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Optimization of Linear Alkyl Benzene Yield through Modelling and Simulation

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Abstract: *Demand for consumer products such as detergents, soap, shampoos, cosmetics and emulsifiers continues to rise due to the increase in population. As a result of this, the production of linear alkyl benzene, a key ingredient in detergent and cosmetics production has increased. The need for the specification of linear alkyl benzene is essential in the production of the best quality detergent. A side reaction is one of the major problems in detergent production that occurs during paraffin conversion to olefins in the linear alkyl benzene (LAB) production process which leads to undesirable olefins. Also, instability of the thermodynamic variables such as temperature, pressure and flow rate are the factors that affect the equipment performance for LAB production. This research was aimed at improving the product yield of the linear alkyl benzene plant of Kaduna Refining and Petrochemical Company (KRPC) using Aspen HYSYS®. The results obtained from the modelling and simulation of the LAB production process using ASPEN HYSYS® revealed that the developed model was successful as the model was able to converge when simulated with all the selected fluid packages. However, Peng-Robison as a fluid package gave a better (compared to other property models used) LAB yield of 3800 kg/h, which, is very close to the actual LAB plant yield of 3788 kg/h at the same feed rate. Moreover, the linear model equation developed for the LAB yield using Design-Expert 13.0.0 may be very useful in representing the behaviour of the KRPC LAB plant as the model was statistically significant and had a high value of the coefficient of determination (0.7075). The R-squared value implied that the first-order polynomial model adequately represented the experimental data. Furthermore, the Response Surface Methodology (RSM) numerical optimization result was able to show a remarkable improvement in LAB yield value up to 2.10%, while with the particle swarm optimization method 1.85% improvement was recorded at the optimum operating PACOL (paraffin conversion to olefins) temperature, pressure and DETAL (detergent alkylation) temperature, pressure of 500 ℃, 3.5 kg/cm^2.g and 280 ℃, 4.5 kg/cm^2.g for particle swarm and 457.349 ℃, 2.320 kg/cm^2.g , 275.692 ℃ and 2.815 kg/cm^2.g for RSM respectively. It can be said that the process variables considered in the current study gave better yield of the LAB product of KRPC LAB plant section.*

Keywords: *LAB, CCD, Particle Swarm, Peng-Robinson, RSM.*

1. INTRODUCTION

Linear alkyl benzene (LAB) is an aromatic hydrocarbon family with a general molecular formula, $C_6H_6 - C_nH_{2n+1}$ (n is between 10 and 16). LAB is majorly used in the manufacturing of nature-friendly detergents, soap and emulsifiers [1]. The industries that use raw materials like LAB is quite growing rapidly. This growth can be noticed from the emergence of new brands of cleaning and cosmetic products in Nigerian markets. Along with the swift demand for chemical products in Nigerian (domestic) market, most industries began using LAB to replace branched alkyl benzene due to environmental issue [2]. In the same vein, chemical experts have intensified research towards production of a detergent whose use is not associated with environmental pollution. One of the research results is the production of environmentally friendly LAB [1]. Kerosene is the main feedstock for the production of LAB. Catalytic dehydrogenation of kerosene yields olefins, which in turn react with benzene in the presence of catalyst to produce LAB [3, 4].

In process development, modelling and simulation plays a very crucial role. Process modelling and simulation allows process engineers to design, optimize, control and analyse complex systems such as refinery and petrochemical plants satisfactorily and efficiently. It also generates realistic thermodynamic data, equipment design specifications and process efficiency prior to the practical implementation. This can reduce large-scale production risk substantially as post-

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implementation modification of projects is generally difficult [5]. Among available modern process simulation software are Aspen plus, Aspen HYSYS®, CHEMCAD®, and Pro II® [6].

Aspen HYSYS® is conceptual simulation software built-in with many chemical components from DECHEMA database, it is widely employed, especially in conceptual and detailed engineering design to develop, control, optimize and monitor various processes of plants at the industrial level [7] The most important applications of Aspen HYSYS® are found in the simulation of the industrial processes in oil & gas and product manufacturing plants. The most attractive advantage of the simulator is that it permits the conversion of steady-state model to dynamic model or vice versa. This flexibility in handling the system under investigation in the two modes make it possible to evaluate with ease, the dynamic nature of system which helps in making design decision with respect to controllability of the system. [8]. Aspen HYSYS® performs high standard calculation with quick convergence and short time simulation, and it is a user-friendly guaranteed software [9].

