



Techno-Economic Modelling of Bioclarified Water Recovery from Petroleum Wastewater Using ASPEN Software and Box-Behnken Design

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Article History

Received: 25-01-24

Revised: 30-04-24

Accepted: 07-05-24

Published: 18-05-24

ABSTRACT

Application and efficiency of bio-coagulants for petroleum wastewater biocoagulation, flocculation, and sedimentation (bioclarification) are still confined to laboratory proof-of-concept practice. The scale-up process design of bio-clarified water recovery from petroleum wastewater has been a major research lacuna. This paper presents ASPEN Base Case Scale-Up Simulation (BCSUS) using optimum laboratory experimental data and techno-economic predictive models for bioclarified water production from petroleum wastewater. The BCSUS, process design, and economics were performed in the ASPEN Batch Process Developer V10 environment. Predictive models for predicting and optimizing techno-economic parameters such as return on investment (ROI), payback time (PBT), and production rate (PR) were achieved in RSM via the Box-Behnken Design (BBD) technique of Design Expert V13. The base case techno-economic model gave batch size, annual production cost, Total Capital Investment (TCI), PBT, and ROI of 406kg, \$9195, \$631484, 5.18 years, and 17%, respectively, at the selling price of \$0.225. The regression models gave R^2 values of 0.9984 for ROI and 0.9920 for PBT, while the production rate was 0.8867. This study shows that a petroleum wastewater bioclarification scale-up design is feasible.

Keywords: Modeling; simulation; bioclarified water; bio-coagulation; flocculation

1. Introduction

Petroleum wastewater, also referred to as produced water (PW), contains complex mixtures of both inorganic and organic compounds and has been adjudged to be the highest by-product generated during oil and gas operations. This wastewater is a mixture of injection water, formation water, aqueous residues of treatment chemicals, and chemical additives from drilling, fracturing, or operating the well, and some of them have been established to contain toxic properties (Danforth et al., 2020). These also include demulsifiers, biocides, corrosion inhibitors from oil fields (Jiménez et al., 2018), methanol, and diethylene glycol; others are dissolved and dispersed oil; and mixtures of hydrocarbons (benzene, ethylbenzene, xylenes, toluene, poly-aromatic, phenol, and hydrocarbons (PAH)) from gas fields (Iggunniet al., 2014).

Treatment methods for PW are grouped into three types: chemical, physical, and biological methods. Coagulation-Flocculation-Sedimentation (CFS) is an important and conventional method of treating wastewater with the overall aim of reducing or removing turbidity, color, COD, and TSS (Farajnezhad and Gharbani, 2012). CFS has been achieved by adding chemicals (coagulants) for destabilizing stable dispersed particles in wastewater, which subsequently agglomerate as well as settle down from the water body. CFS offers a superior viable primary treatment option for wastewater with high treatment efficiency, easy-on-site implementation, and low operating costs (Menkiti et al., 2018; Yu et al., 2011; Wang et al., 2014). CFS has also been reported as one of the integrated treatment processes used for PW clarification in order to significantly reduce the pollution load (Menkiti et al., 2016). Conventional coagulants (inorganic salts) such as aluminum sulfate, ferric chloride, ferric sulfate, and sodium sulfate are commonly used for wastewater clarification owing to their proven performance efficiency (Subramonian et al., 2015). However, the application of chemical-based coagulants produced large and non-biodegradable sludge, and the residual chemicals in clarified water are linked to health-related problems in the human body system (Okolo et al., 2016). Utilization of biocoagulants in the treatment of wastewater has been found to be efficient, environmentally sustainable, and safe for human consumption (Kurniawan et al., 2020).

A review of the literature shows that petroleum wastewater treatments through biocoagulation-fluoculation-sedimentation (BFS) techniques have been confined to laboratory practices, despite their efficiency and cost-effectiveness for wastewater treatments. Menkiti and Ezemagu (2015) and Menkiti et al. (2016) demonstrated the application as well as performance of *Typanotonos fuscatus* and *mucuna* seed-based bio-coagulants for BFS of Petroleum Produced Water (PPW). The above investigations established process optimal conditions and kinetic parameters for possible scale-up process design and economics, and soft-computational prediction and optimization of petroleum wastewater BFS were also reported by Ezemagu et al. (2021). A review of the literature has shown that bio-clarification of PWW has been confined to laboratory practices, and the process has neither been scaled up nor advanced to the level of industrial utilization.

