metrics for validation of the ORC section.

Parameter	This Work	Reference	Unit	Error (%)
Inlet turbine Temperature	104.1	104.15	°C	0.05
Outlet turbine Temperature	51.04	51.05	°C	0.01
Total Work	726.87	726.27	kW	0.08
Work pump	16.07	16.05	kW	0.15

Table 8 presents a comprehensive comparison of key operational parameters between the model predictions and established reference values. The validation results presented in this study demonstrate that the developed Aspen Plus model achieves outstanding predictive accuracy for the ORC turbine performance. The observed errors, ranging from 0.01% to 0.15%, fall well within acceptable tolerances for engineering simulations and are comparable to, or exceed, the accuracy levels reported in similar modeling studies of ORC systems [36].

4.2 Machine learning model development by adaptive LHS

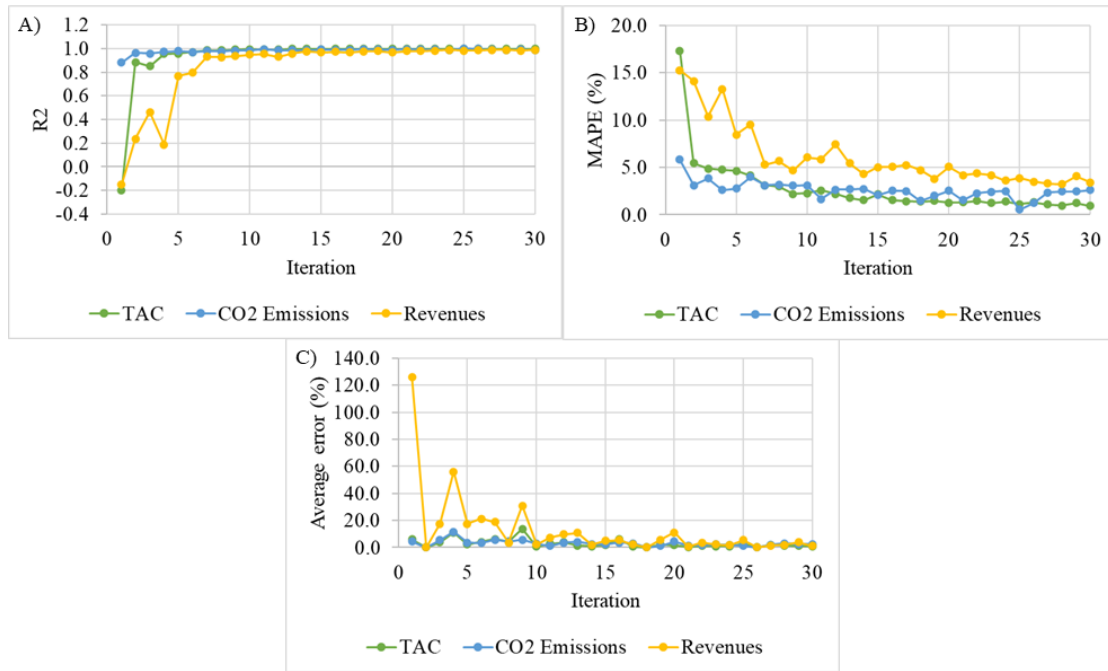


Figure 9 Performance of MLP models of the HPA-RD process: A) 10-fold CV (R^2), B) 10-fold CV (MAPE), and C) Average error of small Pareto front.

The performance of the MLP models developed for HPA-RD through the adaptive LHS is presented in Figure 9, which illustrates the model performance across 30 iterations for three objective functions: TAC, CO₂ emission, and revenues. Figure 9A demonstrates the progression of the R^2 through 10-fold CV across the iterative training process. The TAC and CO₂ emissions models exhibited rapid convergence, achieving R^2 values exceeding 0.95 within the 4 iterations. These models maintained consistently high R^2 values above 0.98 throughout subsequent iterations, indicating robust predictive capability. In contrast, the revenues model displayed notably slower convergence, with initial R^2 values near zero and even negative values in early iterations. The revenues model required approximately 10 iterations to achieve R^2 values above 0.95 and stabilized around 0.98 after iteration 14, suggesting greater complexity or nonlinearity in the underlying relationship between process parameters and economic revenues.

The MAPE trends are presented in Figure 9B. The TAC and CO₂ emissions models achieved MAPE values below 5% within three iterations, subsequently declining to approximately 3% by iteration 8 and stabilizing near 1-2% for the remaining iterations. The revenues model exhibited substantially high initial MAPE values, reaching approximately 15%, with considerable fluctuation during early training stages. The MAPE for the revenues model decreased progressively, falling below 5% by iteration 14 and converging to approximately 3% after iteration 25.

Figure 9C illustrates the average error when the trained models were applied to predict the small Pareto front. The TAC and CO₂ emission models demonstrated exceptional performance, maintaining average errors below 10% throughout nearly all iterations and consistently achieving errors below 5% after iteration 10. The revenues model showed higher prediction errors during initial iterations, with average errors

exceeding 100% at the first iteration and exhibiting substantial volatility through iteration 10. Beyond iteration 27, the revenues model stabilized with average errors consistently below 5%, demonstrating acceptable predictive performance for Pareto front estimation.

The performance of the MLP models developed for DPTC-RD through the adaptive LHS is presented in Figure 10. The R^2 trends displayed in Figure 10A reveal distinct convergence patterns among the three objective function models. The TAC model demonstrated rapid stabilization, achieving an R^2 value approaching unity within the 5 iterations and maintaining this exceptional performance throughout all subsequent iterations. The CO₂ emission model exhibited similarly swift convergence, reaching an R^2 value above 0.95 by iteration 4 and sustaining near-perfect predictive accuracy thereafter. In contrast, the revenues model displayed substantially delayed convergence, with an initial R^2 value of approximately -6 at iteration one, indicating that early predictions performed worse than a naive mean-based estimator. The revenues model required 4 iterations to achieve positive R^2 values and did not stabilize until iteration 22 with R^2 approximately 0.95.

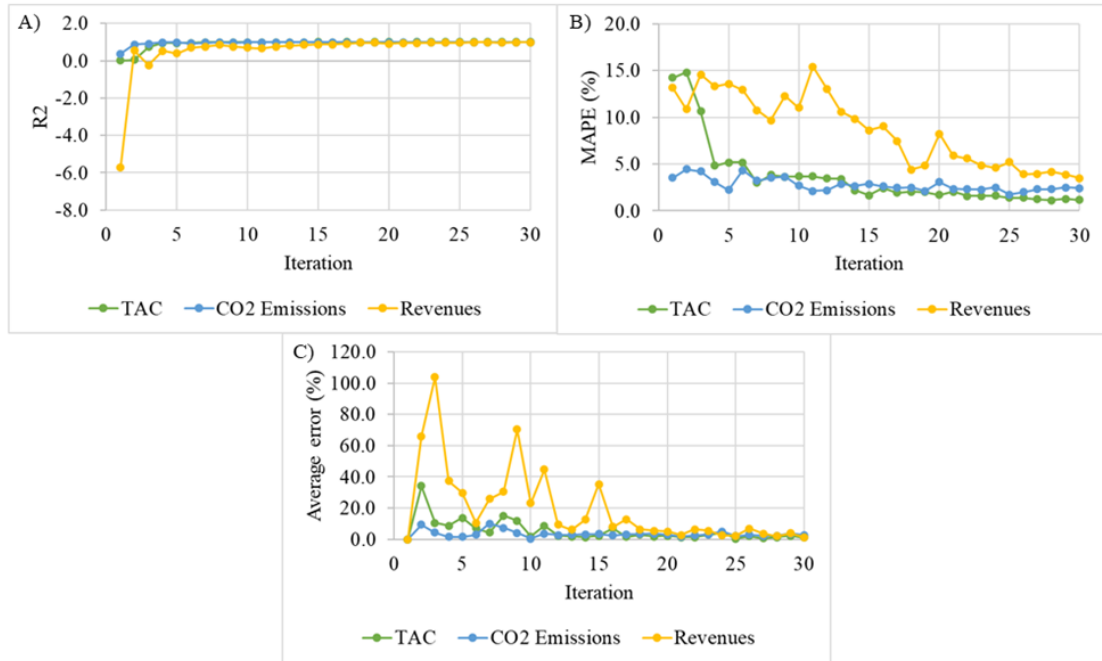


Figure 10 Performance of MLP models of the DPTC-RD process: A) 10-fold cross validation (R^2), B) 10-fold cross validation (MAPE), and C) average error of small Pareto front.

Figure 10B illustrates the MAPE evolution throughout the adaptive LHS. The TAC model achieved MAPE values below 5% by iteration 7, declining steadily to approximately 3% by iteration 14 and stabilizing near this level through iteration 30. The CO₂ emissions model reducing MAPE from approximately 5% at iteration one to below 3% by iteration 10, with sustained performance below 3% for all remaining iterations. The revenues model exhibited markedly elevated MAPE values during initial training, reaching approximately 15% at iteration one and displaying considerable fluctuation between 10% and 15% until iteration 13, followed by progressive improvement. By iteration 18, the revenues model MAPE had declined below 5%.

The average error in predicting the small Pareto front, presented in Figure 10C, provides critical validation of model performance for MOO. The TAC model demonstrated exceptional reliability, maintaining average errors below 10% from iteration 9 and achieving errors consistently below 5% after iteration 17. The CO₂ emissions model exhibited comparable performance, with average errors remaining below 10% throughout all iterations and stabilizing below 5% after iteration 9. The revenues model showed substantially higher prediction errors during early training phases, with a dramatic spike exceeding one hundred percent at iteration 3 and several fluctuations above 40% through iteration 15. After iteration 15, the revenues model stabilized significantly, maintaining average errors consistently below 10% and frequently achieving errors below 5% through iteration 27.

Consequently, MLP model for HPA-RD and DPTC-RD configurations were trained based on datasets of iteration 30. The datasets of HPA-RD and DPTC-RD including 560 and 436 datapoints without abnormal, respectively. Moreover, R^2 and MAPE of HPA-RD were 0.9992 ± 0.0003 and 0.9239 ± 0.1915 for TAC, 0.9893 ± 0.0026 and 2.6324 ± 0.2364 for CO₂ emissions, and 0.9889 ± 0.0069 and 3.412 ± 0.8162 for revenues, respectively. R^2 and MAPE of DPTC-RD were 0.9985 ± 0.0007 and 1.1732 ± 0.3165 for TAC, 0.9896 ± 0.0024 and 2.4239 ± 0.2167 for CO₂ emissions, and 0.9851 ± 0.0077 and 3.5001 ± 0.8532 for revenues, respectively.

Table 9 Accuracy of Pareto front for HPA-RD and DPTC-RD configurations.

Parameter	HPA-RD	DPTC-RD
Average error of TAC (%)	0.54	0.99
Average error of CO ₂ emissions (%)	2.00	1.84
Average error of revenues (%)	3.83	4.62

The accuracy of the Pareto front obtained through the NSGA-II algorithm coupled with the trained MLP models was validated against Aspen Plus simulations for both process configurations. Table 9 presents the average prediction errors for the three objective functions across the Pareto fronts generated for the HPA-RD and DPTC-RD processes. These results confirm that the ML-based optimization framework successfully identified Pareto optimal solutions that closely approximate those that would be obtained through computationally prohibitive direct optimization using FPM. The comprehensive accuracy across all objectives and both process configurations establishes confidence in the subsequent comparative analysis and decision-making based on these Pareto fronts.

4.3 Multi-objective optimization

Figure 11 illustrates the Pareto front obtained from the MOO of the HPA-RD process, considering TAC, CO₂ emissions, and revenues. CO₂ emission increased from approximately 6,000 to 20,000 kg/h; both TAC (5-30 M\$/yr) and revenue (6-35 M\$/yr) were rising, indicating that higher operating intensities lead to enhanced production rates but at the expense of greater energy consumption and associated costs. The correlation between TAC and revenue demonstrates a strong positive trend, suggesting that economically optimal designs inherently require higher capital and utility expenditures to achieve elevated product yields. Moreover, this Pareto front was clustered in two groups, separated by CO₂ emission lower than 8,000 kg/h and CO₂ emission higher than 12,000 kg/h due to limitations of the Aspen Plus model.

Figure 12 illustrates the Pareto front derived from the MOO of the DPTC-RD process. CO₂ emissions increase from approximately 6,000 to 20,000 kg/h; both TAC

(5-27 M\$/yr) and revenue (9-35 M\$/yr) exhibit a strong positive correlation, indicating that higher production capacities or intensified operating conditions lead to greater profitability but at the expense of elevated energy consumption and environmental impact. The relationship between TAC and revenue demonstrates a nearly linear trend, suggesting that economic improvement is closely linked to higher capital and utility requirements inherent to more energy-demanding operation modes.

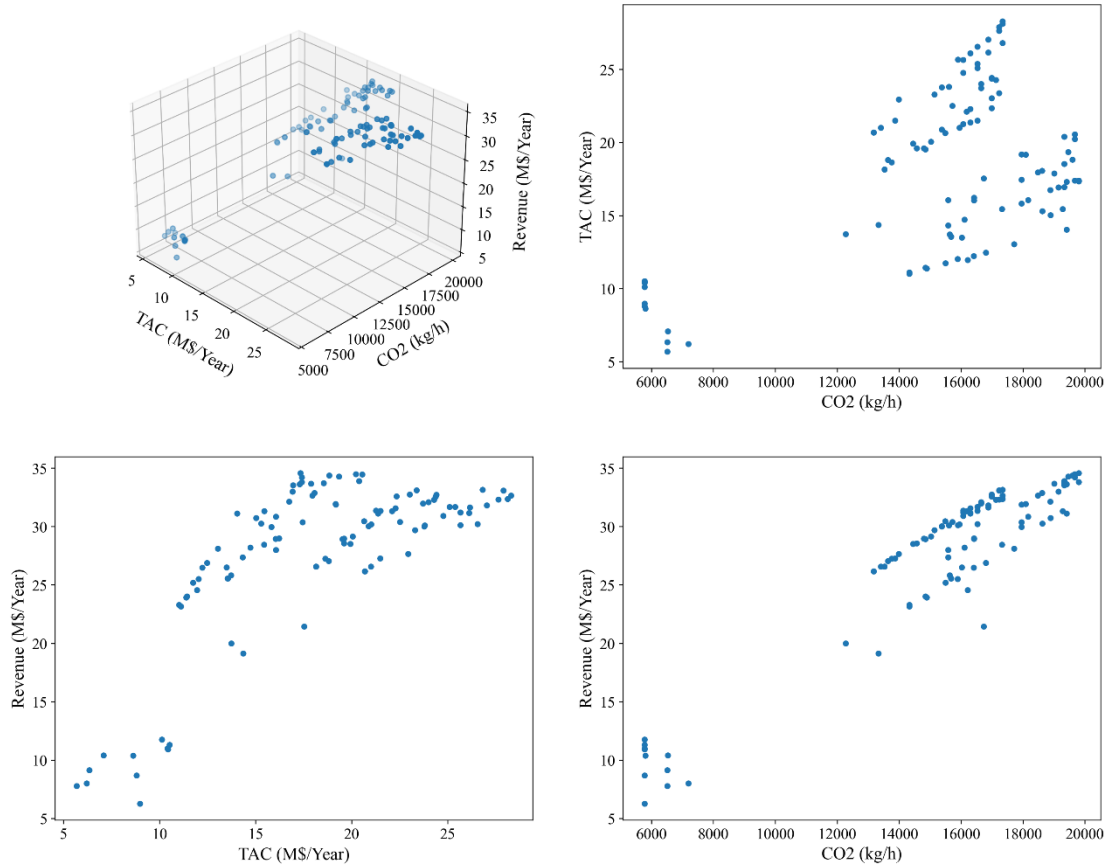


Figure 11 The Pareto front obtained from the multi-objective optimization of the HPA-RD process.

Table 10 and Table 11 summarize the optimized operating conditions of the HPA-RD and DPTC-RD configurations under four optimization scenarios: minimum TAC (HPA-1 and DPTC-1), maximum revenues (HPA-2 and DPTC-2), minimum CO₂ emission (HPA-3 and DPTC-3), and the TOPSIS approach (HPA-4 and DPTC-4). The TOPSIS analysis represents a multi-objective compromise, where the final case was evaluated using equal weighting for all objectives. For the minimum TAC, both configurations yielded relatively low total revenues and CO₂ emission, with TAC values of 5.69 M\$/year and 5.78 M\$/year for HPA-RD and DPTC-RD, respectively. The DPTC-RD configuration demonstrated higher revenue (9.54 M\$/year) than HPA-RD (7.77 M\$/year) with similar CO₂ emissions. Under the max revenues condition, both systems exhibited significantly increased TAC and CO₂ emission due to high feedstock size, with revenues rising sharply to 34.57 M\$/year for HPA-RD and 35.00 M\$/year for DPTC-RD. These results reveal that maximizing profitability strongly correlates with higher energy consumption and larger column dimensions, as also reflected in the increased reflux ratios and reactive stages. When CO₂ minimization

was prioritized, both processes operated at reduced feedstock and lower CO₂ emission (5780-6026 kg/h), though at the expense of reduced revenues (10.68-11.76 M\$/year). The DPTC-RD configuration again slightly outperformed HPA-RD in terms of overall efficiency, maintaining comparable emissions but achieving lower TAC (8.46 M\$/year). Finally, the TOPSIS evaluation identified DPTC-RD as the superior configuration with a TAC of 11.38 M\$/year, CO₂ emissions of 11,619 kg/h, and a revenue of 21.39 M\$/year. This balanced performance demonstrates that DPTC-RD offers better overall trade-offs between economic and environmental factors compared to HPA-RD. Overall, the results confirm that while HPA-RD achieves strong energy integration benefits, DPTC-RD provides greater flexibility and superior multi-objective performance.

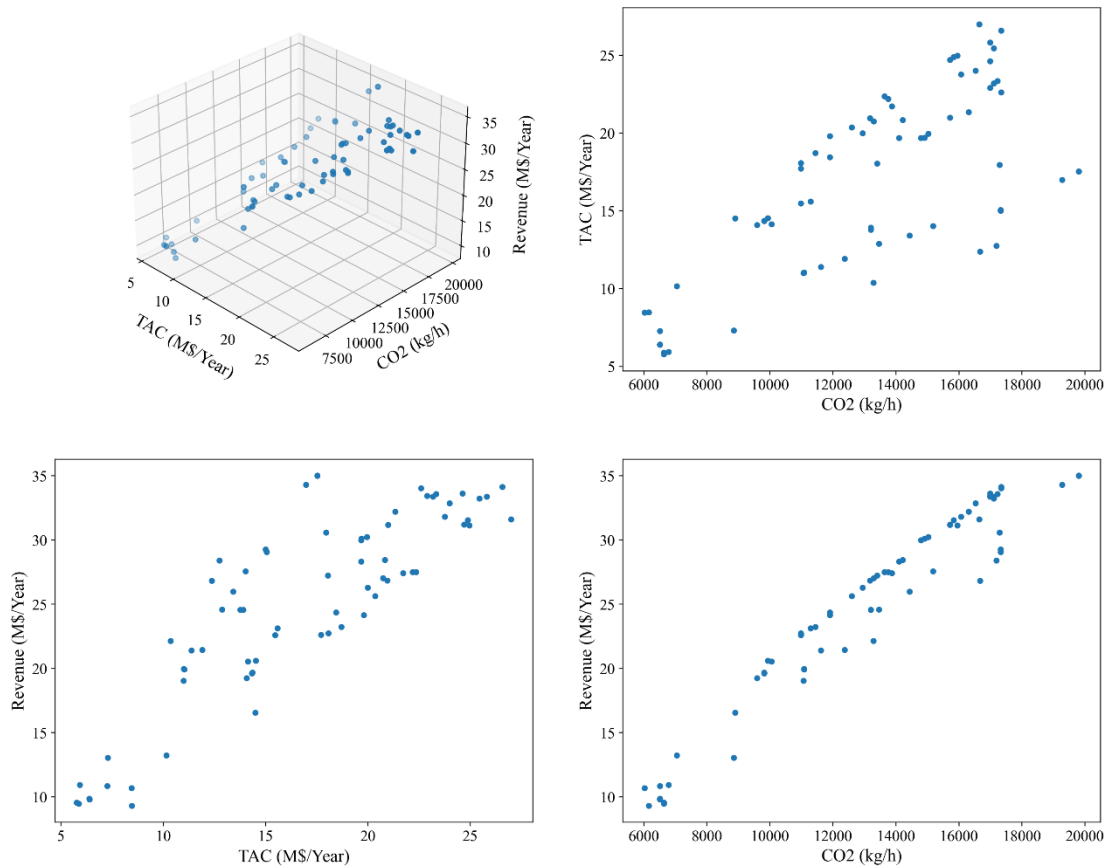


Figure 12 The Pareto front obtained from the multi-objective optimization of the DPTC-RD process.

Table 12 and

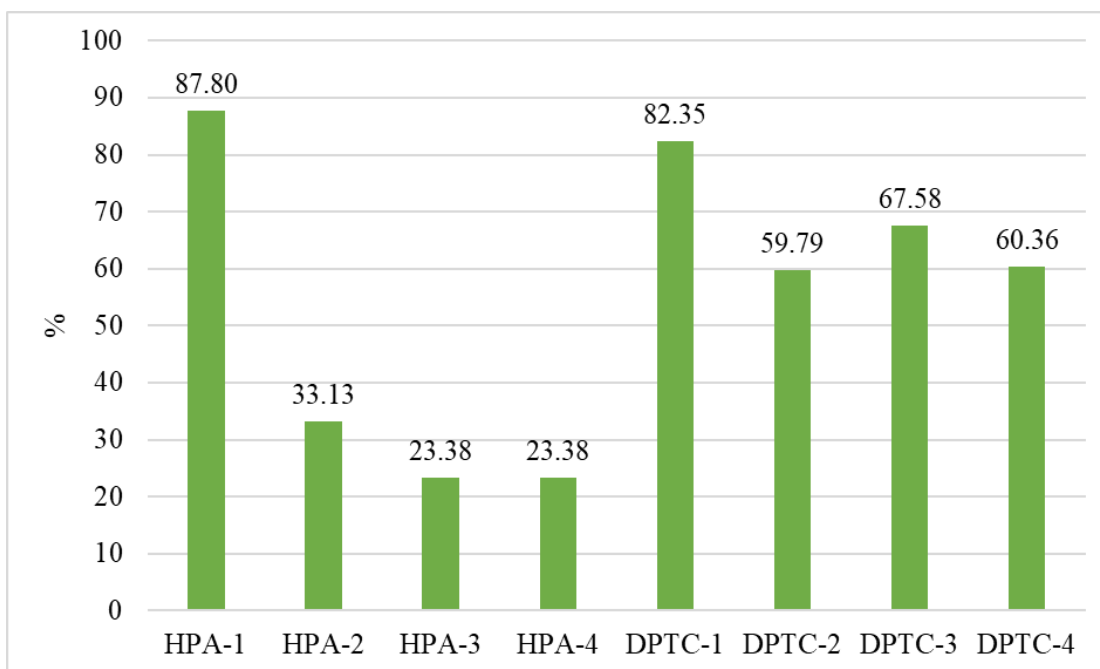


Figure 13 The percentage of electricity supplied from ORC to total electricity consumption.

Table 13 summarize the mass and energy of HPA-RD and DPTC-RD configurations under four optimization scenarios. Across all scenarios, the DPTC-RD shows higher furfural production and electricity generation than the HPA-RD except in scenario DPTC-3, in which furfural production was lower than in scenario HPA-3 by around 174 kg/h. CO₂ emissions have the same trend as electricity generation and total biomass, with DPTC pathways generally emitting equal or slightly more than HPA for comparable conditions. In terms of energy demand, heating and cooling demands were slightly different for comparable conditions. However, the electricity demand of HPA-RD was significantly higher than DPTC-RD. This is because the HPA-RD configurations were operated with high reboiler duty, which generated large vapor at the top of the RD column, leading to high electricity consumption in the compressor. In scenarios HPA-1 and DPTC-1, electricity generated from ORC can supply more than 82% of the contribution for production. In other scenarios, the ORC process of HPA-RD and DPTC-RD configurations can supply electricity about 23-33% and 60-67%, respectively. The percentage of electricity supplied from ORC was shown in Figure 13.

Table 10 Features of optimal solution for HPA-RD process.

Parameter	HPA-1	HPA-2	HPA-3	HPA-4
Type of biomass	SB	WS	CS	CS
Size of biomass (kg/h)	5000	15000	5000	5000
Split biomass to biorefinery	1	1	1	1
Acetic acid (mol/l)	0.12	0.14	0.31	0.31
Reflux ratio of RD	3.31	4.99	5	5
Reflux ratio of DC	4.08	0.18	4.27	4.27
Reboiler duty RD (MW)	5.75	29.17	29.2	29.2
Pressure ratio	1.41	1.42	1.4	1.4

Pressure RD (bar)	8.06	11.42	11.9	11.9
Diameter of RD (m)	2.17	3.5	3.53	3.53
Reactive stages	11	18	17	17
Stripping stages	5	10	10	10
Rectifying stages	10	10	10	10
TAC (M\$/year)	5.69	17.34	10.12	10.12
CO ₂ emissions (kg/h)	6513	19804	5780	5780
Revenues (M\$/year)	7.77	34.57	11.76	11.76

Table 11 Features of optimal solution for DPTC-RD process.

Parameter	DPTC-1	DPTC-2	DPTC-3	DPTC-4
Type of biomass	SB	WS	CS	WS
Size of biomass (kg/h)	5100	15000	5000	8800
Split biomass to biorefinery	1	1	0.89	1
Acetic acid (mol/l)	0.15	0.1	0.1	0.14
Reflux ratio of RD	4.71	2.87	2.82	1.41
Reflux ratio of DC	4.75	4.22	0.37	4.81
Reboiler duty RD (MW)	7.39	29.97	9.7	28.61
Pressure ratio	1.29	1.21	1.22	1.24
Pressure RD (bar)	8.11	11.62	11.61	11.09
Diameter of RD (m)	2.1	3.82	2.03	3.56
Reactive stages	17	20	20	20
Stripping stages	5	6	9	5
Rectifying stages	9	9	5	10
TAC (M\$/year)	5.78	17.53	8.46	11.38
CO ₂ emissions (kg/h)	6643	19804	6026	11619
Revenues (M\$/year)	9.54	35.00	10.68	21.39

Table 12 Mass and energy of each scenario for HPA-RD.

Parameter	HPA-1	HPA-2	HPA-3	HPA-4
Biomass Type	SB	WS	CS	CS
Total biomass (Dry) (kg/h)	5000	15000	5000	5000
Biomass feed to biorefinery	5000	15000	5000	5000
Consumption (kg/h)				
Sulfuric acid	74	222	95	95
Lime	56	168	72	72
Water	19311	35616	13178	13178
Acetic acid	0	0	202	202
Production rate (kg/h)				
Furfural	242	1486	647	647
Net electricity from CHP (kW)	3707	11636	1918	1918
Net electricity from ORC (kW)	250	484	308	308
Net electricity (kW)	3957	12120	2225	2225

Waste (kg/h)				
Gypsum	102	305	131	131
Ash	246	488	279	279
Waste water	23242	46827	17255	17255
CO2 emissions	6513	19804	5780	5780
Energy demand (MW)				
Heating	2.98	8.33	4.03	4.03
Cooling	9.58	29.65	9.57	9.57
Electricity (kW)	284.98	1460.14	1316.97	1316.97

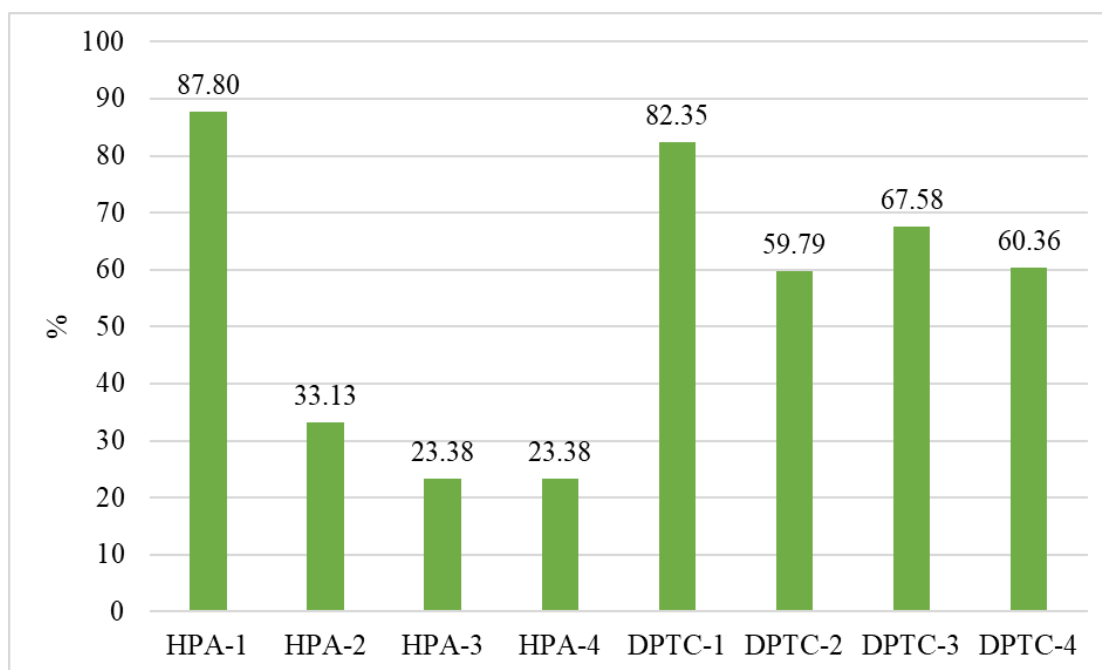


Figure 13 The percentage of electricity supplied from ORC to total electricity consumption.

Table 13 Mass and energy of each scenario for DPTC-RD.

Parameter	DPTC-1	DPTC-2	DPTC-3	DPTC-4
Biomass Type	SB	WS	CS	WS
Total biomass (Dry) (kg/h)	5100	15000	5000	8800
Biomass feed to biorefinery	5100	15000	4450	8800
Consumption (kg/h)				
Sulfuric acid	76	222	85	130
Lime	57	168	64	98
Water	15287	52668	11805	20895
Acetic acid	0	0	4	0
Production rate (kg/h)				
Furfural	358	1497	473	980
Net electricity from CHP (kW)	3777	11765	3336	6099
Net electricity from ORC (kW)	261	597	221	587
Net electricity (kW)	4038	12362	3557	6686

Waste (kg/h)				
Gypsum	104	305	117	179
Ash	251	488	280	286
Waste water	19184	63865	15362	27362
CO2 emissions	6643	19804	6026	11619
Energy demand (MW)				
Heating	2.94	9.76	2.95	7.52
Cooling	9.82	29.25	8.66	17.87
Electricity (kW)	316.88	998.55	327.39	972.21

To ensure a reaction occurs in the reactive stage, temperature and composition profiles in each stage should be analyzed. For example, the temperature and composition profile of scenario HPA-2 were shown in Figure 14 and Figure 15, respectively. The temperature of this column ranges from 183 to 186°C, and these temperatures can cause reactions along the stages. However, the xylose concentration is high within the reactive zone (stages 11–28), its concentration in the remaining sections of the column is low. Consequently, xylose dehydration does not take place outside the reactive zone.

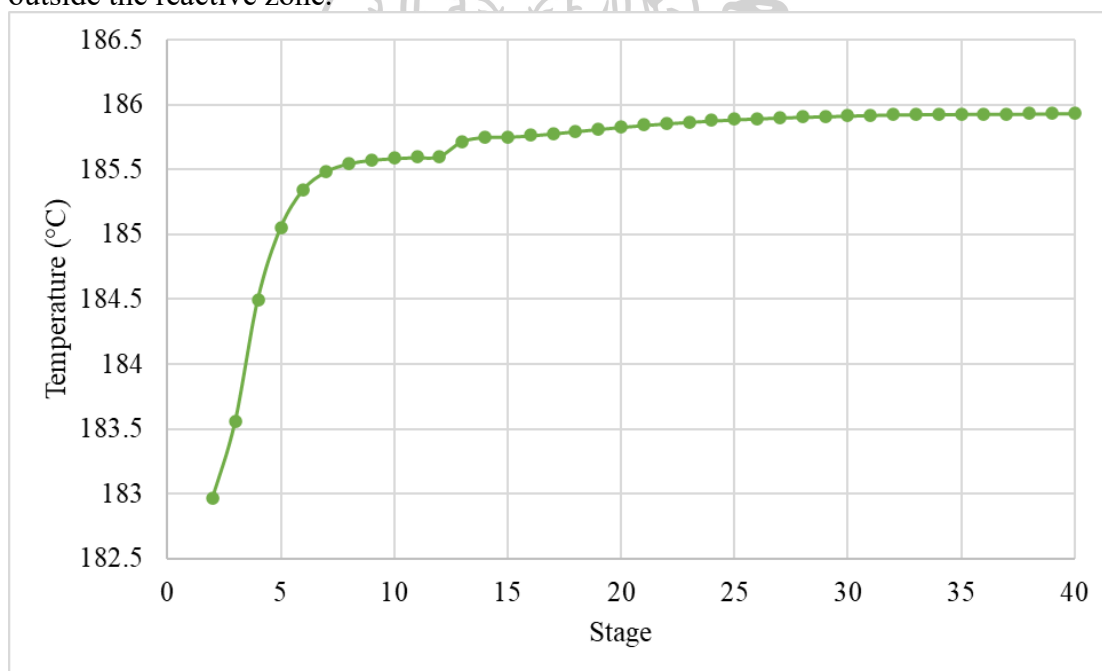


Figure 14 Temperature profile in the reactive distillation column (scenario HPA-2).

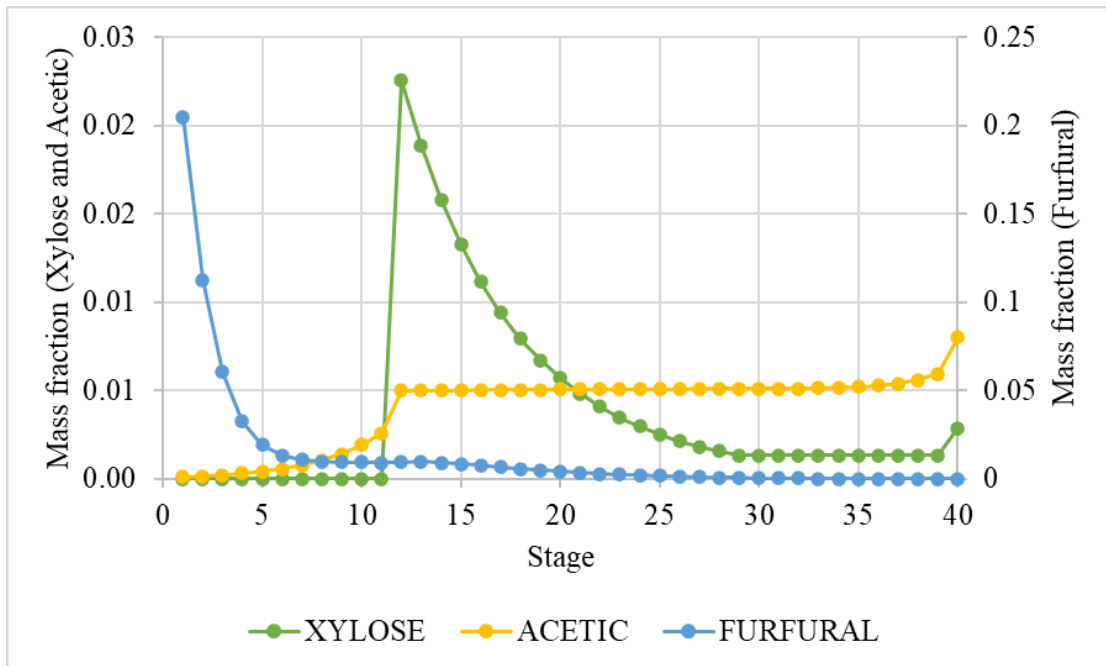


Figure 15 Composition profile in the reactive distillation column (scenario HPA-2).

4.4 SHAP Analysis

The feature importance analysis, conducted using SHAP values, provides critical insight into the factors driving the model outputs for TAC, revenues, and CO₂ emissions across both the HPA-RD (A) and DPTC-RD (B) configurations as shown in Figure 16, Figure 17, and Figure 18, respectively.

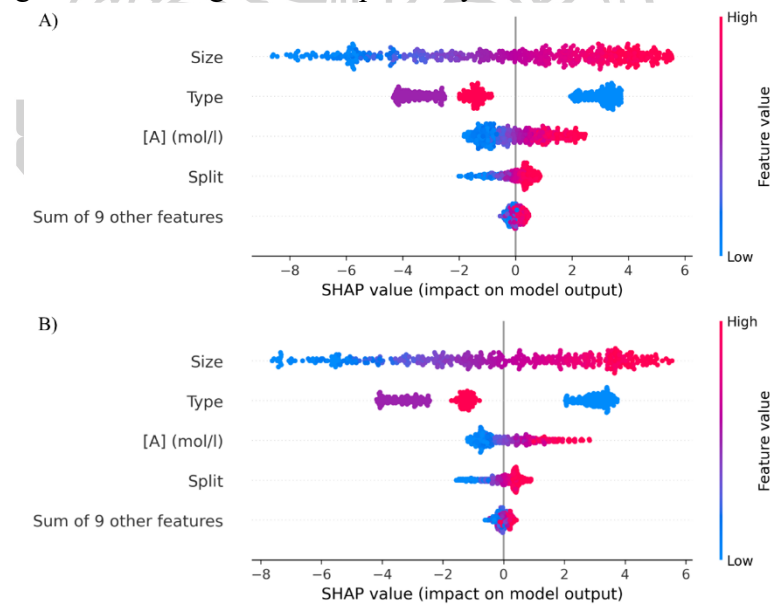


Figure 16 SHAP value of TAC for each configuration; A) HPA-RD, B) DPTC-RD.

The SHAP value analysis presented in Figure 16, Figure 17, and Figure 18 reveals the relative importance and directional impact of key design and operating variables on TAC, revenues, and CO₂ emissions for two HIRD configurations: HPA-RD and DPTC-RD. This analysis provides critical insights into the objective function

of individual process parameters, thereby elucidating which variables exert the greatest influence on economic viability and environmental sustainability.

The size of biomass feedstock had a highest impact on all objectives and all configurations, as increasing the size led to higher TAC, revenues, and CO₂ emissions. The concentration of acetic acid had a significant effect on the TAC, primarily due to the high cost associated with acetic acid. However, variations in acetic acid concentration had a negligible influence on revenue. Therefore, production without the addition of extra acetic acid is recommended to minimize costs without compromising profitability. The ratio of biomass allocated to the biorefinery (Split) significantly influenced the TAC, revenues, and CO₂ emissions. Increasing the Split led to higher TAC and revenues but resulted in lower CO₂ emissions. This trend can be attributed to the larger amount of biomass processed in the biorefinery, which enhanced profits from furfural production while converting more of the carbon in biomass into furfural. Moreover, the diameter and reactive stage of the reactive column had a greater effect than operating parameters such as reboiler duty, reflux ratio, and pressure. This finding suggests that optimizing the internal configuration of the column is crucial to ensure an appropriate residence time for the reaction within the reactive zone.

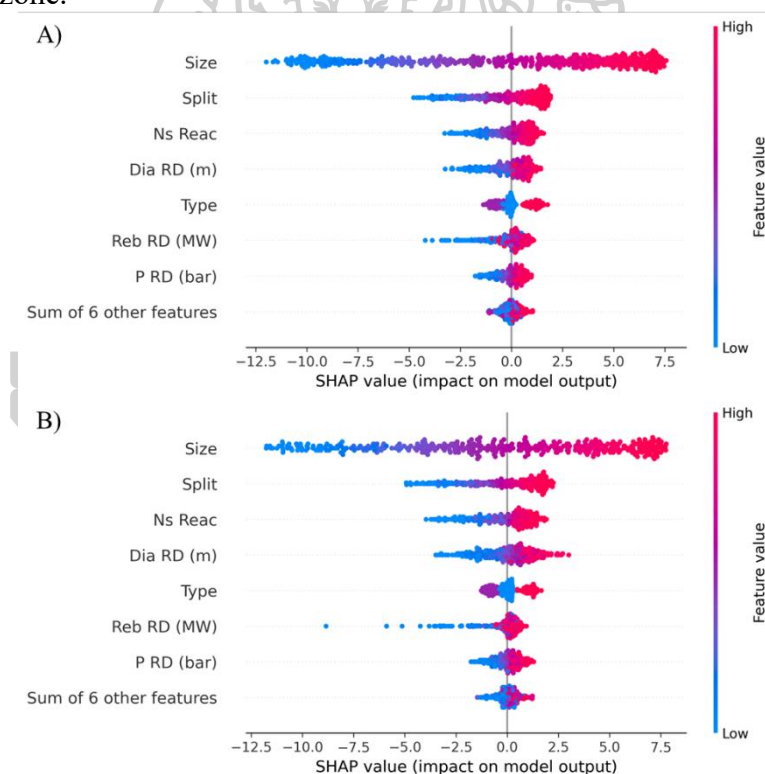


Figure 17 SHAP value of revenues for each configuration; A) HPA-RD, B) DPTC-RD.

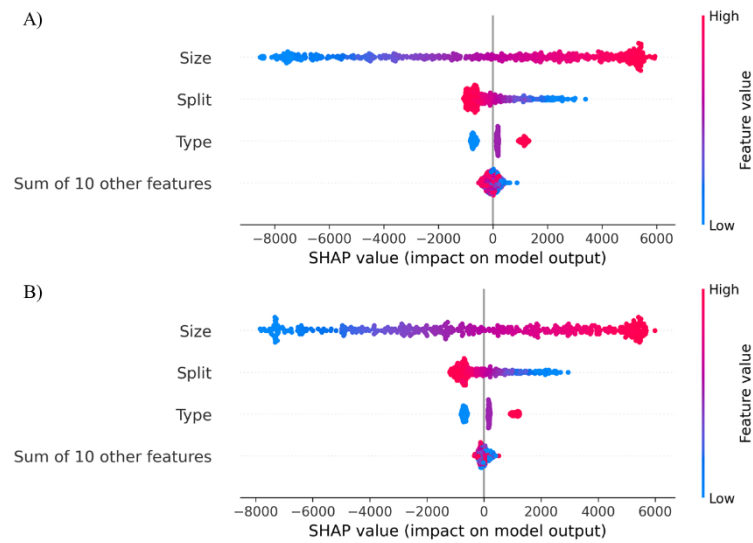


Figure 18 SHAP value of CO₂ emissions for each configuration; A) HPA-RD, B) DPTC-RD.

4.5 Economic evaluation

Table 14 and Table 15 summarize the detailed economic evaluation obtained under each scenario. The range of variation in revenues, costs, and investment parameters is substantial across the eight evaluated scenarios, indicating that the selected optimization objective fundamentally determines the economic scale of the optimal solution.

The economic evaluation comparing the HPA-RD and DPTC-RD systems across four distinct optimization configurations demonstrates that the DPTC-RD process is generally more resilient and effective in maintaining profitability under various operational and environmental constraints. The total revenues ranged from \$7,771,305 to \$35,004,229, with the revenue from furfural representing the largest share, about 45-80% of total revenues. The highest total revenues are obtained under the scenario DPTC-2, reaching \$35,004,229 per year. Raw material cost constituted the largest share of the operating expenses, primarily due to the high cost of biomass, about 80-95% of total operating cost. Moreover, the cost of acetic acid in scenarios HPA-3 and HPA-4 was a large share of the total operating cost. The total capital investment ranged from \$54,096,648 to \$114,765,748, with the CHP (S200) unit representing the largest share, about 25-32% of TCI. Moreover, Pretreatment (S100), Furfural (S300), and ORC (S400) accounted about 13%, 8-16%, and 3%, respectively. In the maximum revenues configuration, both systems exhibit comparable performance, achieving the shortest possible DPP of 6 years. However, the DPTC-RD system yields a slightly higher NPV than HPA-RD. When optimization is directed toward minimizing the TAC (HPA-1 and DPTC-1), DPTC-RD demonstrates clear superiority, with a higher IRR and a substantially shorter payback period. The DPTC-RD successfully decouples profitability from emission reduction constraints, achieving a notably strong TOPSIS solution (DPTC-4) with an IRR of 16.74% and a rapid DPP of 8 years. The NPV of DPTC-4 was decreased by approximately 44%, while CO₂ emission was reduced by about 41%. The IRR ranged from 6.87% to 20.85%, with four scenarios exceeding the minimum discount rate of 9.6% and thus

considered acceptable. The minimum TAC (DPTC-1) and TOPSIS (DPTC-4) scenarios resulted in reductions in IRR of approximately 43.6% and 19.7% compared to the highest IRR (20.85%), respectively. The DPTC-RD configurations outperformed the HPA-RD configurations. The results demonstrate greater profitability, resilience, and adaptability under varying conditions.

The ORC section for all scenarios can generate electricity for supply in production for about 23-87% of total electricity consumption. The revenue from this electricity ranged from 270,535 to 645,550 M\$/yr, which was a small portion when compared to the CHP section. However, the purchase cost of the ORC section was lowest when compared to other sections, which ranged from \$1,511,626 to \$2,640,020, leading to this section being able to rapidly return the capital investment. Consequently, the ORC section can be applied to the process for recovering waste heat.

The required selling price of furfural on economic feasibility in different scenarios was studied. As shown in Figure 19, the minimum selling price was obtained at an IRR of 9.6%. According to the economic results in Table 14 and Table 15, scenarios HPA-1, HPA-3, HPA-4, and DPTC-3 were not profitable at a furfural selling price of 1,700 \$/ton. However, scenarios HPA-1, HPA-3, and HPA-4 were profitable when furfural selling prices increased to 2,000 \$/ton, and scenario DPTC-3 was economically feasible when the furfural selling price increased to 1,800 \$/ton. In addition, the selling price of furfural in scenarios HPA-2 and DPTC-2 can be adjusted to approximately \$800/ton for acceptable IRR, and the selling price of furfural in scenarios DPTC-1 and DPTC-4 was \$1,400 and \$1,000/ton.

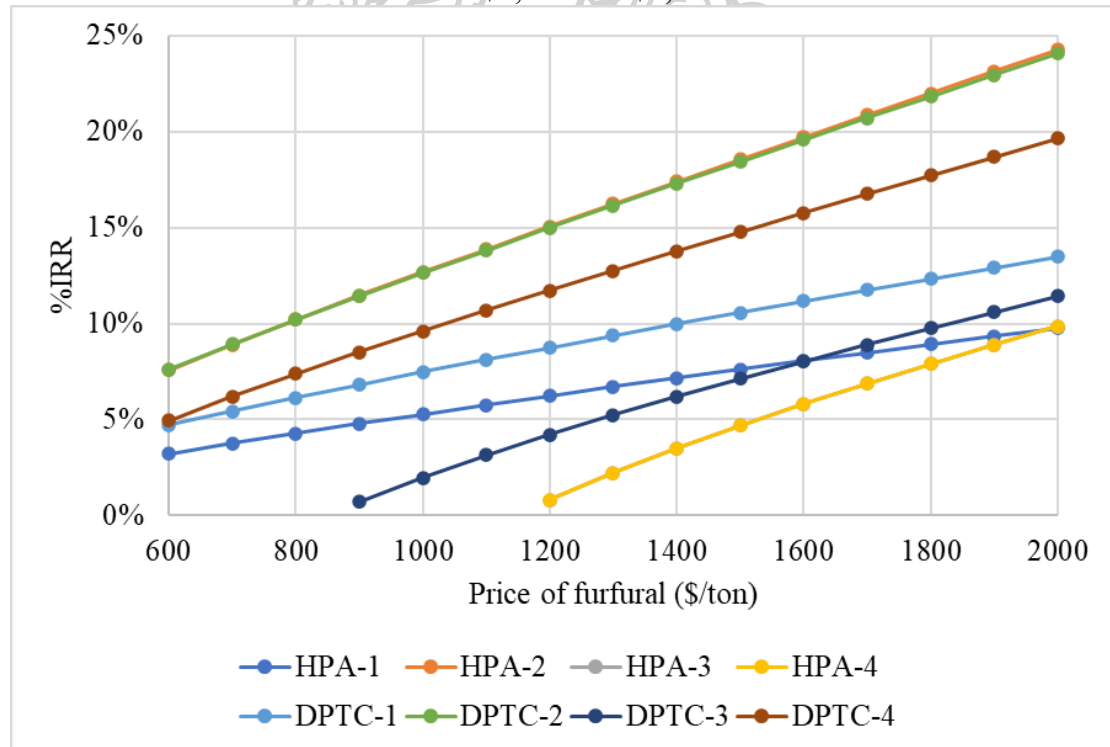


Figure 19 Effect of furfural selling price on IRR.

Table 14 Economic evaluation of optimal solution from HPA-RD.

Parameters	HPA-1	HPA-2	HPA-3	HPA-4
Total Revenues (\$/year)	7,771,305	34,570,170	11,755,356	11,755,356
Furfural	3,492,548	21,466,329	9,349,114	9,349,114
Electricity from CHP	4,008,221	12,580,873	2,073,369	2,073,369
Electricity from ORC	270,535	522,968	332,873	332,873
Total Raw Material (\$/year)	2,336,232	10,476,818	6,269,767	6,269,767
Biomass	2,125,000	9,906,750	4,972,500	4,972,500
H ₂ SO ₄	68,038	204,037	87,596	87,596
Lime	89,026	266,127	114,695	114,695
Water	54,168	99,904	36,963	36,963
Acetic acid	-	-	1,058,013	1,058,013
Total Waste Treatment (\$/year)	139,588	322,774	160,764	160,764
Gypsum	45,356	135,581	58,435	58,435
Ash	83,169	164,903	94,116	94,116
Waste water	11,063	22,290	8,214	8,214
Total Utility (\$/year)	103,758	321,211	103,661	103,661
Cooling water	103,758	321,211	103,661	103,661
Total Purchase Cost (\$)	31,106,586	62,191,177	35,822,183	35,822,183
Purchase cost of pretreatment	7,043,151	13,354,859	7,023,799	7,023,799
Purchase cost of CHP	18,061,143	35,662,016	16,476,752	16,476,752
Purchase cost of furfural production	4,377,733	10,818,824	10,490,889	10,490,889
Purchase cost of ORC	1,624,560	2,355,479	1,830,743	1,830,743
Total capital investment (TCI)	55,860,459	112,077,103	65,616,796	65,616,796
IRR (%)	8.49%	20.85%	6.87%	6.87%
NPV (\$) (i = 5%)	23,949,110	248,397,143	14,645,292	14,645,292
DPP (year) (i = 5%)	16	6	21	21

Table 15 Economic evaluation of optimal solution from DPTC-RD.

Parameters	DPTC-1	DPTC-2	DPTC-3	DPTC-4
Total Revenues (\$/year)	9,536,283	35,004,229	10,676,887	21,386,250
Furfural	5,170,519	21,638,552	6,831,174	14,157,711
Electricity from CHP	4,083,614	12,720,127	3,606,490	6,594,063
Electricity from ORC	282,150	645,550	239,223	634,476
Total Raw Material (\$/year)	2,370,584	10,524,648	5,206,794	6,146,406
Biomass	2,167,500	9,906,750	4,972,500	5,811,960
H ₂ SO ₄	69,398	204,037	77,960	119,704
Lime	90,806	266,127	102,079	156,131
Water	42,880	147,735	33,112	58,610
Acetic acid	-	-	21,143	-
Total Waste Treatment (\$/year)	140,227	330,884	153,897	189,309
Gypsum	46,264	135,581	52,007	79,542
Ash	84,832	164,903	94,578	96,743
Waste water	9,132	30,400	7,312	13,024
Total Utility (\$/year)	106,342	316,823	93,775	193,541
Cooling water	106,342	316,823	93,775	193,541
Total Purchase Cost (\$)	31,587,486	63,567,611	30,041,273	48,524,985
Purchase cost of pretreatment	7,126,647	13,354,859	6,553,806	9,705,370
Purchase cost of CHP	18,292,386	35,514,083	16,994,449	25,555,909
Purchase cost of furfural production	4,503,729	12,058,649	4,981,394	10,648,127
Purchase cost of ORC	1,664,723	2,640,020	1,511,626	2,615,578
Total capital investment (TCI)	56,733,771	114,765,748	54,096,649	87,889,262
IRR (%)	11.76%	20.69%	8.91%	16.74%
NPV (\$) (i = 5%)	49,630,216	251,588,568	26,184,763	140,499,151
DPP (year) (i = 5%)	11	6	15	8

Chapter 5 Conclusions and recommendation

5.1 Conclusions

The MOO of furfural and electricity co-production via heat-integrated reactive distillation was presented. The proposed process of furfural production consists of HPA-RD and DPTC-RD processes. These processes were simulated and optimized using Aspen Plus and Python programs. MLP models for TAC, revenues, and CO₂ emissions were developed using adaptive LHS, incorporating a small Pareto front and targeted LHS sampling around high-error sample and design-spec regions into new datapoints. The R^2 of 10-fold CV for all models exceeds 0.98, with a maximum MAPE of 3.5%. Moreover, the average error of the Pareto front for all models was accepted.

The NSGA-II with the ML-based surrogate model and TOPSIS were selected to find the Pareto front and optimal solution. The optimization results show that while both HPA-RD and DPTC-RD perform well under single-objective conditions, the DPTC-RD configuration consistently provides superior overall performance. Under minimum TAC, both systems achieve similar TAC, though DPTC-RD offers higher revenues. Maximizing revenues greatly increases TAC and CO₂ emissions for both configurations, reflecting the strong link between profitability and energy demand. CO₂ minimization scenarios reduce emissions but lower revenues, with DPTC-RD again achieving slightly better cost-emission trade-offs. The TOPSIS identified DPTC-RD as the superior configuration with a TAC of 11.38 M\$/year, CO₂ emissions of 11,619 kg/h, and a revenue of 21.39 M\$/year. This TOPSIS scenarios of DPTC-RD were balancing TAC, revenues, and emissions more effectively than HPA-RD. Consequently, HPA-RD achieves strong energy integration benefits, DPTC-RD provides greater flexibility and superior multi-objective performance.

The SHAP-based feature importance analysis reveals that biomass feed size is the dominant factor influencing TAC, revenues, and CO₂ emissions for both the HPA-RD and DPTC-RD configurations. Acetic acid concentration strongly affects TAC due to its cost but has little impact on revenues, indicating that operating without additional acetic acid is economically favorable. The biomass split into biorefinery also plays a major role, simultaneously increasing TAC and revenues while reducing CO₂ emissions as more biomass is processed into furfural. Furthermore, column design variables—particularly diameter and number of reactive stages—exert a stronger influence on model outputs than operating parameters such as reflux ratio, pressure, or reboiler duty. This underscores the importance of internal column configuration in achieving efficient reaction–separation performance. Overall, the feature importance results highlight which parameters most critically shape economic and environmental outcomes and provide clear guidance for targeted process optimization.

The DPTC-RD configuration demonstrates superior economic robustness compared to HPA-RD. DPTC-RD consistently delivers higher profitability than HPA-RD, including NPV, IRR, and shorter payback periods. In contrast, the HPA-RD system shows limited financial resilience, with its weakest performance observed under CO₂ minimization and TOPSIS. Key cost contributors include biomass feed and the CHP unit, which share about 80-95% of operating cost and 25-32% of TCI, respectively. In scenario DPTC-4, this process configuration offers a balance between

profitability and environmental impact, for which this process obtained an IRR of 16.74%, a DPP of 8 years, and an NPV of about \$140,499,151. The NPV of DPTC-4 was decreased by approximately 44%, while CO₂ emission was reduced by about 41%. In addition, the minimum selling price of furfural of scenario DPTC-4 can decreased to 1,000 \$/ton, which reduced from 1700 \$/ton about 41%.

5.2 Recommendation

In this work, the reactive columns were simulated by a rate-based model, for which the validation of NRTL and kinetic models is not sufficient for validating the rate-based model. Therefore, these models required more experimental results to validate mass and energy transfer behavior inside the reactive column. In the optimization framework, the boundaries of the decision variables must be carefully defined to avoid convergence issues in the Aspen Plus simulations, which could otherwise lead to inefficient or invalid optimization outcomes.



Appendix A

Multi-objective optimization

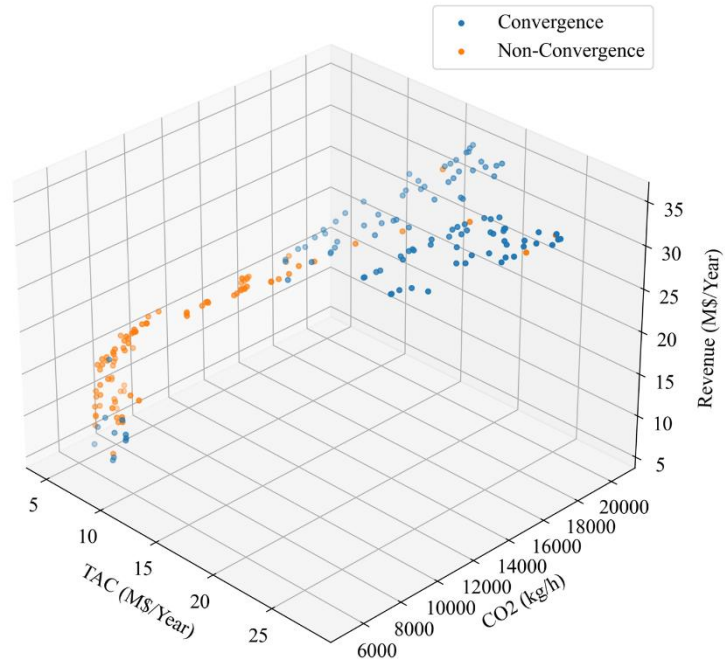


Figure 20 Pareto front of HPA-RD with non-convergence samples.

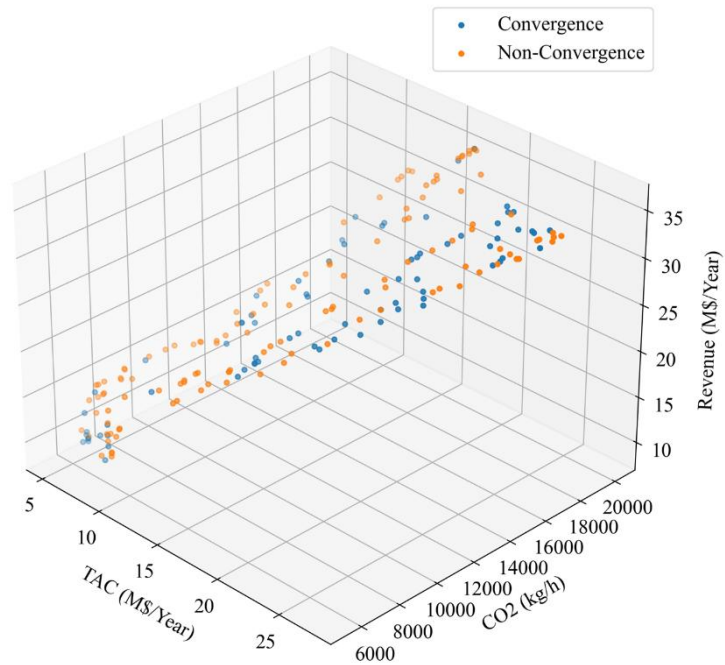


Figure 21 Pareto front of DPTC-RD with non-convergence samples.

Appendix B

Economic evaluation

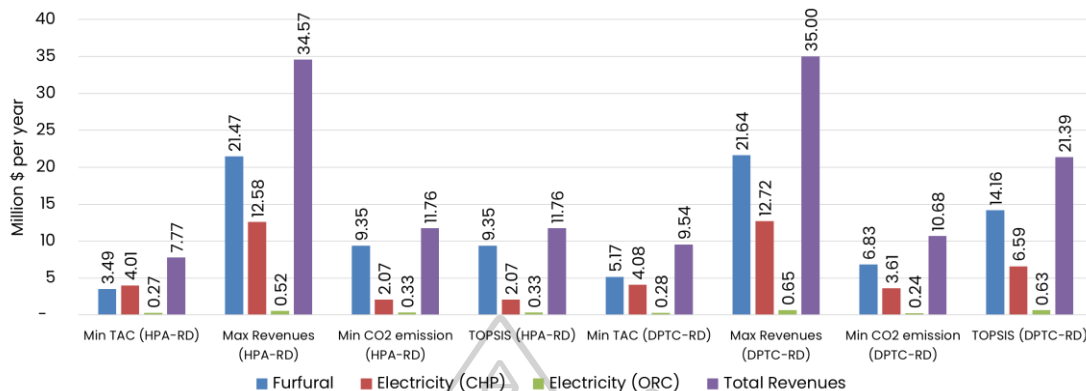


Figure 22 Revenues of each configuration.

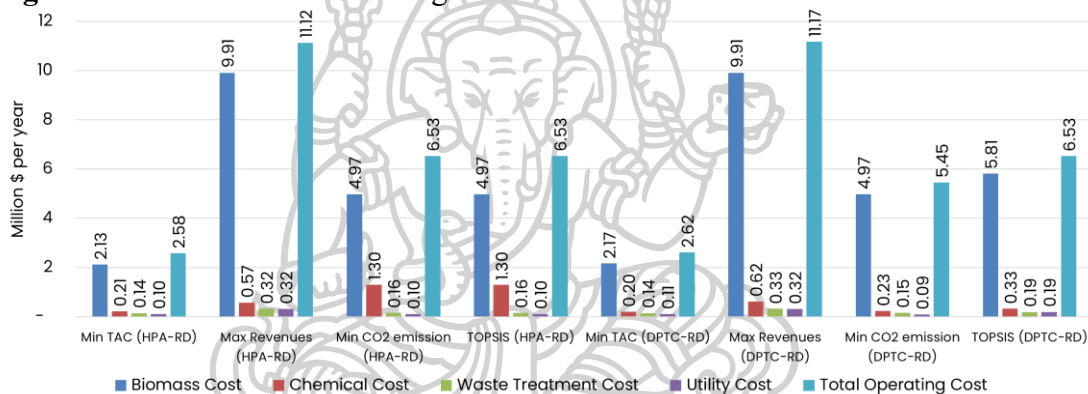


Figure 23 Operating cost of each configuration.

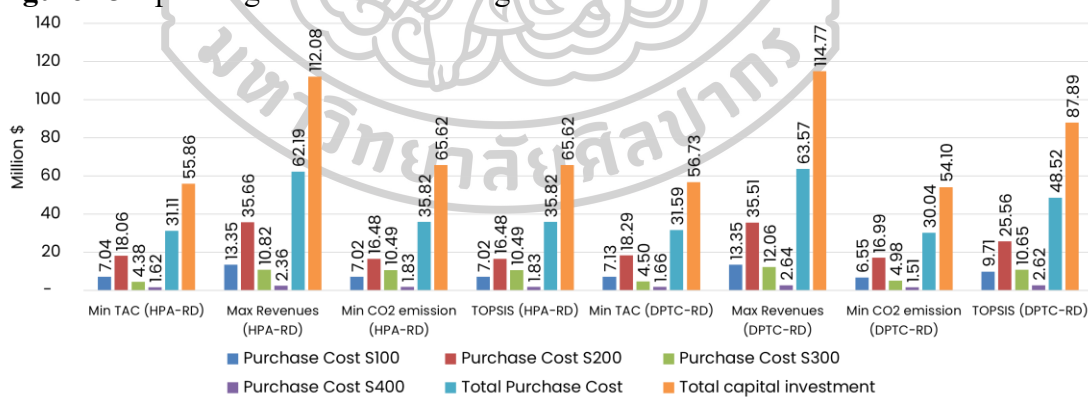


Figure 24 TCI of each configuration.

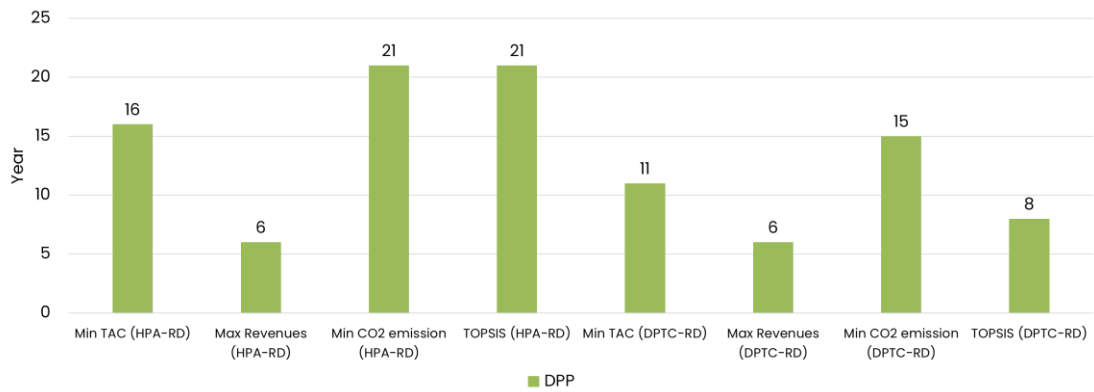


Figure 25 DPP of each configuration.

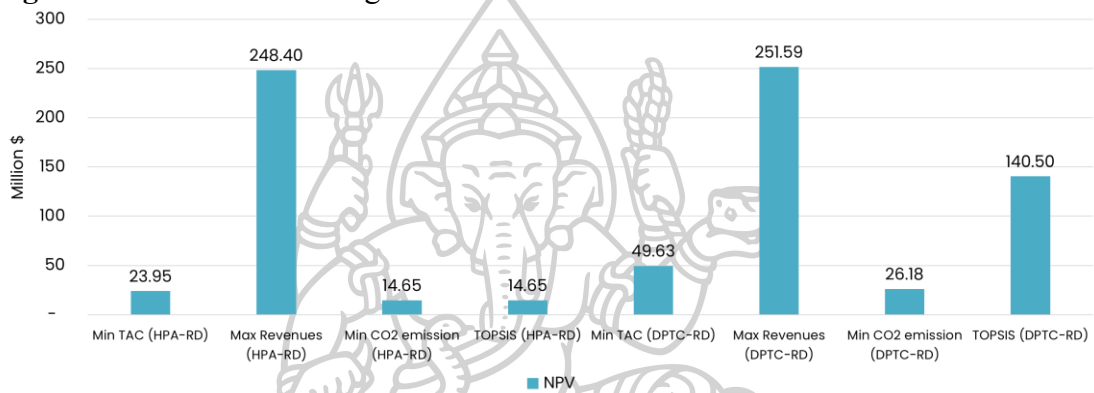


Figure 26 NPV of each configuration.

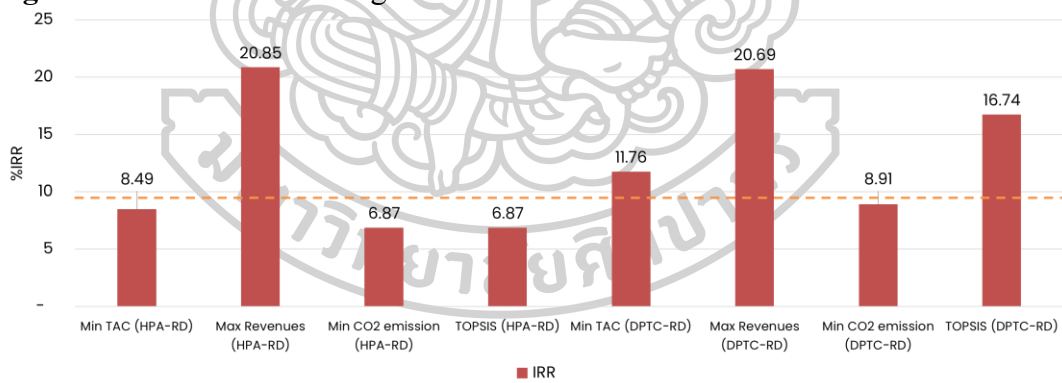


Figure 27 IRR of each configuration.

REFERENCES

- [1] IEA. "Key World Energy Statistics 2021." <https://www.iea.org/reports/key-world-energy-statistics-2021> (accessed 08/04/2025).
- [2] EPA. "Global Greenhouse Gas Overview." <https://www.epa.gov/ghgemissions/global-greenhouse-gas-overview> (accessed 08/04/2025).
- [3] NREL. "Biomass Energy Basics." <https://www.nrel.gov/research/re-biomass> (accessed 08/04/2025).
- [4] EIA. "Biomass explained." <https://www.eia.gov/energyexplained/biomass/> (accessed 08/04/2025).
- [5] T. Werpy and G. Petersen, "Top Value Added Chemicals from Biomass: Volume I -- Results of Screening for Potential Candidates from Sugars and Synthesis Gas," National Renewable Energy Lab (NREL), 2004.
- [6] K. J. Yong *et al.*, "Furfural production from biomass residues: Current technologies, challenges and future prospects," *Biomass and Bioenergy*, vol. 161, p. 106458, 2022/06/01/ 2022, doi: <https://doi.org/10.1016/j.biombioe.2022.106458>.
- [7] K. J. Zeitsch, *The chemistry and technology of furfural and its many by-products*. Elsevier, 2000.
- [8] Z. Liu, Z. Cui, M. Wang, B. Liu, and W. Tian, "A machine learning proxy based multi-objective optimization method for low-carbon hydrogen production," *Journal of Cleaner Production*, vol. 445, p. 141377, 2024/03/15/ 2024, doi: <https://doi.org/10.1016/j.jclepro.2024.141377>.
- [9] T. Shi, J. Zhou, Y. Ayub, S. Toniolo, and J. Ren, "Novel process optimization based on machine learning: A study on biohydrogen production from waste resources," *Biomass and Bioenergy*, vol. 185, p. 107222, 2024/06/01/ 2024, doi: <https://doi.org/10.1016/j.biombioe.2024.107222>.
- [10] G. Contreras-Zarazúa, M. Martin-Martin, E. Sánchez-Ramirez, and J. G. Segovia-Hernández, "Furfural production from agricultural residues using different intensified separation and pretreatment alternatives. Economic and environmental assessment," *Chemical Engineering and Processing - Process Intensification*, vol. 171, p. 108569, 2022/01/01/ 2022, doi: <https://doi.org/10.1016/j.cep.2021.108569>.
- [11] K. Wiranarongkorn, K. Im-orb, J. Panpranot, F. Maréchal, and A. Arpornwicheanop, "Exergy and exergoeconomic analyses of sustainable furfural production via reactive distillation," *Energy*, vol. 226, p. 120339, 2021/07/01/ 2021, doi: <https://doi.org/10.1016/j.energy.2021.120339>.
- [12] L. C. Nhien, N. V. D. Long, and M. Lee, "Novel Hybrid Reactive Distillation with Extraction and Distillation Processes for Furfural Production from an Actual Xylose Solution," *Energies*, vol. 14, no. 4, p. 1152, 2021. [Online]. Available: <https://www.mdpi.com/1996-1073/14/4/1152>.
- [13] J. Köchermann and M. Klemm, "Hydrothermal Reactive Distillation of Biomass and Biomass Hydrolysates for the Recovery and Separation of Furfural and Its Byproducts," *Industrial & Engineering Chemistry Research*, vol. 62, no. 18, pp. 6886-6896, 2023/05/10 2023, doi: 10.1021/acs.iecr.3c00259.
- [14] A. K. Jana, "Heat integrated distillation operation," *Applied Energy*, vol. 87, no.

- 5, pp. 1477-1494, 2010/05/01/ 2010, doi: <https://doi.org/10.1016/j.apenergy.2009.10.014>.
- [15] Z. Mekidiche, J. A. Labarta, J. Javaloyes-Anton, and J. A. Caballero, "From power to heat: Strategies for electrifying distillation for sustainable chemical processes," *Applied Thermal Engineering*, vol. 257, p. 124316, 2024/12/01/ 2024, doi: <https://doi.org/10.1016/j.applthermaleng.2024.124316>.
- [16] M. Adami, K. Farheen, and M. Skiborowski, "Electrifying distillation – Optimization-based evaluation of internally heat-integrated distillation columns," *Separation and Purification Technology*, vol. 360, p. 131061, 2025/07/08/ 2025, doi: <https://doi.org/10.1016/j.seppur.2024.131061>.
- [17] K. Wiranarongkorn, K. Im-Orb, D. Saebea, Y. Patcharavorachot, and A. Arpornwichanop, "Energy analysis and life cycle assessment of furfural and 5-hydroxymethylfurfural integrated biorefinery processes with heat pump-assisted reactive distillation," *Energy*, vol. 319, p. 134720, 2025/03/15/ 2025, doi: <https://doi.org/10.1016/j.energy.2025.134720>.
- [18] J. Li, H. Zhou, L. Sun, and N. Zhang, "Design and control of different pressure thermally coupled reactive distillation for synthesis of isoamyl acetate," *Chemical Engineering and Processing - Process Intensification*, vol. 139, pp. 51-67, 2019/05/01/ 2019, doi: <https://doi.org/10.1016/j.cep.2019.03.014>.
- [19] K. Wiranarongkorn, K. Im-orb, Y. Patcharavorachot, F. Maréchal, and A. Arpornwichanop, "Comparative techno-economic and energy analyses of integrated biorefinery processes of furfural and 5-hydroxymethylfurfural from biomass residue," *Renewable and Sustainable Energy Reviews*, vol. 175, p. 113146, 2023/04/01/ 2023, doi: <https://doi.org/10.1016/j.rser.2023.113146>.
- [20] G. Zang, A. Shah, and C. Wan, "Techno-economic analysis of an integrated biorefinery strategy based on one-pot biomass fractionation and furfural production," *Journal of Cleaner Production*, vol. 260, p. 120837, 2020/07/01/ 2020, doi: <https://doi.org/10.1016/j.jclepro.2020.120837>.
- [21] M. Nieder-Heitmann, K. F. Haigh, and J. F. Görgens, "Process design and economic analysis of a biorefinery co-producing itaconic acid and electricity from sugarcane bagasse and trash lignocelluloses," *Bioresource Technology*, vol. 262, pp. 159-168, 2018/08/01/ 2018, doi: <https://doi.org/10.1016/j.biortech.2018.04.075>.
- [22] J. F. L. Silva, M. A. Selicani, T. L. Junqueira, B. C. Klein, S. Vaz, and A. Bonomi, "Integrated furfural and first generation bioethanol production: Process simulation and technoeconomic analysis," *Brazilian Journal of Chemical Engineering*, Article vol. 34, no. 3, pp. 623-634, 2017, doi: 10.1590/0104-6632.20170343s20150643.
- [23] K. Aliyon, F. Rajaei, and J. Ritvanen, "Use of artificial intelligence in reducing energy costs of a post-combustion carbon capture plant," *Energy*, vol. 278, p. 127834, 2023/09/01/ 2023, doi: <https://doi.org/10.1016/j.energy.2023.127834>.
- [24] A. Samad, H. Saghir, A. Musawwir, I. Ahmad, and H. Caliskan, "A data-driven multi-objective optimization approach for enhanced methanol yield and exergy loss minimization in direct hydrogenation of CO₂," *Applied Thermal Engineering*, vol. 251, p. 123517, 2024/08/15/ 2024, doi: <https://doi.org/10.1016/j.applthermaleng.2024.123517>.
- [25] M. Lahafdoozian, H. Khoshkroudmansouri, S. H. Zein, and A. A. Jalil,

- "Hydrogen production from plastic waste: A comprehensive simulation and machine learning study," *International Journal of Hydrogen Energy*, vol. 59, pp. 465-479, 2024/03/15/ 2024, doi: <https://doi.org/10.1016/j.ijhydene.2024.01.326>.
- [26] J. Eason and S. Cremaschi, "Adaptive sequential sampling for surrogate model generation with artificial neural networks," *Computers & Chemical Engineering*, vol. 68, pp. 220-232, 2014/09/04/ 2014, doi: <https://doi.org/10.1016/j.compchemeng.2014.05.021>.
- [27] C. Nentwich and S. Engell, "Surrogate modeling of phase equilibrium calculations using adaptive sampling," *Computers & Chemical Engineering*, vol. 126, pp. 204-217, 2019/07/12/ 2019, doi: <https://doi.org/10.1016/j.compchemeng.2019.04.006>.
- [28] C. Nentwich, J. Winz, and S. Engell, "Surrogate Modeling of Fugacity Coefficients Using Adaptive Sampling," *Industrial & Engineering Chemistry Research*, vol. 58, no. 40, pp. 18703-18716, 2019/10/09 2019, doi: 10.1021/acs.iecr.9b02758.
- [29] P. Borisut and A. Nuchitprasittichai, "Adaptive Latin Hypercube Sampling for a Surrogate-Based Optimization with Artificial Neural Network," *Processes*, vol. 11, no. 11, p. 3232, 2023. [Online]. Available: <https://www.mdpi.com/2227-9717/11/11/3232>.
- [30] D. Humbird *et al.*, "Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover," National Renewable Energy Laboratory (NREL), Golden, CO., United States, 2011. [Online]. Available: <https://www.osti.gov/biblio/1013269>
- [31] Q.-Q. Wu, Y.-L. Ma, X. Chang, and Y.-G. Sun, "Optimization and kinetic analysis on the sulfuric acid – Catalyzed depolymerization of wheat straw," *Carbohydrate Polymers*, vol. 129, pp. 79-86, 2015/09/20/ 2015, doi: <https://doi.org/10.1016/j.carbpol.2015.04.053>.
- [32] M. Ali Mandegari, S. Farzad, and J. F. Görgens, "Economic and environmental assessment of cellulosic ethanol production scenarios annexed to a typical sugar mill," *Bioresource Technology*, vol. 224, pp. 314-326, 2017/01/01/ 2017, doi: <https://doi.org/10.1016/j.biortech.2016.10.074>.
- [33] Z. Chen, W. Zhang, J. Xu, and P. Li, "Kinetics of xylose dehydration into furfural in acetic acid," *Chinese Journal of Chemical Engineering*, vol. 23, no. 4, pp. 659-666, 2015/04/01/ 2015, doi: <https://doi.org/10.1016/j.cjche.2013.08.003>.
- [34] Y. Benjamin, H. Cheng, and J. F. Görgens, "Optimization of Dilute Sulfuric Acid Pretreatment to Maximize Combined Sugar Yield from Sugarcane Bagasse for Ethanol Production," *Applied Biochemistry and Biotechnology*, vol. 172, no. 2, pp. 610-630, 2014/01/01 2014, doi: 10.1007/s12010-013-0545-z.
- [35] D. J. Schell, R. Torget, A. Power, P. J. Walter, K. Grohmann, and N. D. Hinman, "A technical and economic analysis of acid-catalyzed steam explosion and dilute sulfuric acid pretreatments using wheat straw or aspen wood chips," *Applied Biochemistry and Biotechnology*, vol. 28, no. 1, pp. 87-97, 1991/03/01 1991, doi: 10.1007/BF02922591.
- [36] J. Nondy and T. K. Gogoi, "Exergoeconomic investigation and multi-objective optimization of different ORC configurations for waste heat recovery: A comparative study," *Energy Conversion and Management*, vol. 245, p. 114593,

2021/10/01/ 2021, doi: <https://doi.org/10.1016/j.enconman.2021.114593>.



VITA

NAME

Patcharapuek Pattaramanon

**INSTITUTIONS
ATTENDED**

Bachelor degree of Engineering (CHEMICAL
ENGINEERING)
Department of CHEMICAL ENGINEERING
Graduate School, Silpakorn University