In chemical engineering, when a process is confirmed scale up, this means the plant is in commercial scale [7] Due to aging and other factors, matter may arise to optimize the process in order to improve the product yield, reduce operating and investment cost in order to maximize profit. In this case, the aspect of chemical engineering job is to optimize the LAB plant of Kaduna Refining and Petrochemical Company. However, due to the composite nature of reactions and separations taking place in the production process, distillation columns exhibit complex behaviours [5,10] such as steady-state multiplicity, changes in process gain sign (bidirectionality) and strong interactions between process variables [7]. These complexities which have made the modelling of the reactive process extremely difficult [11]. And also, have made its optimization a challenging task to chemical engineers because this process is a multivariable type [10].

Traditionally, finding the optimum conditions of multivariate systems is achieved by using One-factor optimization technique, in which variation of a factor is done at a time while other factors are held at constant values. This approach requires large number of experimental runs which later need more time to perform and consequently, leads to increasing cost of project. Aside, by this method, the interaction between the factors is not accounted for. Thus, this optimum given by this approach may not be real optimum. These problems can be eliminated by using optimization approaches such as Response Surface Methodology (RSM) [7].

RSM is a very useful tool in designing experiments for systems that have no mechanistic information and optimizing the same [12]. With conventional software such as Design Expert and Minitab, optimization using RSM can be performed via three steps, namely, (1) Design of experiment, this step requires stating or entering the ranges of independent variables and in return, a set of experimental runs according to which experiments are carried out is given. In this step also, the dependent variable (response) values are collected and entered to response column in the design matrix (2) Development of the empirical model and statistical analysis, at this stage the experimental (input-output) data are modelled mathematically and the validity of the model is evaluated using analysis of variance (ANOVA) (3) Optimization, in this step, the model developed in step 2 in maximized or minimized based on objective of the study [7, 8]

Actually, some research works have been done on LAB production. Otaraku *et al.* [1] carried out research on the effect of temperature on LAB yield from a Rerun Column of LAB Plant using Aspen HYSYS®, their findings gave 99.4% LAB yield at the 280 °C and 115 kPa from the bottom of the rerun column of LAB production process using Peng-Robison as fluid package. In addition, Ivanchina [3] reported on the application of mathematical modelling to the optimization of LAB sulphonation mode in a film reactor. Their findings revealed that the detergent alkylation reactor kinetic modelling improved the raw material compositions. This technique is quite robust as it allows acquisition of data related to the kinetic study of the detergent alkylation reactor. Khlebnikova *et al.* [13] reported on the optimization of linear alkyl benzene production, their findings revealed that the mathematical model of the reacting system and optimization of the system using Pareto criterion showed 99.15% yield of olefin, 0.6% diolefins and 7625 kg/h LAB with feed rate of 1000 kg/h of kerosene. Also, their findings showed that temperature had significant effect on the LAB production process. Abdulla [10] and Abdel-Rahman and Latef [14] reported on the process simulation analysis of HF stripping column using Aspen HYSYS® process simulator. Their findings revealed that feed temperature, bottom temperature and top pressure of 120 ℃, 200 ℃ and 461.3 kPa were the best operating conditions for the stripping operation using Margules thermodynamic model.

According to the literature review carried out, it has been discovered that it is very necessary to simultaneously simulate the LAB plant in order to achieve the maximum yield of LAB, due to the rigorous nature of the LAB production process. This makes it impossible to ascertain the yield of LAB with a single unit and one variable [15]. Similarly, the work reported by Otaraku *et al.* [1] and Abdulla [10] may not actually improve the yield of LAB since it is only a single system considered. More so methods of optimization employed by Khlebnikova *et al.* 13] had the possibility of missing the true optimum conditions that can lead to an improved yield of LAB since these works did not employ the design of experiment that allows wide variation of factors within certain ranges. Therefore, this work was carried out to contribute toward improving the yield of LAB plant of KRPC by applying Aspen HYSYS® to model and simulate the plant. In addition, the optimization of the plant was carried out using response surface methodology and particle swarm method. The former approach was achieved by employing the central composite design with aid of Design Expert 13. While the latter was accomplished in MATLAB® 2018b environment. Also, in order to evaluate the performance of each of the optimization methods, optimum conditions obtained were validated using the plant data.