Modeling bioclarified water production is essential for process techno-economic analyses as well as process design and control. Previous reports (Liu et al., 2020; He et al., 2020; Oke et al., 2020, 2021) have used modeled and optimized chemical processes via RSM owing to its efficiency in modeling and optimizing experimental process data without prior knowledge of process mechanisms. Computer-aided process simulation performs material flow balance, process scale-up, and equipment sizing of the unit operations of chemical processes.

Techno-Economic Analysis (TEA) is suitably adopted to investigate the technical and economic performance of production processes. The TEA technique has been performed for various processes in order to evaluate the feasibility of process technologies through the use of commercial process simulators such as Aspen Batch Process Developer (ABPD), Superpro Designer, Aspen Plus, and Aspen Hysys (Adeniyi et al., 2019; Lee et al., 2020; Liu et al., 2021; Oke et al., 2021). This study is aimed at carrying out techno-economic modeling of PWW bioclarification using ASPEN-RSM software.

2. Materials and Method

2.1 ASPEN batch base case process simulation environment

The laboratory experimental optimum conditions and proximate compositions of the biocoagulant as detailed in Menkiti et al. (2016) were utilized in performing batch base case process simulation of the bio-clarified water production from petroleum wastewater using the ASPEN Batch Process Developer (ABPD) Version 10. The characteristics of the raw petroleum wastewater are shown in Table 1, while the proximate compositions of the *mucuna* seed biocoagulant are shown in Table 2. These were declared in the pure mixture user-defined environment of ABPD.

Table 1: Characteristics of Produced Water (PW)

Parameter	Value	Unit
pH	8	
Fe	0.711	mg/L
SO	26	mg/L
NO ₃ ²	12.8	mg/L
Alkalinity	1820.5	mg/L
Acidity	202	mg/L
Ca	Nil	mg/L
Mg ²⁺	Nil	mg/L
Salinity	3842	mg/L
Turbidity	1435	NTU
Conductivity	12.17	ms/mc
Total dissolved solids	1899	mg/L
Total suspended solids	1473	mg/L
COD	10	mg/L
Hydrocarbon	99.7	ppm

Source: Menkiti et al., (2016)

Table 2: Proximate analysis results of mucuna seed

Parameter	Value	Unit
Bulk density	0.53	g/mol
Oil content	5.30	%
Ash content	2.80	%
Moisture content	11.0	%
Protein content	22.7	%
Weight loss	10.9	%
Yield	89.0	%

Source: Menkiti et al., 2016

2.2 Base Case Process Simulation Description and Design

The first step involves the pumping of the raw petroleum wastewater from Tank 2 and the bio-coagulant solution that has already been charged in the second tank (Tank 1) into the mixing tank (C-Tank), as shown in Figure 1. From the process flow sheet in Figure 1, bio-coagulation and flocculation of the wastewater take place in the mixing tank (C-Tank). The coagulation process involves rapid mixing in the mixing tank at 250 revolutions per minute for 3 minutes, followed by flocculation, which involves slow agitation at 30 revolutions per minute for 40 minutes. After the slow mixing, the treated petroleum wastewater is pumped into the SET-TANK, where it is allowed to settle, and the sludge separated from the clarified water is placed in the sludge tank, as depicted in Figure 1. The bioclarified water from the SET-TANK is further pumped for filtration at the micro/ultrafiltration unit (MC-UL Filters) as a stand-alone unit. Colloidal matter and suspended solid particles of pore size ranging from 0.05–0.1µm, as well as the accompanied viruses, emulsified oils, metal hydroxides, colloids, proteins, and other large molecular weight materials, are removed at this stage from the water. The filtered water is finally sent to the storage tank (Tank 4), while the residue is sent to the residue tank (Tank 5).

