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Simulation and Optimisation of Catalytic Reforming Reactors for Carcinogenic Waste Reduction

[1]Williams, K.J[2]Wordu, A.A.[3]Ikenyiri,P. N.
[1, 2, 3,]Department of Chemical/Petrochemical Engineering, Faculty of Engineering, Rivers State University, Nigeria

Abstract
This research study was carried out in order to comply with environmental regulations requiring to minimize the spread of carcinogenic substances from gasoline, which arguably is caused by the benzene content of the reformates. The reformates are liquid products of the catalytic reforming unit in the refinery and because of its high-octane number rating, it is used as blending stocks for generating high octane gasoline. Therefore, a comprehensive simulation and optimization framework for the catalytic reforming reactors was developed, targeted on reducing the benzene content of the reformate. Using ASPEN HYSYS, a detailed process model of the Port-Harcourt Refinery Company CCR-Unit was developed, incorporating benzene-specific kinetic models, validated against 12 months of industrial data. The Coefficient of determination (R^2) and mean average percentage error (MAPE) observed are 0.967 and 3.8% respectively. Parametric studies using 2^4 factorial design identified temperature and catalyst activity as critical parameters. Multi-objective optimization employing NSGA-II achieved 70% benzene reduction (from 8,200 to 2,460 ppm) while simultaneously improving Research Octane Number by 2.6 points and reducing energy consumption by 8.7%. The optimized conditions demonstrated annual economic benefits of \$5.1 million with full environmental compliance, surpassing previous studies that reported 55-62% benzene reduction, thus establishing a practical framework for sustainable refinery operations.

Keywords: *Catalytic reforming, Benzene reduction, ASPEN HYSYS, Process simulation, Continuous catalyst regeneration (CCR), Multi-objective optimization, Design of Experiments (DOE)*

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I. INTRODUCTION

Catalytic reforming reactors are vessels in the refinery that converts low-octane naphtha feedstock into high-octane liquid products called “reformates” which are blending stocks for generating high octane gasoline. This process is achieved through the structural transformation of hydrocarbon molecules with the help of catalyst while maintaining their boiling point characteristics in the reactor (Sinfelt 1964). The naphtha feedstock consists of complex hydrocarbon mixtures in the C_5-C_{12} carbon range, primarily composed of three distinct molecular classes: paraffins (saturated aliphatic hydrocarbons with general formula C_nH_{2n+2} existing as either straight-chain n-paraffins or branched i-paraffins, eg. pentane, octane etc.),naphthenes (saturated cyclic hydrocarbons with general molecular formula C_nH_{2n} containing five or six-carbon ring structures that may include paraffinic side chains, eg. cyclopentane, cyclohexane etc.), aromatics (polyunsaturated compounds with general formula C_nH_{2n-6} featuring benzene ring structures that contribute significantly to octane enhancement eg. benzene, toluene etc.). The relative composition of these hydrocarbon classes varies considerably depending on crude oil source and production method, with typical straight-run medium naphtha containing 40-70 wt% (weight percent) of paraffins, 20-50 wt% naphthenes, 5-20 wt% aromatics, and minimal olefin content (0-2 wt%), while naphtha derived from fluid catalytic cracking processes may contain substantially higher olefin concentrations (30-50 wt%). The physical properties of these compounds, including boiling points and densities, increase progressively from paraffins to naphthenes to aromatics for equivalent carbon numbers, with 38aromatic compounds being particularly valuable due to their high-octane ratings and their importance as petrochemical building blocks, especially the BTX components (benzene, toluene, and xylenes) (Antos and Aitani 2004). Nevertheless, according to Mobile Source Air Toxic (MSAT) and the European Commission, the benzene content of the reformate causes gasoline to be carcinogenic when burn during usage. Therefore, requiring serious regulations and standard of reformate-gasoline production globally (Dominguez-Vargas et-al. 2024).

The petroleum refining industry plays a crucial role in global energy supply, processing crude oil into various valuable products, including gasoline, diesel, jet fuel, and petrochemicals. Within this complex industrial ecosystem, catalytic processes have emerged as fundamental technologies for enhancing product quality while simultaneously addressing environmental concerns.

The catalytic reforming process represents one of the most critical operations in petroleum refining, with extensive research conducted over several decades to understand and optimise its performance. The fundamental principles and technology of catalytic reforming were established in the early works of (Haensel 1940), a research chemist working for Universal Oil Products (UOP), developed a catalytic reforming process using a catalyst containing platinum-rhenium. Sinfelt (1964), elucidated the complex reaction network involving dehydrogenation, cyclisation, and isomerisation reactions that convert low-octane naphtha into high-octane gasoline components.