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2. MATERIALS AND METHODS

2.1 Materials

The materials used for this research work are:

i. Aspen HYSYS® version V 11.0
ii. Design Expert V 13.0
iii. MATLAB® 2018b software
iv. Flow and data sheet of linear alkyl benzene production process (KRPC)

2.2 Methods

2.2.1 Data Collection

Process data were collected from the LAB plant data log sheet of KRPC, feed data such as mass flowrate, temperature and pressure were used as equipment operating conditions to simulate the PACOL and DETAL units of the production system.

2.2.2 Aspen HYSYS® Modelling and Simulation Procedure

Aspen HYSYS® was used to model the PACOL and DETAL unit of the LAB production plant in order to test it virtually, based on the condition and parameters obtained from the LAB plant of KRPC Kaduna. Detail of the modelling and simulation procedure is presented Figure 1.

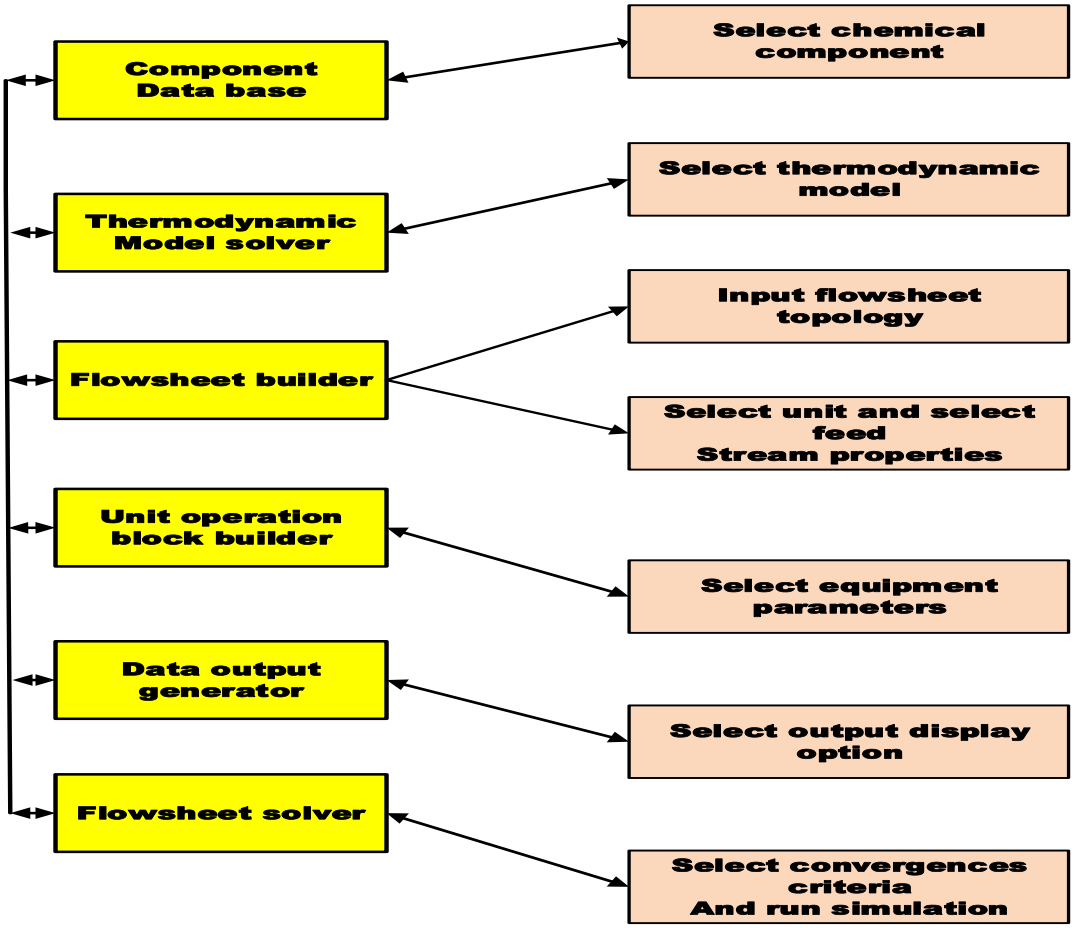

Figure 1: Basic Simulation Steps [16]