In this study, using run 1 of the BBD experimental design matrix as the base case (Table 6), a daily target production rate of 1,818.18 liters per day and an annual process design of 600,000 liters per year for bioclarified water production were designed. The assumption of 24-hour, annual operations of 330 days was made, and the plant was designed to produce 600,000 liters per year of bio-clarified water from petroleum wastewater, 391kg per batch, with a total number of 1,535 batches designed in order to meet the production target of 600,000 liters per year. Production rate was 1.24 kg/min, while campaign time was 484,522.92 min. This production target of 600,000 liters was the maximum and allowable size in the design algorithm environment without exceeding the campaign production time. Campaign production time is the total time required for producing all the batches per year.

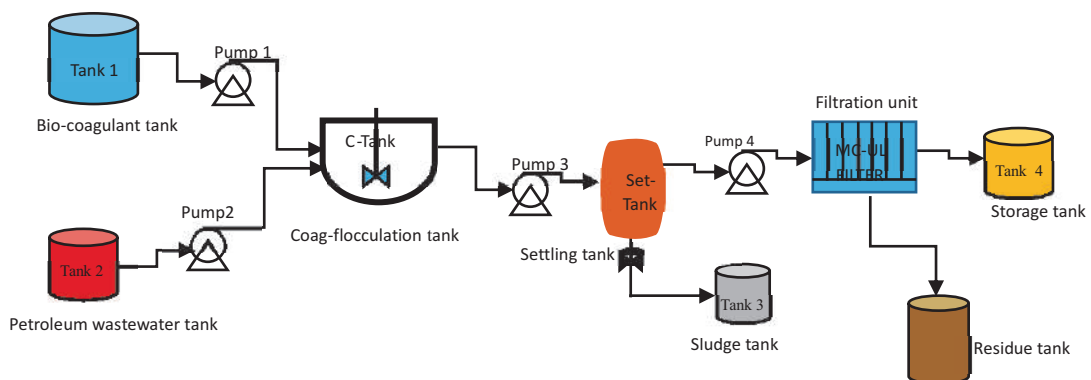


Figure 1: Process flowsheet for bio-clarified water reclamation from PPW

2.3 Process: Economic and Profitability Evaluation

Economic analysis of chemical production processes involves total capital investment (TCI) and total production cost (TPC). The total production cost is direct production cost (labor, consumables, packaging cost, and raw material cost) plus indirect production cost (administrative, supervision, lab charges, distribution and marketing, research and development, and royalty cost). Total Capital Investment (TCI) is made up of Working Capital (WC) and Fixed Capital Investment (FCI). The WC used in this study is 15% of the FCI obtained in the previous study (Oke et al., 2021). The FCI was the sum of the total equipment purchase cost and the installed cost of the production equipment purchase. The installed cost factors for purchase equipment such as equipment installation (2.13), engineering (1.65), contingencies (1.60), instrumentation (0.96), auxiliary materials (0.69), miscellaneous supplies (0.52), utilities (0.42), structure (0.42), and transportation (0.17) used in this study were obtained in an ASPEN environment. The labor cost (\$1.2/h) used in this work was obtained from Nigerian chemical process industries and benchmarked with the National Minimum Wages and Income Commission (NMWIC) in Nigeria. The price of the pieces of equipment was obtained from Alibaba.com.

Return on investment (ROI) and payback time (PBT) as profitability indices were used to measure the feasibility and performance of bioclarified water production from petroleum wastewater. PBT means the time required to recover the invested capital; in other words, the length of time required for the investment to reach the break-even point, while ROI is the profitability performance index that measures the amount of return on investment relative to the investment's cost (Mellichamp, 2019). In this work, the discount rate and tax percentage were varied against the base-case simulation cumulative cash flow of the project. PW was freely discharged and attracted zero fees. The bio-coagulant cost used was \$0.02/kg, as obtained from the Alibaba.com website. The price of the bio-clarified water was set at \$0.225 per liter since the purified water output is close to the drinkable quality of the water.

2.4 Techno-Economic Modeling and Optimization Study

The RSM via Box-Behnken Design (BBD) technique was applied to optimize the process parameters. Production cost (coded as A), fixed capital investment (coded as B), selling price (coded as C), discounted rate (coded as D), and efficiency removal (coded as E) were selected as independent variables, while PBT, ROI, and production rate were selected as dependent variables. A multiple regression model in equation 1 was used to determine the interaction effects of the process parameters on the responses. The process parameters significance and their responses were validated using the p-value obtained from the Analysis of Variance (ANOVA) (Oke et al., 2021).

$$Y = \beta_0 + \sum_{i=1}^3 \beta_i X_i + \sum_{i=1}^3 \beta_{ii} X_i^2 + \sum_{i < j}^3 \beta_{ij} X_i X_j \quad (1)$$

Where Y represents the measured response, β_0 , β_i , β_{ii} , and β_{ij} are the intercept, linear, quadratic, and interaction coefficients, respectively, of the model, and X_i and X_j are levels of independent variables. The variable $X_i X_j$ shows the first-order interaction between X_i and X_j for ($i < j$).

The range of numbers for the independent and dependent variables is given in Table 3. The BB design gives forty-six experiments, and once the range of independent variables for each coagulant was incorporated with design expert software, the set of different experimental conditions was obtained, which is provided as the experimental design matrix. The experiments using the software as a virtual laboratory were performed under these conditions and incorporated into the design expert software as actual dependent variables.

Table 3: Properties of the independent variable selected for the BBD method

Factor	Name of independent variable	Minimum	Maximum	Mean	Std. Dev.
A	Production Cost (\$)	8276	10114	9195.00	547.99
B	Fixed Capital Investment (\$)	494205	604029	5.49117	32743.19
C	Selling Price (\$)	0.05	0.4	0.2250	0.1043
D	Discounted Rate (%)	0	10	5.00	2.98
E	Efficiency Removal (%)	88	99	93.50	3.28

3. Results and Discussion

Table 4 shows ASPEN base-case batch simulation results of bioclarified water production from petroleum wastewater. The batch size, production rate, cycle time, and campaign time estimation from the simulation results were 406 kg/batch, 0.12 kg/min, 316 min, and 464,295.76 min, respectively. Assuming a 24-hour operation and a 330-day annually operated bioclarified water plant, the plant produces 600,000 liters per year of bioclarified water production from petroleum wastewater in 1,469 batches per year, or 1818 liters per day. The total capital investment cost, fixed capital investment, and annual production cost for the base-case facility that produces 600,000 liters are \$631484, \$549117, and \$9195, respectively. PBT and ROI of the base case simulation model are 5.18 years and 17% at the selling price of \$0.225, respectively. The profitability indices, such as ROI and payback time, in this study are similar to previous works (Zhao et al., 2016; Lee et al., 2020). The summary of the material stream balance is presented in Table 5. The results validated the 95% removal from the laboratory data as it was compared with the experimental result (95%) in Menkiti et al. (2016); this shows that the mean relative deviation error (MRDE) between the simulated and experimental results is 0.000%. Previous works (Oke et al., 2020; Oke et al., 2014) reported that MRDE with less than 10% shows high performance of the simulation model. This similarity confirms the convergence and performance of the ASPEN simulation of the process.

Table 4: Bioclarified water production base case techno-economic parameters

S/N	Process parameters	Values
1	Batch Size (kg)	406
2	Cycle Time (min)	316.00
3	Batch Time (min)	409.00
4	Production Rate (kg/min)	0.12
5	Number of Batches	1,469
6	Campaign Time (min)	464,295.76
7	Annual production capacity (Litres)	600,000
8	Daily production (Litres)	1818
9	Total capital investment (\$)	631484.55
10	Annual production cost (\$)	9195
11	Payback time (year)	5.18
12	Return on investment (%)	17
13	Selling price (\$)	0.225
14	Fixed capital investment (\$)	549117
15	Profit (\$)	113224.5
16	Discounted rate (%)	0

Table 5: Material Stream balance summary

From Unit	TANK 1	TANK 2	C-TANK	SET-TANK	SET-TANK	MC UL FILTERS	MC UL FILTERS	MC UL FILTERS	MC UL FILTERS	MC UL FILTERS
To Unit	C-TANK	C-TANK	SET-TANK	MC UL FILTERS	TANK 3	MC UL FILTERS	MC UL FILTERS	MC UL FILTERS	TANK 4	TANK 4
Total (kg)	39,352.4733	39.5970	10,067.6242	10,067.6242	1,869.2425	8,198.3818	8,198.3818	7,788.4627	409.9191	409.9191
WATER (kg)	9,000.0006	0.00	8,550.0006	8,550.0006	427.5000	8,122.5006	8,122.5006	7,716.3755	406.1250	406.1250
TPD (kg)	30,352.4726	0.00	1,517.6236	1,517.6236	1,441.7425	75.8812	75.8812	72.0871	3.7941	3.7941
Moisture (kg)	0.0	4.6391	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
protein (kg)	0.0	10.2176	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
fat (kg)	0.0	2.0614	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
carbohydrate (kg)	0.0	20.3342	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
fiber (kg)	0.0	1.5684	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ash (kg)	0.0	0.7764	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass (Kg)	39,352.47	39.60	10,067.62	10,067.62	1,869.24	8,198.38	8,198.38	7,788.46	409.92	409.92
Total Volume (litre)	39,597.42	39.84	10,129.36	10,129.36	1,879.99	8,249.37	8,249.37	7,836.90	412.47	412.47
Phase	Liquid1	Liquid1	Liquid1+Solid	Liquid1+Solid	Liquid1+Solid	Liquid1+Solid	Liquid1+Solid	Liquid1+Solid	Liquid1+Solid	Liquid1+Solid

3.1 RSM Techno-Economic Model Fitting

The BBD model legitimized the development of mathematical equations shown in equations 2 to 4, where the predicted response (Y) was assessed as a function of production cost (A), fixed capital investment (B), selling price (C), discounted rate (D), and efficiency removal (E). Table 7 presents the statistical fit summary for the production of bioclarified water from petroleum wastewater, while Figure 2 presents the relation between the predicted and experimental values of the responses.

Table 6: The BBD experimental design matrix

Std	Run	Production cost (\$)	Fixed Capital Investment (\$)	Selling Price (\$)	Discounted Rate (%)	Efficiency Removal (%)	PBT (Years)	ROI (%)	Production Rate (%)
17	1	9195	549117	0.225	0	88	5.18	17	0.12
34	2	10114	549117	0.225	5	88	5.98	14	0.13
30	3	9195	549117	0.4	5	88	3	28.5	0.16
33	4	8276	549117	0.225	5	88	6.63	15.04	0.14
10	5	9195	604029	0.225	5	88	7.14	12.95	0.19
29	6	9195	549117	0.05	5	88	0	0	0.15
9	7	9195	494205	0.225	5	88	5	16.11	0.17
18	8	9195	549117	0.225	10	88	8.17	11.17	0.155
23	9	9195	494205	0.4	5	93.5	3.02	33.16	1.275
42	10	9195	549117	0.225	5	93.5	6.21	14.01	1.264
45	11	9195	549117	0.225	5	93.5	6.71	14.91	1.28
5	12	9195	549117	0.05	0	93.5	6.41	15.6	1.297
21	13	9195	494205	0.05	5	93.5	7.04	14.2	1.256
40	14	9195	604029	0.225	10	93.5	9.98	10.02	1.29
43	15	9195	549117	0.225	5	93.5	6	13.97	1.26
41	16	9195	549117	0.225	5	93.5	6.71	14.91	1.275
27	17	8276	549117	0.225	10	93.5	8.48	11.8	1.3
8	18	9195	549117	0.4	10	93.5	3.81	26.25	1.58
7	19	9195	549117	0.05	10	93.5	0	0	0.04
46	20	9195	549117	0.225	5	93.5	6.36	13.78	1.58
16	21	10114	549117	0.4	5	93.5	3.4	29.41	1.78
37	22	9195	494205	0.225	0	93.5	5.01	19.92	1.48
1	23	8276	494205	0.225	5	93.5	5.37	17.02	1.38
15	24	8276	549117	0.4	5	93.5	3.37	29.67	1.2568
22	25	9195	604029	0.05	5	93.5	0	0	1.245
14	26	10114	549117	0.05	5	93.5	0	0	1.28
28	27	10114	549117	0.225	10	93.5	8.67	11.54	1.77
6	28	9195	549117	0.4	0	93.5	3.04	32.89	1.878
3	29	8276	604029	0.225	5	93.5	7.45	13.42	1.98
2	30	10114	494205	0.225	5	93.5	5.57	16.33	1.58
4	31	10114	604029	0.225	5	93.5	7.58	13.19	1.58
44	32	9195	549117	0.225	5	93.5	6.21	13.49	1.38
25	33	8276	549117	0.225	0	93.5	5.54	18.06	1.568
38	34	9195	604029	0.225	0	93.5	6.13	16.3	1.65
26	35	10114	549117	0.225	0	93.5	5.62	17.8	1.49
13	36	8276	549117	0.05	5	93.5	0	0	1.656
39	37	9195	494205	0.225	10	93.5	7.32	13.65	1.48
24	38	9195	604029	0.4	5	93.5	3.75	26.63	1.978
35	39	8276	549117	0.225	5	99	6.65	15.04	2.48
19	40	9195	549117	0.225	0	99	5.58	17.93	2.61
31	41	9195	549117	0.05	5	99	0	0	2.5
12	42	9195	604029	0.225	5	99	7.54	13.25	2.42
20	43	9195	549117	0.225	10	99	8.57	11.67	2.53
36	44	10114	549117	0.225	5	99	6.76	14.78	2.41
11	45	9195	494205	0.225	5	99	5.92	16.88	2.4
32	46	9195	549117	0.4	5	99	3.39	29.5	2.38

Table 7: Fit summary for the production of bioclarified water from petroleum wastewater

	Std. Dev	Mean	R ²	Adjusted R ²	Predicted R ²	Adeq Precision	C.V. %	p-value
PBT	0.2196	6.01	0.9920	0.9837	0.9682	43.8381	3.66	<0.0001
ROI	0.3652	17.64	0.9984	0.9968	0.9946	85.9727	2.07	<0.0001
Production rate	0.2669	1.39	0.8867	0.8725	0.8456	27.7285	19.16	<0.0001

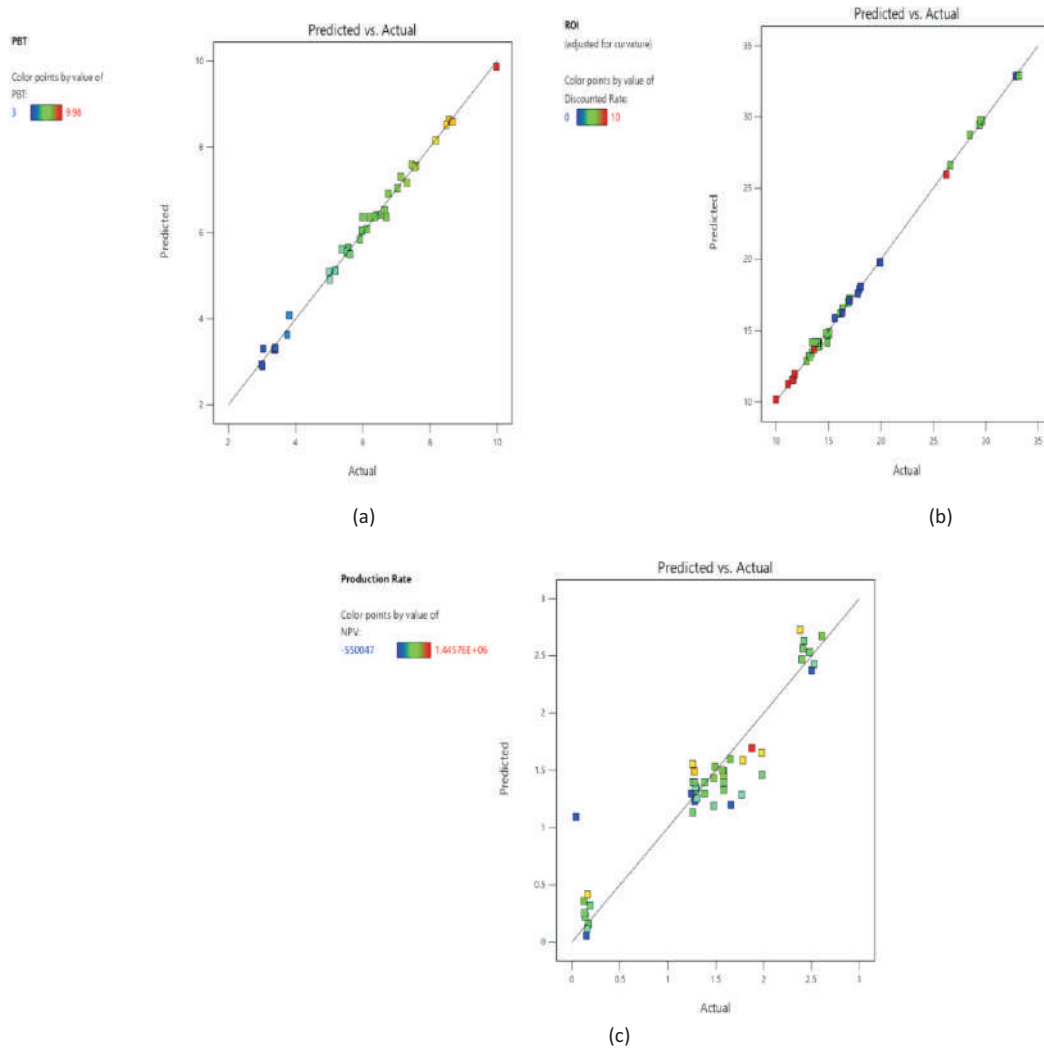


Figure 2: Design expert plot, predicted vs. actual plot for (a) PBT (b) ROI, and (c) Production rate

3.2 Effect of the cost factors on PBT, ROI, and production rate

The regression model in Equations 2 to 4 is adequate for the evaluation of the payback time, return on investment, and production rate of bio-clarified water production, as the model statistical parameter p-values are far less than 0.05, as depicted in Table 7. The relationship between the predicted and experimental values of payback time is shown in Figure 2. This Figure 2 clearly shows that both the actual and predicted values of the PBT, ROI, and production rate are in close agreement, which indicates that the models developed are well-matched to form a relationship among the cost factors and payback time. The values of the correlation coefficient (R^2) for the PBT, ROI, and production rate were found to be 0.9920, 0.9984, and 0.8867. They show reliable relationships between dependent and independent variables. The R^2_{adj} for PBT was found to be 0.9837, 0.9968, and 0.8725, which were very close to R^2 values. Thus, the prediction of experimental data is satisfactory, indicating the fitness and significance of the models (Franco *et al.*, 2017). This result also agrees comparably with that reported by several authors (Oke *et al.* (2019; 2020; 2021).