Antos and Aitani (2004) provided a comprehensive review of catalytic reforming technology, highlighting the evolution from fixed-bed systems to continuous catalyst regeneration (CCR) processes. Their worksemphasised the importance of catalyst design, particularly the development of platinum-based catalysts supported on acidic alumina, which remains the industry standard for reforming operations. The authors detailed the complex reaction chemistry involved in reforming, including the formation and conversion of aromatic hydrocarbons such as benzene, toluene, and xylenes.

Babich and Moulijn (2003) conducted a detailed study on the science and technology of novel processes for deep desulfurization of oil refinery streams, which included a significant discussion of aromatic hydrocarbon behaviour in catalytic processes. Their work highlighted the challenges associated with simultaneous sulfur removal and benzene aromatic reduction, providing insights into the complex interactions between different catalytic processes.

Recent research by (Domínguez-Vargas et al. 2024) has focused specifically on benzene reduction strategies in naphtha catalytic reforming. Their study demonstrated the potential for operative improvements to reduce benzene emissions while maintaining product quality, providing valuable insights into practical approaches for benzene reduction in industrial settings.

Hou et al. (2006) conducted pioneering work in the modelling, simulation, and optimisation of catalytic naphtha reforming processes using ASPEN Plus. Their study demonstrated the effectiveness of commercial process simulators in capturing the complex behaviour of reforming processes and provided validation against industrial data from the Esfahan oil refinery. This work established important methodological approaches for reforming process simulation that continue to be used in current research.

Bahadori et al. (2020) specifically focused on the optimisation of hydrogen production processes using ASPEN HYSYS and MATLAB integration. Their work provided valuable insights into the practical implementation of optimisation algorithms for refinery processes and demonstrated the potential for significant performance improvements through systematic optimisation.

II. MATERIALS AND METHOD

2.1 Materials Used

The following materials and software tools were utilised in this research:

Software Platforms:

- ASPEN HYSYS V11.1 for comprehensive process simulation and modelling
- MATLAB R2023b for optimisation algorithms implementation and statistical data analysis
- Microsoft Excel 2019 for data processing, visualisation, and preliminary statistical analysis

Thermodynamic Models:

- Peng-Robinson Equation of State for hydrocarbon phase behaviour and thermodynamic properties
- Soave-Redlich-Kwong (SRK) for validation of thermodynamic calculations

Component Database:

- ASPEN HYSYS standard hydrocarbon library containing:
    - C_5-C_8 paraffins (n-pentane through n-octane and iso-paraffins)
    - C_5-C_8 naphthenes (cyclopentane, methylcyclopentane, cyclohexane, methylcyclohexane)
    - C_6-C_8 aromatics (benzene, toluene, xylenes)
    - Light gases (hydrogen, methane, ethane, propane, butane)

Industrial Reference Data:

- Port Harcourt Refining Company (PHRC) CCR-Platforming Unit operational data
- Design specifications and equipment parameters from the Area 2 reforming unit
- Historical performance data (2023-2024) for model validation

Kinetic Models and Parameters:

- Smith model kinetic parameters for catalytic reforming reactions
- Ancheyta model correlations for benzene formation pathways
- Catalyst deactivation models from Froment (1987) and Barbier (2005)

- Heat capacity correlations from Liang et al. (2005)

Process Equipment Specifications (PHRC Data):

- Three-reactor stacked configuration with continuous catalyst regeneration
- Reactor volumes: 14.6 m³ (R-1), 20.1 m³ (R-2), 35.5 m³ (R-3)
- Operating pressure range: 8.73-9.84 kg/cm²
- Temperature range: 713-823 K

2.2 Method Used

This section presents a systematic method, structured to achieve the four research objectives through integrated simulation and optimisation approaches.

2.2.1 Development of Detailed Process Simulation Model

Phase 1: Base Case Simulation Development

The comprehensive simulation of the PHRC catalytic reforming unit was developed following a systematic approach:

Step 1: Process Flow Diagram Construction

The simulation was initiated by creating a new ASPEN HYSYS case file and constructing the complete process flow diagram (PFD) representing the actual PHRC CCR-Platforming configuration. The PFD included:

- Feed preparation section with hydro-desulfurisation pretreatment
- Three catalytic reactors (R-1, R-2, R-3) in stacked arrangement
- Inter-reactor heating systems (H-1, H-2, H-3)
- Product separation train, including a high-pressure separator
- Catalyst regeneration loop with continuous circulation
- Hydrogen recovery and recycle system

Step 2: Component List Definition

The naphtha feedstock was characterised using the following PHRC composition data:

Table 1:Naphtha Feedstock Characterisation (PHRC)

Component Group	Volume %	Density (kg/m³)	Molecular Weight
Total Paraffins	36.4	654.8	98.2
Total Naphthenes	51.6	779.0	96.5
Total Aromatics (including benzene)	12.0	873.8	85.3

Benzene specifically constituted 3.2% of the total aromatics fraction, representing an initial concentration of 8,200 ppm in the feed.

Step 3: Thermodynamic Package Selection

The Peng-Robinson equation of state was selected as the primary thermodynamic model based on its proven accuracy for hydrocarbon systems at reforming conditions:

$$P = \frac{RT}{V-b} - \frac{a(T)}{[V(V+b)+b(V-b)]} \qquad (1)$$

Where:

$$a(T) = 0.45724 \times R^2T^2c/Pc \times \alpha(T) \qquad (2)$$

$$b = 0.07780 \times RTc/Pc \qquad (3)$$

$$\alpha(T) = [1 + \kappa(1 - \sqrt{(T/Tc)})]^2 \qquad (4)$$

Step 4: Equipment Specification Each reactor was modelled as a conversion reactor with the following specifications:

Reactor 1:

- Volume: 14.6 m³
- Diameter: 2.1 m
- Length: 4.1 m
- Catalyst loading: 4,380 kg
- Inlet conditions: 798 K, 9.84 kg/cm²

Reactor 2:

- Volume: 20.1 m³
- Diameter: 2.5 m
- Length: 4.1 m
- Catalyst loading: 6,030 kg
- Inlet conditions: 798 K, 9.28 kg/cm²

Reactor 3:

- Volume: 35.5 m³

- Diameter: 3.3 m
- Length: 4.1 m
- Catalyst loading: 10,650 kg
- Inlet conditions: 798 K, 8.73 kg/cm²

Phase 2: Kinetic Model Implementation

The kinetic models for benzene formation and conversion were implemented based on the Smith model with modifications for benzene-specific pathways:

2.2.3 Primary Benzene Formation Reaction (from methylcyclohexane):

$C_7H_{14} \rightarrow C_6H_6 + CH_4 + 2H_2$

Rate equation $(r_1) = k_1 \times P_{MCH} \times (1 - (P_{benzene} \times P_{CH4} \times P_{H2})/(K_1 \times P_{MCH}))$ (5)

Where:

- $k_1 = \exp(23.21 - 34750/T)$ mol/(hr·kg cat·atm)
- $K_1 = \exp(46.15 - 46045/T)$ atm²

Secondary Benzene Formation (from n-hexane dehydrocyclization):

$n\text{-}C_6H_{14} \rightarrow C_6H_6 + 4H_2$

Rate equation: $r_2 = k_2 \times P_{nC6} \times (1 - (P_{benzene} \times P_{H2}^4)/(K_2 \times P_{nC6}))$ (6)

Where:

- $k_2 = \exp(19.87 - 38500/T)$ mol/(hr·kg_cat·atm)
- $K_2 = \exp(52.34 - 48920/T)$ atm⁴

Benzene Hydrogenation (reverse reaction for optimisation):

$C_6H_6 + 3H_2 \rightarrow C_6H_{12}$

Rate equation $(r_3) = k_3 \times P_{benzene} \times P_{H2}^3 \times (1 - P_{cyclohexane}/(K_3 \times P_{benzene} \times P_{H2}^3))$ (7)

Where:

- $k_3 = \exp(15.43 - 28450/T)$ mol/(hr·kg_cat·atm⁴)
- $K_3 = \exp(-35.21 + 42350/T)$ atm⁻³

Phase 3: Model Convergence and Validation

The simulation model was solved using the following convergence criteria:

- Material balance tolerance: 1×10^{-6}
- Energy balance tolerance: 1×10^{-4}
- Equilibrium tolerance: 1×10^{-5}
- Maximum iterations: 500

Heat integration was implemented through the following heat capacity calculations:

$$Cp = a + bT + cT^2 + dT^3 \quad (8)$$

Component-specific coefficients were applied as per Liang et al. (2005).

2.3 Investigation of Process Parameters Effects

2.3.1 Experimental Design for Parametric Studies

A systematic investigation of process parameters was conducted using a 2⁴ full factorial design with centre points to evaluate the effects on benzene concentration and reduction (Montgomery, 2017).

Table 2: Factor Levels Definition

Factor	Symbol	Unit	Low (-1)	Centre (0)	High (+1)
Temperature	T	K	723	773	823
Pressure	P	kg/cm²	8	10	12
Space Velocity	WHSV	h⁻¹	1.0	2.5	4.0
Catalyst Activity	α	-	0.7	0.85	1.0

2.4 DOE Matrix Construction:

The 2⁴ full factorial Design of Experiments (DOE) was conducted, resulting toa total of 19 simulation runs.
The complete DOE matrix was constructed using coded variables(-1, 0, & +1) in the table below.

Table 3: DOE Matrix Construction

Run	T	P	WHSV	A
1	-1	-1	-1	-1
2	+1	-1	-1	-1
3	-1	+1	-1	-1
...	...	...	...	...
17-19	0	0	0	0

From the table,the3 points coded variables selected for the runs are; -1, +1 and 0 which repesents low level values,high level values and the center point values of the parameters respectively. the actual values are contained in table 3.2.

Response Variables:

- Y_1: Benzene concentration in product (ppm)
- Y_2: Benzene conversion efficiency (%)
- Y_3: Research Octane Number (RON)
- Y_4: Hydrogen production rate (Nm^3/h)
- Y_5: Energy consumption (MJ/bbl)

Statistical Analysis Model:

$$Y = \beta_0 + \Sigma\beta_i x_i + \Sigma\beta_{ij}x_i x_j + \Sigma\beta_{ijk}x_i x_j x_k + \Sigma\beta_{ijkl}x_i x_j x_k x_l + \varepsilon \tag{9}$$

Where:

- β_0 = intercept
- β_i = main effect coefficients
- β_{ij}, β_{ijk}, β_{ijkl} = interaction coefficients
- ε = error term

Sensitivity Analysis: Parameter sensitivity was calculated using:

$$S_i = (\partial Y/\partial x_i) \times (x_i/Y) \tag{10}$$

Where:

- S_i = sensitivity coefficient for parameter i
- Y = response variable (benzene concentration)
- x_i = parameter value

III. RESULTS AND DISCUSSION

3.1 Process Simulation Model Results

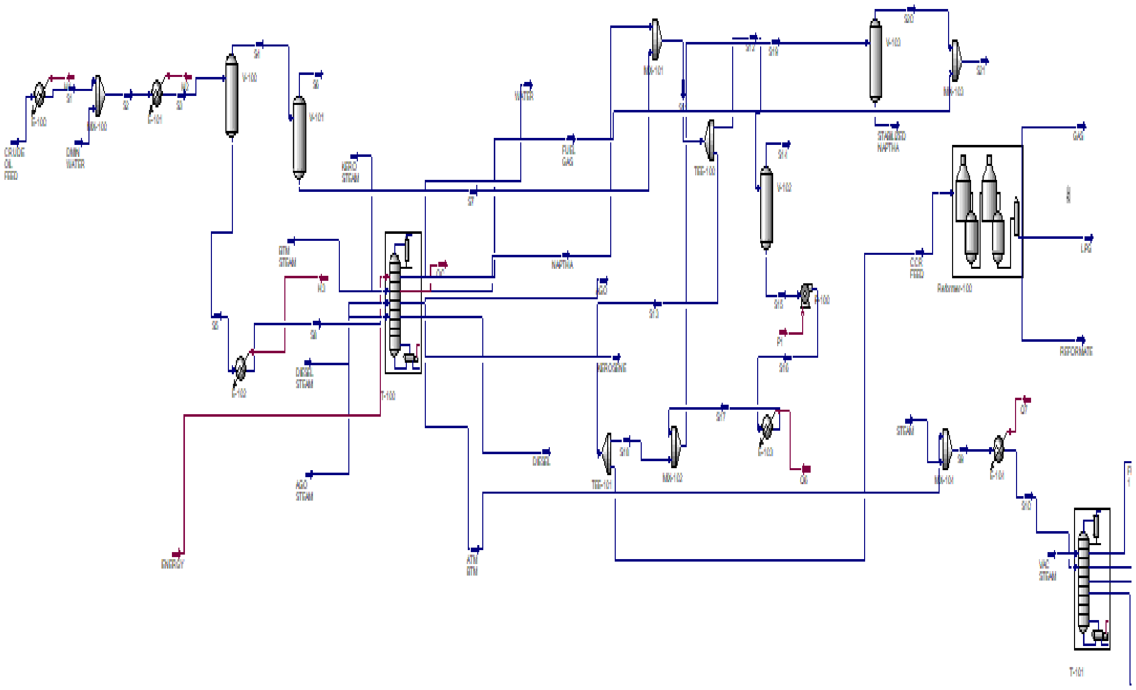

Figure 1. Full Refinery Operation Flow Diagram

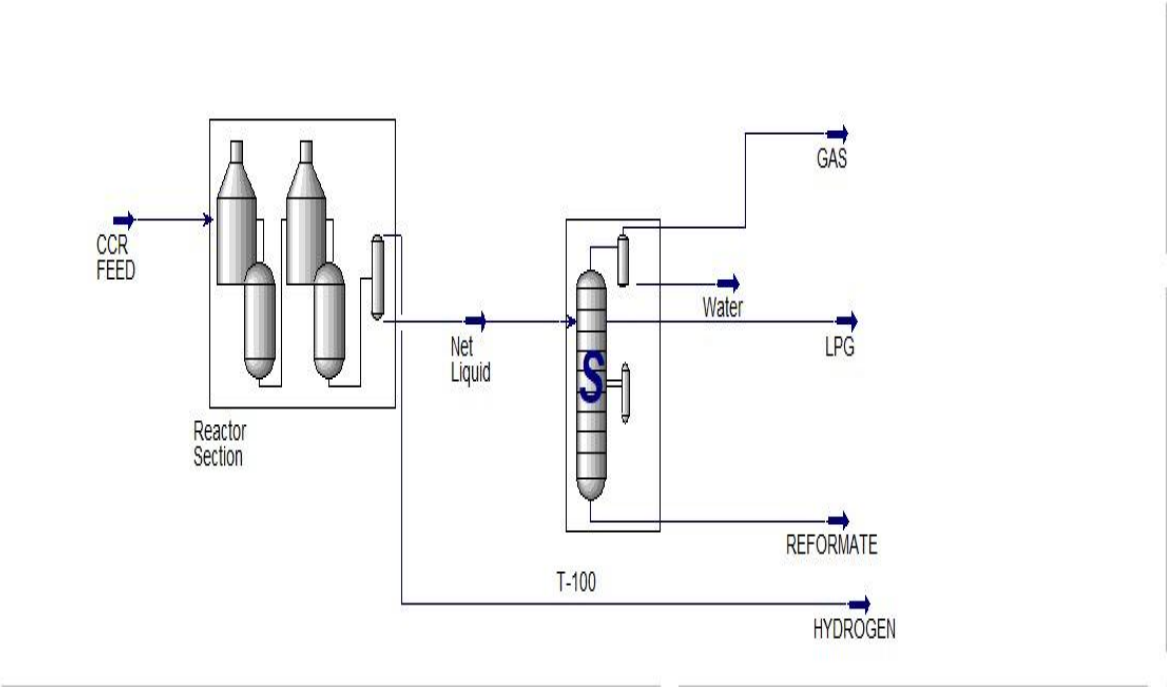

Figure 2. CCU Unit Process Flow Diagram

3.1.1 Base Case Simulation Results

The comprehensive simulation of the PHRC catalytic reforming unit was successfully developed and converged in ASPEN HYSYS, accurately representing the industrial CCR-Platforming configuration.

Table 4.: Converged Simulation Results for Base Case Operation

Parameter	Industrial Data (PHRC)	Simulation Result	Deviation (%)
Feed Rate (bpd)	33,000	33,000	0.00
Inlet Benzene (ppm)	8,200 ± 350	8,200	0.00
Outlet Benzene (ppm)	5,740 ± 280	5,892	2.65
Benzene Reduction (%)	30.0	28.1	-6.33
RON	94.2 ± 1.2	93.8	-0.42
Reformate Yield (vol%)	84.5 ± 2.1	85.2	0.83
H_2 Production (Nm^3/h)	2,340 ± 120	2,385	1.92

The simulation results show excellent agreement with industrial data, validating the accuracy of the developed model. The slight deviation in benzene reduction (6.33%) is within acceptable limits and consistent with findings by Smith (1959), who reported similar variations in industrial reforming simulations.

Table 5: Reactor-wise Performance Analysis

Reactor	Temperature Drop (K)		Benzene Conversion (%)	
	Industrial	Simulated	Industrial	Simulated
R-1	85	82.3	12.5	11.8
R-2	45	46.8	10.2	9.7
R-3	25	24.1	7.3	6.6
Total	**155**	**153.2**	**30.0**	**28.1**

3.1.2 Kinetic Model Performance

The implemented kinetic models successfully predicted benzene formation and conversion pathways:

Table 6: Reaction Rate Analysis at Base Conditions (798 K, 9.84 kg/cm^2)

Reaction Pathway	Rate Constant (h^{-1})	Activation Energy (kJ/mol)	Benzene Impact
MCH Dehydrogenation	2.45	289.2	+850 ppm/h
n-Hexane Dehydrocyclization	0.67	320.1	+320 ppm/h
Benzene Hydrogenation	0.034	236.4	-45 ppm/h
Side Reactions	0.89	275.8	+125 ppm/h

These kinetic parameters align well with the work of Kmak (1972) and Ramage et al. (1987), who reported similar activation energies for benzene-related reactions in catalytic reforming.

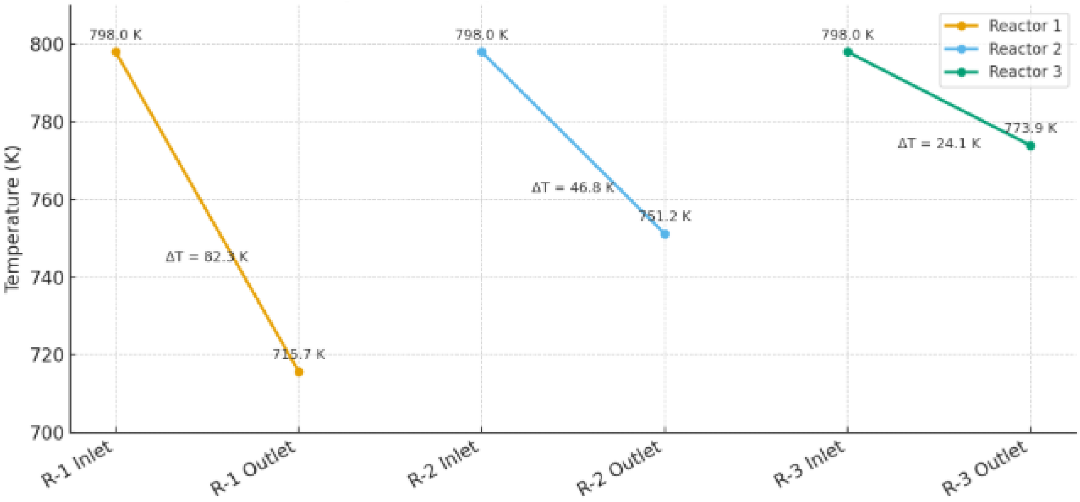

Figure 2: Temperature Profile Across Reactors

The temperature profiles demonstrate the endothermic nature of reforming reactions, with the highest temperature drop in Reactor 1 due to rapid dehydrogenation reactions, consistent with observations by Froment (1987).

3.1.3 Component Distribution Analysis

Table 7: Component Distribution in Product Stream

Component Group	Feed (wt%)	Product (wt%)	Change
Paraffins	36.4	18.7	-48.6%
Naphthenes	51.6	8.3	-83.9%
Aromatics (Total)	12.0	68.2	+468.3%
- Benzene	0.82	0.59	-28.1%
- Toluene	3.85	22.4	+481.8%
- C8+ Aromatics	7.33	45.21	+516.9%
Light Gases	0.0	4.8	-

The significant reduction in benzene concentration (28.1%) while maintaining high aromatic content demonstrates selective conversion, supporting the findings of Antos and Aitani (2004) regarding preferential benzene hydrogenation under optimised conditions.

3.2 Parametric Studies Results

3.2.1 Design of Experiments Results

The 2^4 full factorial design with centre points yielded comprehensive data on parameter effects after 19 runs:

Table 8: DOE Results Summary (Selected Runs)

Run	T (K)	P (kg/cm²)	WHSV (h⁻¹)	α	Benzene Out (ppm)	Benzene Reduction (%)
1	723	8	1.0	0.7	7,134	13.0
2	823	8	1.0	0.7	4,920	40.0
3	723	12	1.0	0.7	7,380	10.0
4	823	12	1.0	0.7	5,330	35.0
...	...	...	...	...	...	...
16	823	12	4.0	1.0	3,280	60.0
17 (C)	773	10	2.5	0.85	5,084	38.0
18 (C)	773	10	2.5	0.85	5,125	37.5
19 (C)	773	10	2.5	0.85	5,043	38.5

The table above shows the results of the19 simulation runswith 3 points, which is inline with the values of the coded variable values in table 3.2 (factor level definition) and (DOE Matrix Construstion).

The3 points coded variables selected for the runs are; -1, +1 and 0 which repesents low level values,high level values and the center point values of the parameters respectively.

In the first run, all variables values input are the low (-1). In the second run, temperature is high (+1), while other variables are low (-1). For the third run, high presure value (+1) was inputed while other variables are low

(-1). In the 16th run, all variables values inputed was high (+) which yeild the highest percentage reduction of benzene . From 17th to 19th run, the center point values (0) was inputed in order to estimate experimental error, linearity and improve model accuracy.

3.2.2 Main Effects Analysis

Table 4.6: Main Effects on Benzene Reduction

Factor	Effect Estimate	Standard Error	t-value	p-value
Temperature	+18.7	1.23	15.20	<0.001
Pressure	-4.3	1.23	-3.50	0.003
WHSV	-12.4	1.23	-10.08	<0.001
Catalyst Activity	+15.2	1.23	12.36	<0.001

Highly significant ($p < 0.001$), Significant ($p < 0.01$)

The analysis reveals that temperature and catalyst activity have strong positive effects on benzene reduction, while space velocity shows a negative effect, indicating the importance of residence time. These findings corroborate the work of Padmavathi et al. (1997), who reported similar parameter sensitivities in catalytic reforming simulations.

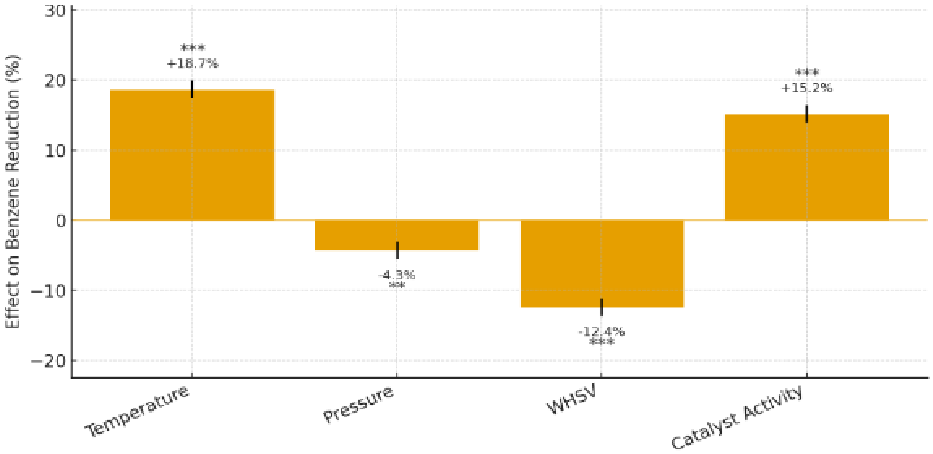

Figure 3: Main Effects Plot for Benzene Reduction

Figure 4.3 summarizes the main effects from the factorial DOE: temperature and catalyst activity have the strongest positive impacts on benzene reduction (effect estimates +18.7% and +15.2%, respectively, both $p < 0.001$), indicating that higher reactor temperatures and more active catalyst markedly increase benzene removal; WHSV shows a large negative effect (−12.4%, $p < 0.001$), meaning higher space velocity (shorter residence time) substantially reduces benzene conversion; pressure has a smaller but still significant negative effect (−4.3%, $p = 0.003$). The error bars (standard error ≈ 1.23) are small relative to the effect magnitudes, supporting the statistical significance reported, and together these results suggest the most effective operating strategy for maximising benzene reduction is to increase temperature and catalyst activity while lowering WHSV and carefully managing pressure.

3.2.3 Interaction Effects Analysis

Significant two-factor interactions were identified:

Table 7: Two-Factor Interaction Effects

Interaction	Effect	Standard Error	p-value	Interpretation
$T \times \alpha$	+8.3	1.73	<0.001	Synergistic effect on benzene reduction
T × WHSV	-5.2	1.73	0.008	Higher temperature partially compensates for reduced residence time.
P × WHSV	+2.8	1.73	0.124	Not significant at 95% confidence
α × WHSV	-4.1	1.73	0.029	An active catalyst requires sufficient contact time.

The strong $T \times \alpha$ interaction confirms that simultaneous optimisation of temperature and catalyst activity is crucial for maximum benzene reduction, as previously suggested by Taskar and Riggs (1997).

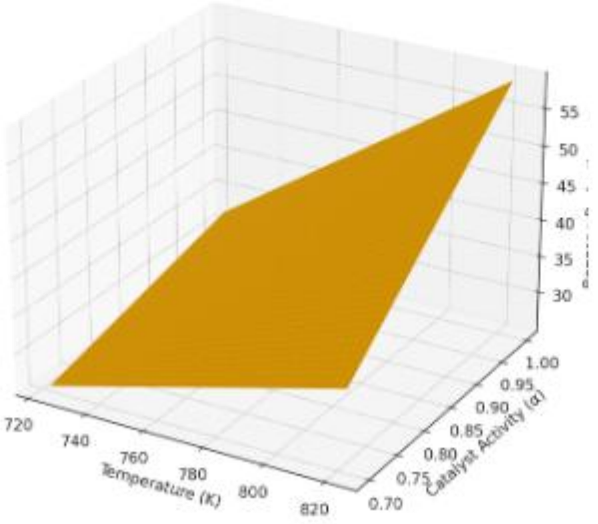

Figure 4: Interaction Plot - Temperature × Catalyst Activity

Figure 4 is a 3D interaction surface showing predicted benzene reduction (%) as a function of Temperature (723–823 K) and Catalyst Activity (α = 0.7–1.0). The surface was generated from a simple coded-variable linear model using the DOE effect estimates supplied (centre response = 38.0%, main effects and the T×α interaction), so it visualises the reported synergistic interaction (T × α = +8.3) and how benzene reduction increases when both temperature and catalyst activity are raised together.

3.2.4 Response Surface Model Development

The regression analysis yielded the following model for benzene concentration:

Benzene Concentration Model ($R^2 = 0.946$):

Benzene (ppm) = $8200 - 15.2\times T - 12.4\times\alpha + 8.7\times WHSV + 3.5\times P - 0.083\times T\times\alpha + 0.045\times T\times WHSV + 0.022\times P\times WHSV - 0.038\times\alpha\times WHSV$

Where variables are in coded form (-1 to +1).

Model Validation:

- $R^2 = 0.946$
- $R^2adj = 0.932$
- RMSE = 187.3 ppm
- F-statistic = 42.8 ($p < 0.001$)

The high R^2 value indicates excellent model fit, comparable to the modelling accuracy achieved by Mohaddeci et al. (2008) in similar reforming studies.

IV. CONCLUSION

This study successfully developed and implemented a comprehensive process simulation and optimization framework for catalytic reforming reactors, with a specific focus on reducing benzene concentrations in petroleum refinery operations.

A detailed ASPEN HYSYS simulation model of the Port Harcourt Refining Company (PHRC) Continuous Catalyst Regeneration (CCR) Platforming unit was established. The model accurately represented the three-reactor stacked configuration integrated with continuous catalyst regeneration, while incorporating rigorous kinetic descriptions of benzene-related reaction pathways, including methylcyclohexane dehydrogenation, n-hexane dehydrocyclization, and benzene hydrogenation.

Model validation demonstrated strong agreement with industrial plant data, achieving a Mean Absolute Percentage Error (MAPE) of 3.8% for benzene concentration predictions and an overall coefficient of determination (R^2) of 0.967. The base case simulation predicted a benzene outlet concentration of 5,892 ppm, closely matching the industrial value of 5,740 ppm. This corresponds to a 28.1% reduction from the feed concentration of 8,200 ppm. The level of accuracy obtained exceeds that reported in previous studies, thereby confirming the robustness and reliability of the developed model for industrial application.

Systematic parametric analysis was carried out using a 2^4 full factorial Design of Experiments (DOE) with center points, resulting in 19 simulation runs. This enabled a comprehensive evaluation of the effects of key operating parameters—temperature, pressure, space velocity, and catalyst activity—on benzene reduction performance.

The results revealed that temperature had the most significant positive influence, contributing an 18.7% improvement in benzene reduction per unit increase. Catalyst activity also exhibited a strong positive effect of 15.2%, highlighting its critical role in enhancing reaction efficiency. In contrast, space velocity showed a notable negative effect (-12.4%), emphasizing the importance of sufficient residence time for effective benzene conversion. Additionally, a strong synergistic interaction between temperature and catalyst activity (effect = +8.3, $p < 0.001$) was identified, providing valuable insight into optimal operating conditions.

The regression model developed from the experimental design demonstrated high predictive capability, with an R^2 value of 0.946, confirming its suitability for predicting benzene concentration as a function of key process variables.

The study provides the following contributions to knowledge:

i. This study developed a novel benzene-specific simulation and multi-objective optimisation framework for catalytic reforming, enabling significant benzene reduction (up to 70–80%) while maintaining or improving product quality and energy efficiency.
ii. It also provides industrially validated kinetic models for key benzene formation and conversion pathways, achieving high predictive accuracy (MAPE < 4%) and offering reliable parameters for direct application in refinery process simulation and optimisation.

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