The simulation process was run at steady-state based on sequential modular approach, five different fluid packages such as UNIQUAC, UNIFAC, Wilson, NRTL and Peng-Robison were used to run the simulation [17]. Then, the best out of these packages was selected for the optimization aspect. The variables considered in this study were the flow rate, temperature and pressure. Given in Tables 1 and 2 are the feed compositions; and in Table 3 are operating conditions data used for the simulation to obtain the most suitable fluid package. Also, Tables 4 and 5 contain the industrial data used for equipment specification. The simulation of various equipment was conducted starting from the PACOL reactor, which is a heterogeneous catalytic system where the conversion of paraffin to olefins takes place. The second reactor is a liquid-phase hydrofluoric alkylation reactor, which produces linear alkyl benzene (LAB) and followed by the columns which are

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hydrofluoric stripper column, benzene column, paraffin column and the rerun column [9]. Figure 2 is the PACOL and DETAL units' process flow diagram.

Table 1: LAB Plant feed composition in weight percent (%)

Components	Chemical Formula	Composition in Mass (wt%)
Hydrogen	H_2	0.6569
N-Decane	$nC_{10}H_{22}$	0.0024
N-Undecane	$nC_{11}H_{24}$	0.1060
N-Dodecane	$nC_{12}H_{26}$	0.1026
N-Tridecane	$nC_{13}H_{28}$	0.0748
N-Tetradecane	$nC_{14}H_{30}$	0.0456
N-Pentadecane	$nC_{15}H_{32}$	0.0010
Cyc-Paraffin	$C\text{-}C_6H_6$	0.0016
Iso-Paraffin	$i\text{-}C_5H_{14}$	0.0044
Aromatics	C_6H_6	0.0045
Heavy Alkane	$n\text{-}C_{24}$	0.0001
Total		1.00
Flowrate (kg/h)		3220

Table 2**:** LAB Plant sub-feed composition in weight (%)

Components	Chemical formula	Composition	Mole fraction	Flowrate (kg/h)
Benzene	C_6H_6	1.0	20.21	1580

Table 3**:** The parameters used in the simulation of LAB production process

Streams	Temperature (°C)	Pressure (kg/cm^2.g)	Flowrate (kg/h)
Feed stream	104	1.05	3220
Stream (3) PACOL Reactor Inlet	499	2.46	------
Stream (4) PACOL Reactor Outlet	480	2.11	------
Stream (21) DETAL reactor (1) Inlet	38	2.467	------
Stream (22) DETAL reactor (1) outlet	308	3.9767	------
Stream (23) DETAL reactor (2) Inlet	260.7	0.4668	------
Stream (25) DETAL reactor (2) Outlet	281	1.967	------

Table 4**:** Industrial data for PACOL rector (31R01)

Parameter	Value	Unit
Reactor Diameter	1525	mm
Reactor length	4300	mm
Reactor position	Vertical	-------
Feed flow rate	43.3	m^3/h.
Inlet pressure	2.1	kg/cm^2.g
Inlet temperature	370	°C
Catalyst bed porosity	0.345-0.55	-------
Bed bulk density	658	kg/m^3
Particle diameter	2*10E^{-3}	m

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Table 5**:** Industrial data for detal rectors & stage acid settlers

Equipment	Position	Diameter (mm)	Length (mm)	Sieve Tray No.	Sieve Tray Spacing	Sieve Tray Type
1st stage Alkylation mixer(32C01)	Vertical	2000	15450	30	450	Perfor trays
2nd stage Alkylation mixer(32C02)	Vertical	1300	13500	14	900	Perfor Trays
1st stage Acid Settler(32D01)	Horizontal	4000	14000	-----	-----	-----
2nd stage Acid settler(32D02)	Horizontal	4000	14000	-----	-----	-----

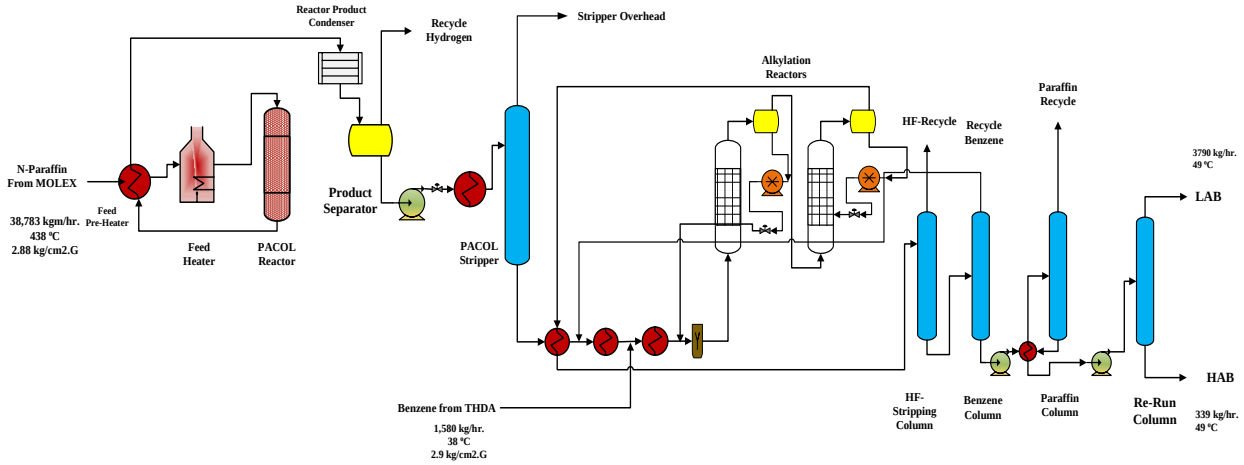

Figure 2: PACOL and DETAL Units Process Flow Diagram [18]

Also, Tables 6 and 7 contain the kinetic data specified for the plug-flow reactors used for both PACOL and DETAL Units; other industrial specifications of the PACOL and DETAL reactors used were as given in Tables 4 and 5 respectively. All the data presented in Tables 1-7 were obtained from the LAB Production Plant manuals of the KRPC Kaduna. The manuals were developed by UOP and Chiyoda Corporation [18].

Table 6: PACOL reactor kinetic reaction data

Reactions	Pre-exponential factor (A^0)	Activation energy (E_a)	Reaction stoichiometric
R1	3.6500e+015	30.5000	1:1
R2	3.2900e+015	80.0000	1:1
R3	3.2500e+015	78.0000	1:1
R4	3.2000e+015	70.0000	1:1
R5	3.1800e+015	68.0000	1:1
R6	3.1500e+015	65.0000	1:1
R7	3.1600e+015	67.0000	1:1
R8	1.5000e+015	42.0000	1:1
R9	3.3000e+015	84.0000	1:1
R10	3.4800e+015	92.0000	1:1

Table 7: DETAL reactor kinetic data

Reaction	Pre-exponential factor (A^0)	Activation energy (E_a)	Reaction stoichiometric
R1	1.89000e-003	45.300000	1:1
R2	1.98000e-003	43.000000	1:1
R3	2.18000e-003	43.290990	1:1
R4	2.20000e-003	42.800000	1:1
R5	2.25000e-003	42.100000	1:1
R6	2.30000e-003	40.500000	1:1

2.2.3 LAB Production Mathematical Modelling and Optimization

In order to develop a mathematical model relating the selected variables, i.e., PACOL temperature, PACOL pressure, DETAL temperature and DETAL pressure with LAB yield as a response, a set of 30 experimental runs were generated according to central composite design of RSM. Thereafter, each of runs was carried out in the Aspen HYSYS model to obtain LAB yield expressed in kg/h. The obtained data were fitted to a linear equation based on suggestion of the Fit Statistics. The developed linear model was then optimized via two different approaches, namely, numerical method of RSM and particle swarm, a heuristic method of optimization for comparison purpose. All the RSM steps were accomplished using Design Expert 13. While the latter optimization was carried using MATLAB 2018b, by creating a function file with the linear model earlier obtained and calling the same function via the command line as bound optimization problem with lower and upper bound as [300 2 38 2.5] and [500 3.5 280 4.5] respectively. In order to validate the optimization results, both predicted set of optimum conditions were run in the Aspen HYSYS prototype plant, the obtained maximum yields were later compared to the existing maximum yield of the plant.

3. RESULTS AND DISCUSSION

3.1 Aspen HYSYS Modelling and Simulation

Modelling and simulation of the process systems is an important tool in reducing risk of operation, investment and operating cost due to systems failures thereby improving the performance of the process systems. