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Surrogate-Based Steady-State Modeling of a Refinery Wastewater Treatment Train Using Aspen Plus

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Abstract
The integration of refinery wastewater treatment systems into refinery-wide optimization workflows remains challenging because commercial process simulators lack native wastewater treatment unit operations. Existing studies also provide limited attention to validated surrogate-based representations and energy-performance tradeoff analysis. This study develops a validated steady-state surrogate framework for modeling and optimizing an integrated refinery wastewater treatment train using Aspen Plus. The treatment configuration included gravity separation, dissolved air flotation (DAF), aerobic biological oxidation, and granular activated carbon polishing. Oil and grease, soluble organics, and dissolved solids were represented using n-decane, phenol, and sodium chloride, respectively. Treatment units were implemented using separator split fractions, flash operations, empirical recycle-dependent DAF relationships, and stoichiometric reactor configurations under the electrolyte non-random two-liquid Redlich-Kwong (ENRTL-RK) property method. Model predictions showed strong agreement with refinery laboratory data, producing effluent concentrations of 9.0 mg/L oil and grease, 0.5 mg/L phenol, and 1296 mg/L dissolved solids, with an overall AARD of 3.43% and $R^2 = 0.998$. *Sensitivity-based optimization demonstrated that recycle ratios between 0.24 and 0.25 minimized pumping duty while maintaining discharge compliance, whereas aeration rates above approximately 60 kg/h produced negligible additional phenol degradation despite increasing compressor energy demand. The study introduces a validated and reproducible methodology for representing non-native wastewater treatment operations within Aspen Plus while demonstrating the potential of surrogate-based process simulation for refinery wastewater optimization, energy minimization, and sustainability-oriented process integration.*
Keywords: *Refinery wastewater treatment, Optimization, Modeling, Aspen Plus*

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I. INTRODUCTION

Petroleum refinery wastewater contains hydrocarbons, phenolic compounds, suspended solids, sulfides, ammonia, heavy metals, and dissolved salts that can severely impair aquatic ecosystems and industrial sustainability when inadequately treated (Wake, 2005; Diya'uddeen et al., 2017; Thorat et al., 2022). Discharge of untreated refinery effluents contributes to aquatic toxicity, oxygen depletion, groundwater contamination, and long-term ecological degradation, thereby increasing pressure on refineries to adopt environmentally sustainable treatment strategies (Crini&Lichtfouse, 2019; Varjani et al., 2020). Simultaneously, increasingly stringent discharge regulations, rising energy costs, and global decarbonization targets have intensified the need for refinery wastewater treatment systems that are not only environmentally compliant but also operationally efficient and energy conscious (World Bank Group, 2017). Conventional refinery wastewater treatment trains commonly integrate gravity separation, dissolved air flotation (DAF), aerobic biological oxidation, and tertiary polishing processes to achieve acceptable discharge quality (Palaniandy et al., 2018; Farzana et al., 2022; Thorat &Sonwani, 2022). However, treatment performance remains highly sensitive to operating variables such as recycle ratio, aeration intensity, hydraulic loading, and contaminant concentration, all of which directly influence pollutant removal efficiency, process stability, and operational energy demand (Flores-Alsina et al., 2016; Ali & Aziz, 2023; Wang et al., 2024; Kato & Kansha, 2024). In industrial practice, these variables are frequently selected conservatively to minimize compliance risk, often resulting in excessive aeration duty, elevated recycle pumping requirements, and unnecessary operating costs (Rivas et al., 2019; Wang et al., 2024; Chen et al., 2020). Consequently, improving the energy-performance efficiency of refinery wastewater treatment systems has become increasingly important for sustainable refinery operation and environmental compliance.

Process simulation has emerged as an important tool for evaluating industrial treatment systems and optimizing operational conditions without disrupting refinery operations (Yao et al., 2022; Wang et al., 2024). Specialized wastewater simulators such as GPS-X, WEST, and BioWin provide detailed biological process modeling capabilities, including activated sludge kinetics and nutrient transformation analysis (Minnana et al., 2021; Hauduc et al., 2013). Nevertheless, petroleum refineries predominantly employ general-purpose process simulators such as Aspen Plus because of their compatibility with refinery process integration, thermodynamic analysis, equipment sizing, and energy-evaluation workflows (Adams, 2022; Bezzera et al., 2021; Haydary, 2019)). Despite these advantages, Aspen Plus lacks native unit operation models for conventional wastewater treatment processes such as API separators, DAF systems, and activated sludge reactors, thereby limiting its direct applicability to refinery wastewater optimization studies (Schneider et al., 2022; Mannina et al., 2016; Yao et al,. 2022). Existing Aspen-based investigations have primarily focused on isolated membrane systems, desalting operations, advanced oxidation technologies, or zero-liquid-discharge processes rather than validated simulations of integrated refinery wastewater treatment trains (Elmobarak et al., Chen et al., 2020; Varjan et al., 2020). Furthermore, many reported studies lack refinery laboratory validation, statistical performance evaluation, and explicit energy-performance optimization under realistic industrial operating conditions (Schneider et al., 2018; Thorat et al., 2022; Wang et al., 2024). Consequently, a significant knowledge gap still exists in the development of validated refinery-applicable simulation frameworks capable of integrating surrogate-based process representation, thermodynamic consistency, statistical validation, and energy-aware operational optimization within a unified refinery engineering platform. To address these limitations, this study develops a validated surrogate-based steady-state simulation and optimization framework for an integrated refinery wastewater treatment train using Aspen Plus. The modeled system incorporates gravity separation, dissolved air flotation, aerobic biological oxidation, and granular activated carbon polishing. Dominant contaminant groups were represented using n-decane, phenol, and sodium chloride as surrogates for oil and grease, soluble organics, and dissolved solids, respectively. Treatment processes were implemented using separator split fractions, empirical recycle-dependent DAF relationships, flash operations, and stoichiometric reactor configurations under the electrolyte non-random two-liquid Redlich-Kwong (ENRTL-RK) thermodynamic framework (Adams, 2022; Haydary, 2019; Henze et al., 2016; Tchobanoglous et al., 2014). Unlike previous studies, the developed framework uniquely integrates surrogate-based process representation, refinery laboratory validation, statistical error analysis, and energy-aware optimization of DAF recycle ratio and biological aeration demand under environmental discharge constraints. The study therefore contributes a validated and reproducible methodology for extending Aspen Plus to refinery wastewater applications while demonstrating the feasibility of surrogate-based simulation for integrated refinery wastewater optimization, operational decision support, environmental compliance assessment, and sustainability-oriented refinery process analysis.

II. MATERIALS AND METHODS

2.1 Research Framework and Simulation Strategy

The integrated methodological framework employed in this study is illustrated in Figure 1. A surrogate-based steady-state Aspen Plus simulation framework was developed to represent, validate, and optimize the performance of a refinery wastewater treatment train under environmental discharge constraints. The approach was designed to bridge the gap between refinery process simulation and wastewater treatment analysis by enabling refinery-compatible representation of conventional treatment operations within a generalized process systems environment. Unlike dedicated wastewater modeling platforms that primarily emphasize microbial kinetics and sludge process dynamics, the present framework focused on process integration, thermodynamic reliability, operational realism, and energy-performance evaluation. The refinery wastewater stream considered in this work represented a combined desalter wastewater generated after equalization of process and utility effluents. Wastewater quality data and operating information used for model development were derived from industrial laboratory measurements and operational records obtained from an operating refinery facility. However, due to industrial confidentiality agreements, refinery identity and proprietary operational details are not disclosed. Accordingly, selected process variables were presented within representative refinery operating ranges while preserving the validity of the simulation, calibration, and optimization analyses. The methodological workflow comprised wastewater characterization, surrogate selection, Aspen Plus flowsheet development, model calibration, statistical validation, and sensitivity-based optimization of key operating variables affecting treatment efficiency and energy demand.