$$\text{PBT} = 6.37 + 0.01A + 0.96B - 2.675C + 1.51D + 0.24E - 0.02AB + 0.01AC + 0.03AD + 0.19AE - 0.60BC + 0.39BD - 0.13BE - 1.13CD - 0.05CE + 0.13A^2 + 0.11B^2 - 0.53C^2 + 0.54D^2 - 0.03E^2 \quad (2)$$

$$\text{ROI} = 14.18 - 0.24A - 1.77B + 8.12C - 3.05D + 0.27E + 0.12AB + 0.10AC + 0AD + 0.20AE - 1.36BC - 0.003BD - 0.12BE - 0.39CD + 0.23CE - 0.11DE + 0.37A^2 + 0.57B^2 + 6.90C^2 + 0.23D^2 + 0.04E^2 \quad (3)$$

$$\text{Production Rate} = 1.39 + 0.02A + 0.08B + 0.18C - 0.12D + 1.16E \quad (4)$$

4. Conclusion

The model in this paper gave batch size, annual production cost, TCI, PBT, and ROI of 406kg, \$9195, \$631484, \$5.18, and 17%, respectively, at the selling price of \$0.225. The outcome of increasing the selling price of the bio-clarified water to \$0.4 reduced the number of years to pay back money obtained from external sources to 3.54 years. The techno-economic regression models gave R^2 values of 0.9984, 0.9920, and 0.8867 for return on investment, payback time, and production rate, respectively, which were close to unity. For the profit of \$99723.65, the optimum ROI and PBT were feasible at 11.55% and 8.66 years, respectively. This reveals a significant decrease in PBT with an increase in selling price. In summary, this work developed the ASPEN Base Case Simulation Model and techno-economic RSM models and feasible optimum profitable conditions for bioclarified water production from petroleum wastewater. The RMSE between ASPEN-simulated and that of the experimental data was 0.00%, revealing that the degree of ASPEN-based simulation model predictability is high and that it is capable of simulating petroleum wastewater bio-clarification. Further study is recommended for the fabrication and construction of a bioclarified water production prototype plant in Nigeria in order to validate the techno-economic results obtained from this study.

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