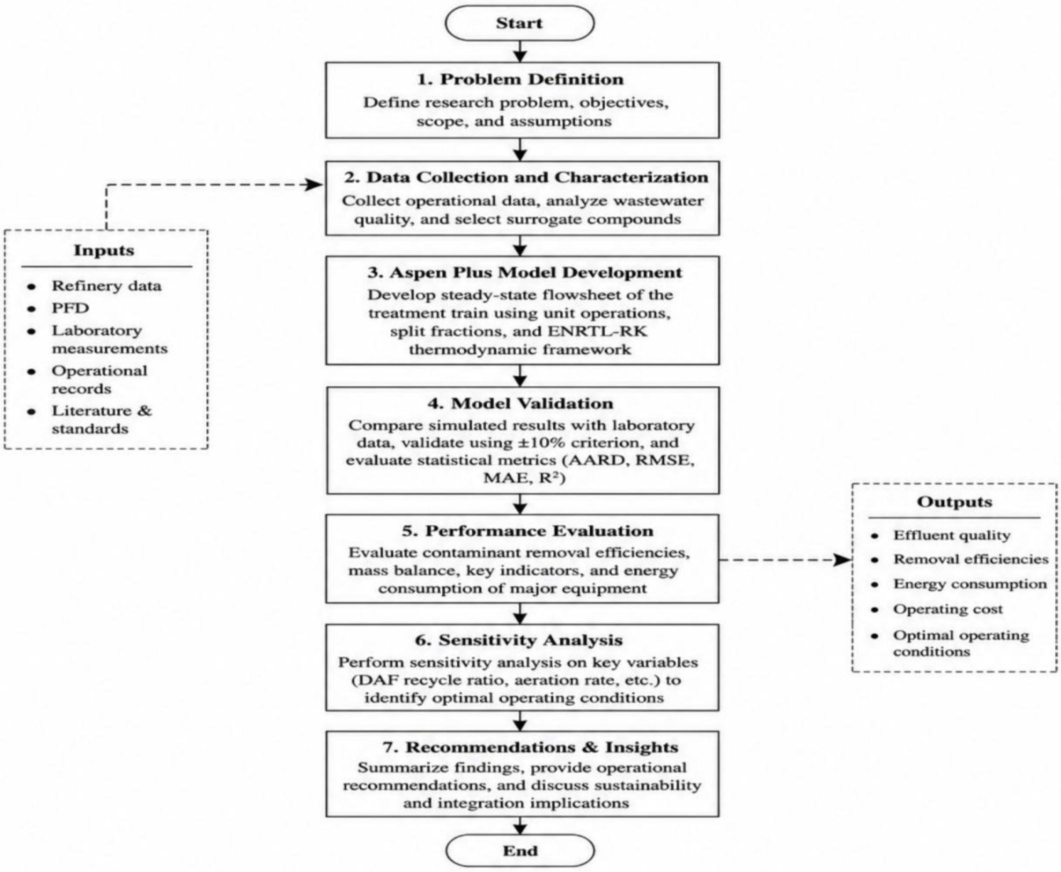


Figure 1. Methodological framework adopted for surrogate-based Aspen Plus modeling and optimization of the refinery wastewater treatment system

The developed treatment train incorporated gravity oil separation, dissolved air flotation (DAF), aerobic biological oxidation, and granular activated carbon (GAC) polishing, as shown in Figure 2. Optimization analysis focused primarily on DAF recycle ratio and biological aeration demand because recycle pumping and compressed-air supply constitute the dominant contributors to operational energy consumption in conventional refinery wastewater treatment systems.

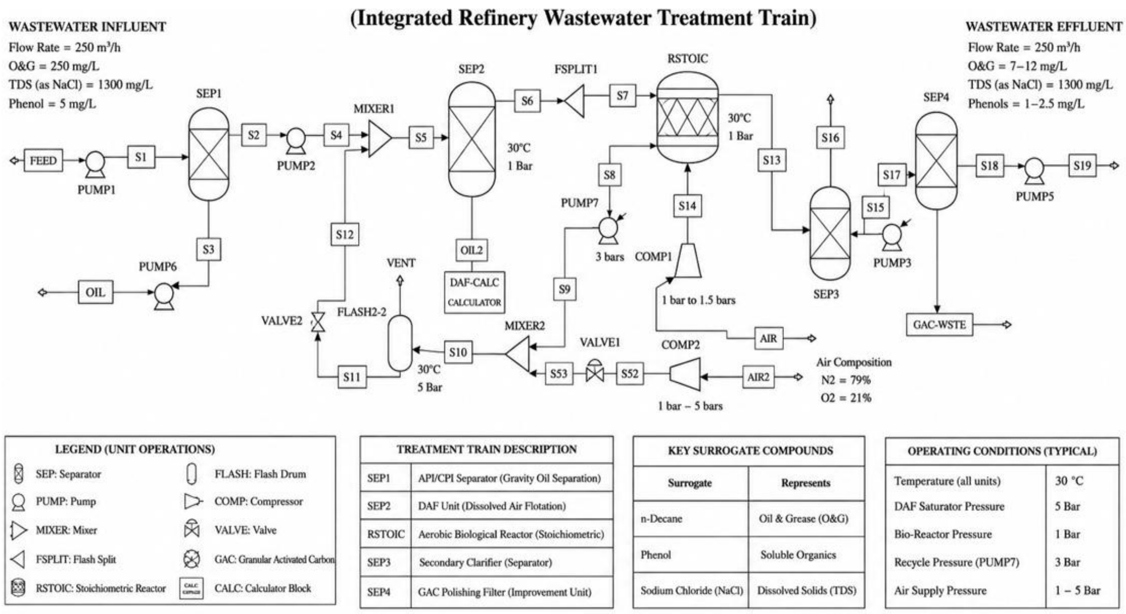


Figure 2. Aspen Plus flowsheet representation of the integrated refinery wastewater treatment train

2.2Aspen Plus Model Development and Process Representation

Aspen Plus flowsheet developed for the integrated refinery wastewater treatment train is shown in Figure 2. The treatment train comprised gravity separation (SEP1), dissolved air flotation (SEP2), aerobic biological oxidation (RSTOIC), secondary clarification (SEP3), and granular activated carbon (GAC) polishing (SEP4), supported by auxiliary pumps, compressors, mixers, flash drums, valves, and recycle splitters. Influent wastewater first passed through the gravity separator (SEP1), where free oil and settleable solids were removed by density-based separation. The partially treated stream then entered the DAF unit (SEP2), where a pressurized recycle stream generated microbubbles for enhanced flotation of dispersed oil droplets. To account for the effect of recycle flow on flotation performance, DAF oil removal efficiency was represented using a recycle-dependent empirical relationship:

$$\eta_{DAF} = \min\left(\eta_{base} + k(R - 0.10), \eta_{max}\right)$$

where: $\eta_{base} = 0.85$, $k = 0.25$, Rrepresents recycle ratio and $\eta_{max} = 0.90$. The relationship captures recycle-enhanced flotation behavior while constraining removal efficiency within realistic operational limits. Biological treatment was represented using a stoichiometric reactor (RSTOIC) under aerobic conditions. Phenol degradation was modeled using the overall oxidation reaction:

$$C_6H_5OH + 7O_2 \rightarrow 6CO_2 + 3H_2O$$

Compressed air supplied through COMP1 maintained aerobic operation, while a downstream separator (SEP3) removed gaseous products prior to final polishing in the GAC unit (SEP4).

2.3 Wastewater Characterization and Surrogate Selection

The refinery wastewater considered in this study was characterized using key regulatory and operational indicators, including oil and grease (O&G), phenols, total dissolved solids (TDS), temperature, pH, and flow rate. The influent composition and effluent discharge specifications adopted for model development and performance evaluation are presented in Tables 1 and 2, respectively. To enable practical implementation of refinery wastewater treatment processes within Aspen Plus, a surrogate-based contaminant representation strategy was adopted. n-decane, phenol, and sodium chloride (NaCl) were selected to represent oil and grease, biodegradable soluble organics, and dissolved solids, respectively. These surrogate compounds were chosen to preserve the dominant separation, transport, and degradation characteristics of the principal pollutant classes while reducing wastewater compositional complexity. Treatment unit performance was represented using literature-derived contaminant removal efficiencies and split fractions for gravity separation, dissolved air flotation, biological oxidation, and granular activated carbon polishing processes (Henze et al., 2016).

Table1. Influent Wastewater Characteristics Used for Model Development

Property	Quantity/Concentration	Unit
Flow Rate	250	m^3/h
Temperature	30 (max)	°C
Oil and Grease	250	mg/L
Phenols	20	mg/L
Total Dissolved Solids	1300	mg/L

Table 2. Effluent Discharge Targets Used for Validation and Optimization

Property	Quantity/Concentration	Unit
pH	6.5–8.5	–
Temperature	<30	°C
Oil and Grease	≤10	mg/L
Phenols	≤0.5	mg/L
Total Dissolved Solids	1300	mg/L

During model calibration, these parameters were adjusted within reported engineering ranges to improve agreement between simulated and measured effluent concentrations. The validated removal efficiencies employed in the final simulation model are summarized in Table 3.

Table 3. Literature-Derived Removal Efficiencies Applied in the Simulation Model

Unit Operation	Component	Removal Efficiency Range (%)
API/CPI Separator	Oil and Grease, TSS	50–70
Coagulation/Flocculation	O&G, TSS, COD	60–90
Dissolved Air Flotation	Oil and Grease	85–90
Biological Treatment	Phenol (COD)	85–95
GAC Polishing	Phenols, COD	40–60
All Units	TDS (NaCl)	0

2.4 Thermodynamic Framework and Block Selection

The refinery wastewater treatment train was modeled in Aspen Plus using separator (SEP), flash (FLASH2), mixer, splitter, compressor, pump, and stoichiometric reactor (RSTOIC) blocks to reproduce the principal physical and chemical treatment processes. Separator blocks were employed to simulate gravity separation, dissolved air flotation, clarification, and adsorption through component-specific split fractions, while the FLASH2 block represented the pressurized saturator section of the DAF recycle loop. Compressors, pumps, and valves were incorporated to capture pressure-dependent aeration and recycle operations within the treatment train.The electrolyte non-random two-liquid Redlich–Kwong (ENRTL-RK) property method was selected to describe phase and thermodynamic behavior within the mixed hydrocarbon–organic–electrolyte system. By integrating electrolyte activity-coefficient calculations with the Redlich–Kwong equation of state, ENRTL-RK provides reliable representation of aqueous non-idealities, electrolyte interactions, and vapor–liquid equilibrium behavior in streams containing dissolved salts, hydrocarbons, and polar organic compounds. The property method was therefore considered appropriate for modeling refinery wastewater characterized by simultaneous organic and inorganic contaminant interactions.

2.5 Model Validation, Statistical Analysis, and Optimization

Model calibration and validation were undertaken to verify the ability of the developed simulation framework to reproduce refinery wastewater treatment performance under steady-state operating conditions. Simulated effluent concentrations of oil and grease (O&G), phenol, and total dissolved solids (TDS) were compared against corresponding refinery laboratory measurements.A maximum deviation of ±10% between simulated and measured values was adopted as the validation criterion, consistent with commonly accepted environmental process modeling practice (Lawan et al., 2023). Where discrepancies exceeded this tolerance, contaminant split fractions, stoichiometric conversion extents, and recycle-dependent removal parameters were iteratively adjusted within literature-supported engineering limits until acceptable agreement was achieved.To further evaluate predictive performance, statistical validation metrics including Absolute Average Relative Deviation (AARD), Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and the coefficient of determination (R^2) were calculated. AARD was determined using:

$$AARD(\%) = \frac{100}{N}\sum_{i=1}^{N} \left| \frac{X_{exp} - X_{sim}}{X_{exp}} \right|$$

where $X_{exp}$and X_{sim}denote experimental and simulated values, respectively, and Nrepresents the number of observations. Low AARD, RMSE, and MAE values, together with an R^2value approaching unity, were interpreted as evidence of satisfactory predictive accuracy and model robustness.

Following validation, sensitivity-based optimization was performed using Aspen Plus Sensitivity Analysis tools. Two operational variables were investigated: DAF recycle ratio and biological reactor airflow rate. The optimization objective was to minimize pumping and compressor energy consumption while maintaining compliance with discharge limits of O&G ≤ 10 mg/L and phenol ≤ 0.5 mg/L. Optimal operating conditions were therefore defined as the minimum recycle ratio and aeration requirement capable of satisfying environmental discharge standards with the lowest practical energy demand.

III. Results and Discussion

3.1 Model Validation and Predictive Performance

The developed surrogate-based Aspen Plus framework was validated by comparing simulated effluent concentrations with refinery laboratory measurements for the principal discharge parameters: oil and grease (O&G), phenol, and total dissolved solids (TDS). Validation was performed using literature-constrained split fractions and removal efficiencies representing the major treatment processes within the refinery wastewater treatment train. The comparison between experimental and simulated values is summarized in Table 4.while the overall validation performance is illustrated in Figure 4.

Table 4. Laboratory and Simulated Effluent Comparison

Parameter (mg/L)	Influent	Laboratory Effluent	Simulated Effluent	% Deviation	Validation Criterion
O&G (asdecane)	250	10.0	9.0	-10.0	±10% ✓
Phenol	20	0.5	0.5	0.0	±10% ✓
TDS (as NaCl)	1300	1300	1296	-0.3	±10% ✓

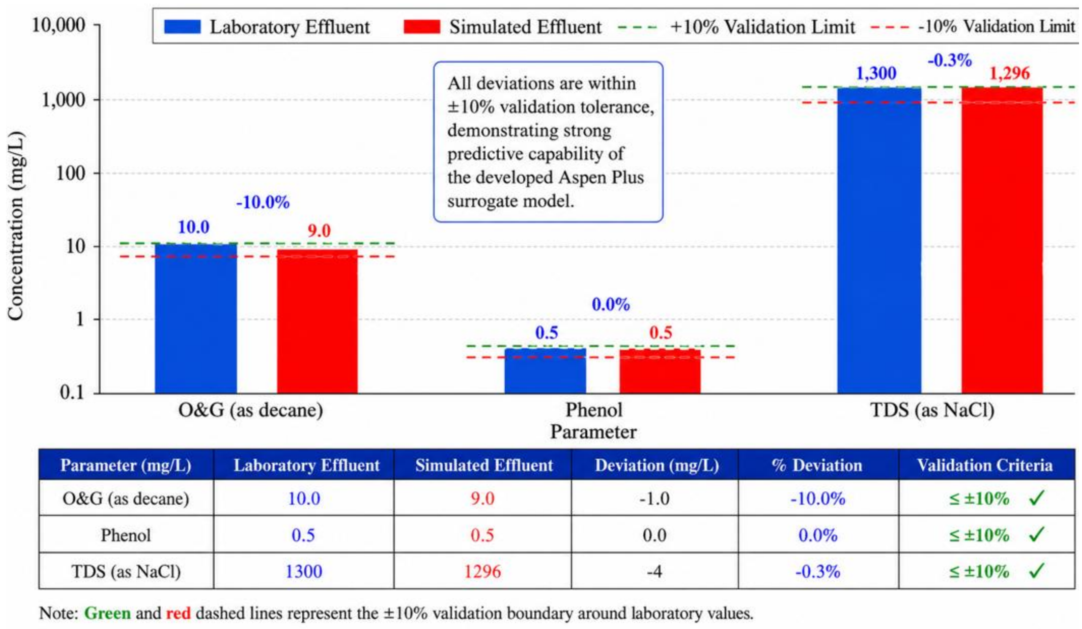


Figure 4. Validation performance of the surrogate-based Aspen Plus model relative to refinery laboratory measurements.

All simulated parameters satisfied the predefined ±10% validation criterion, confirming acceptable predictive capability of the developed framework. The simulated O&G concentration of 9.0 mg/L closely matched the measured refinery value of 10.0 mg/L, corresponding to a deviation of 10%. Similarly, phenol concentration was predicted exactly at the measured value of 0.5 mg/L, while TDS deviation remained negligible at approximately 0.3%.To strengthen statistical rigor, additional validation metrics including Absolute Average Relative Deviation (AARD), Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and coefficient of determination (R^2) were evaluated. The developed framework produced an overall AARD of 3.43%, while the parity between measured and simulated values yielded an R^2 value of 0.998, indicating excellent agreement between model predictions and refinery observations. The low prediction error demonstrates that the selected surrogate compounds and simplified unit representations were sufficient to reproduce the dominant treatment behavior of the refinery wastewater train despite the absence of native wastewater treatment operations within Aspen Plus.

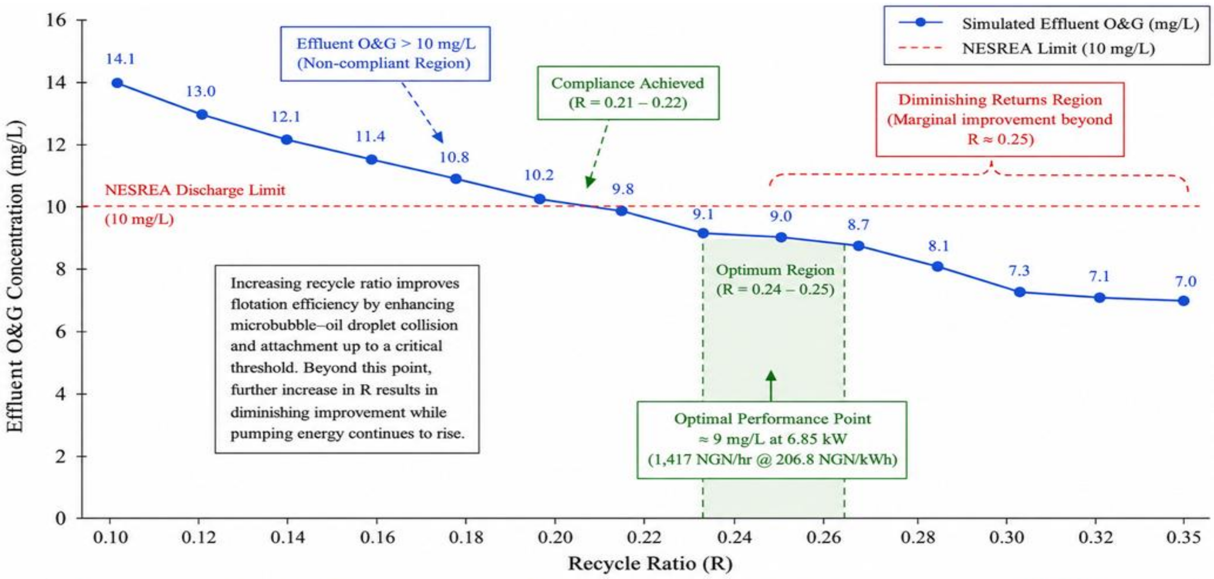
Table 5. Statistical Validation Metrics for Model Predictions

Validation Metric	Value	Interpretation
Absolute Average Relative Deviation (AARD, %)	3.43	Indicates low overall prediction error and strong agreement between experimental and simulated values
Root Mean Square Error (RMSE)	2.38 mg/L	Demonstrates low dispersion between simulated and measured effluent concentrations
Mean Absolute Error (MAE)	1.67 mg/L	Confirms minimal average deviation across all validated parameters
Coefficient of Determination (R^2)	0.998	Indicates excellent correlation and predictive consistency
Validation Criterion	±10%	All simulated parameters satisfied the predefined engineering tolerance

The agreement between measured and simulated effluent quality demonstrates that the developed surrogate-based framework provides a realistic representation of refinery wastewater treatment performance. Accurate prediction of O&G and phenol removal, together with the conservative behavior of TDS, confirms the robustness of the selected surrogate compounds and process models. These results address a key limitation of conventional refinery simulators by providing a practical methodology for integrating wastewater treatment analysis and energy-performance optimization within Aspen Plus.

3.2 Optimization of Dissolved Air Flotation Performance

Sensitivity analysis of the dissolved air flotation (DAF) unit was performed by varying the recycle ratio from 0.10 to 0.35 while maintaining a saturator pressure of 5 bar. The corresponding effect on effluent oil and grease (O&G) concentration is presented in Figure 5.



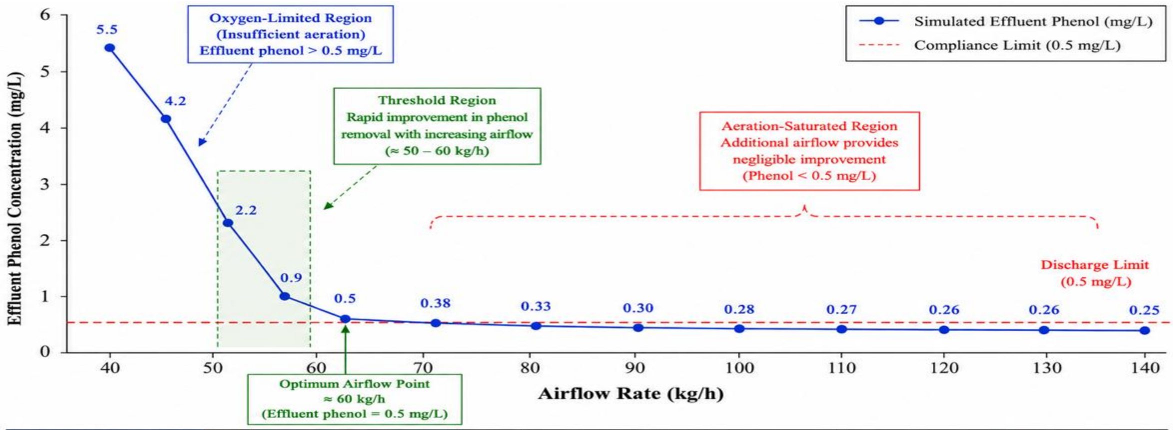
Parameter	Recycle Ratio Range	0.21 – 0.22	0.24 – 0.25 (Optimum)	0.26 – 0.35
Value	11 – 14 mg/L (Non-compliant)	≈ 10 mg/L (Compliance Achieved)	≈ 9 mg/L at 6.85 kW	7 – 8 mg/L (Diminishing Returns)

Figure 5. Effect of DAF recycle ratio on effluent oil and grease concentration.

Effluent O&G concentration decreased with increasing recycle ratio because enhanced microbubble generation improved the flotation of dispersed oil droplets. At recycle ratios below 0.20, predicted O&G concentrations exceeded the NESREA discharge limit of 10 mg/L (NESREA, 2011). Compliance was achieved at approximately 0.21–0.22, after which the rate of improvement declined. Beyond a recycle ratio of 0.25, additional recycle flow produced only marginal reductions in O&G concentration while pumping energy demand continued to increase. The optimum operating range was therefore identified between 0.24 and 0.25, corresponding to an effluent O&G concentration of approximately 9 mg/L and a pumping duty of 6.85 kW. These results highlight the tradeoff between treatment efficiency and energy consumption and demonstrate the suitability of the developed DAF model for refinery wastewater optimization.

3.3 Optimization of Biological Aeration Demand

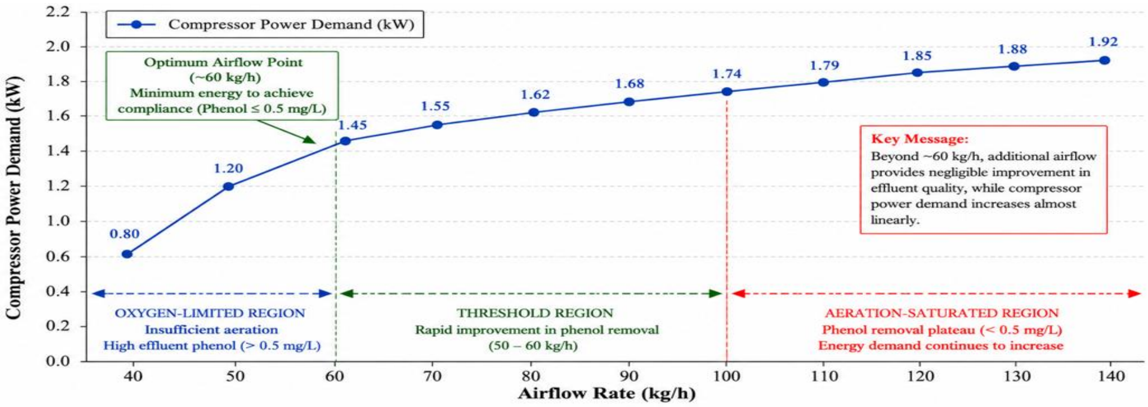
Biological aeration represented the dominant energy-consuming process within the treatment train. Sensitivity analysis was performed by varying airflow rate between 40 and 140 kg/h while monitoring effluent phenol concentration and compressor power demand. The effects of airflow rate on phenol removal and compressor energy consumption are presented in Figures 6 and 7, respectively.



Airflow Range (kg/h)	40 – 50	50 – 60	≥ 60
System Behavior	Oxygen-limited; high effluent phenol	Threshold region; sharp reduction	Aeration-saturated; negligible improvement
Performance	> 0.5 mg/L (Non-compliant)	Drops to 0.5 mg/L	< 0.5 mg/L (Compliant)

Figure 6. Effect of airflow rate on effluent phenol concentration.

At airflow rates below approximately 55 kg/h, oxygen availability was insufficient to sustain complete phenol degradation, resulting in effluent concentrations above the discharge limit of 0.5 mg/L. Increasing airflow enhanced biological oxidation and rapidly reduced phenol concentration. A transition region was observed between approximately 50 and 60 kg/h, where phenol removal improved sharply. Beyond 60 kg/h, further increases in airflow produced negligible additional reduction in phenol concentration, indicating the onset of oxygen-saturated biological conditions.



Airflow Range (kg/h)	40 – 50	50 – 60	> 60
Phenol Removal Behavior	Oxygen-limited; High effluent phenol (> 0.5 mg/L)	Threshold region; Rapid improvement	Aeration-saturated; Negligible additional improvement
Compressor Load Trend	Low but rising	Moderate increase	Continuously increasing
Implication	Non-compliant	Approach optimum	Higher energy cost with no treatment benefit

Figure 7. Compressor power demand as a function of airflow rate.

Compressor energy demand increased continuously with airflow rate, rising from approximately 0.8 kW at 40 kg/h to 1.9 kW at 140 kg/h. Although phenol removal approached saturation beyond 60 kg/h, compressor power continued to increase almost linearly. Consequently, the optimum operating point was identified at approximately 60 kg/h airflow, representing the minimum aeration requirement capable of achieving discharge compliance with the lowest practical energy demand. The combined implications of treatment performance and energy consumption are further examined through the integrated analysis presented in Section 4.4.

3.4 Integrated Energy–Performance Analysis

Figure 8 presents the integrated relationship between treatment performance and energy demand for the principal operating variables investigated in this study.

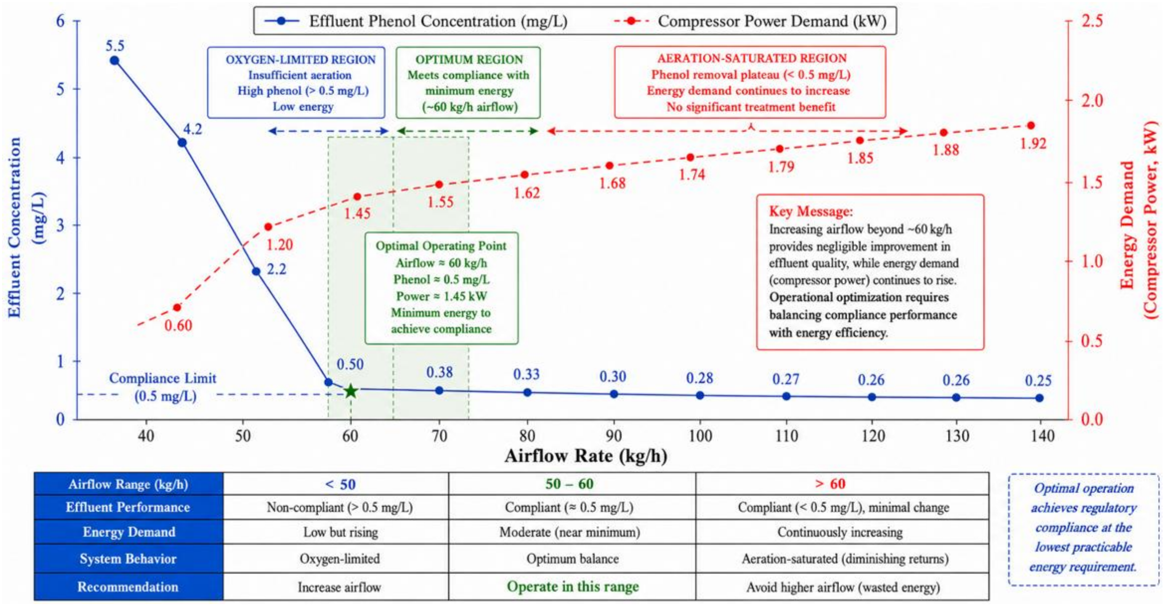


Figure 8. Integrated energy-performance tradeoff for refinery wastewater treatment optimization.

A common threshold-type response was observed in both treatment stages. In the DAF unit, O&G removal improved with recycle ratio until an optimum range of 0.24–0.25 was reached, beyond which additional pumping energy produced only marginal treatment gains. Similarly, biological treatment exhibited an aeration threshold of approximately 60 kg/h, above which phenol removal approached a plateau while compressor energy demand continued to increase. These results demonstrate that treatment efficiency and energy consumption are not linearly related. In both cases, pollutant removal improved rapidly at low-to-moderate operating intensity but approached saturation beyond a critical operating threshold. Consequently, further increases in recycle ratio or airflow generated disproportionately higher energy demand relative to the additional treatment benefit achieved. The identified optimum operating conditions therefore provide a rational basis for balancing environmental compliance and operational efficiency. More broadly, the results demonstrate the capability of the developed surrogate-based Aspen Plus framework to support energy-conscious decision-making and refinery-wide wastewater treatment optimization.

4.5 Integrated Assessment of Treatment Train Performance

The results demonstrate that conventional refinery wastewater treatment operations can be effectively represented within Aspen Plus using a surrogate-based modeling approach despite the absence of dedicated wastewater treatment unit operations. The validated framework accurately reproduced refinery effluent quality and enabled simultaneous evaluation of contaminant removal performance, energy demand, and operational optimization.The integration of surrogate compounds, calibrated separation models, stoichiometric reactor representations, and statistical validation metrics provided a realistic representation of the principal treatment processes while maintaining compatibility with refinery process simulation workflows. Furthermore, the optimization analyses identified energy-efficient operating conditions for both dissolved air flotation and biological treatment without compromising discharge compliance, highlighting the capability of the framework to support operational decision-making and process optimization.

V. Conclusion

A validated surrogate-based steady-state Aspen Plus framework was developed to model and optimize an integrated refinery wastewater treatment train comprising gravity separation, dissolved air flotation (DAF), aerobic biological oxidation, and granular activated carbon polishing. Conventional wastewater treatment operations were successfully represented using surrogate compounds, calibrated removal efficiencies, empirical process relationships, and stoichiometric reactor models within the ENRTL–RK thermodynamic framework.

The model accurately reproduced refinery effluent quality, predicting 9.0 mg/L oil and grease, 0.5 mg/L phenol, and 1296 mg/L total dissolved solids. All predictions satisfied the ±10% validation criterion, while statistical indicators (AARD = 3.43%, RMSE = 2.38 mg/L, MAE = 1.67 mg/L, and R^2 = 0.998) confirmed excellent agreement with refinery laboratory data.

Optimization results identified a DAF recycle ratio of 0.24–0.25 as the most energy-efficient operating range for achieving discharge compliance. Similarly, biological aeration exhibited an optimum threshold of approximately 60 kg/h, beyond which additional airflow produced negligible phenol removal despite increasing compressor energy demand. These findings highlight the importance of balancing treatment performance with energy consumption in refinery wastewater operations.

The proposed framework provides a validated and reproducible methodology for representing non-native wastewater treatment processes within Aspen Plus and demonstrates the potential of surrogate-based simulation for refinery wastewater optimization, energy minimization, and operational decision support.

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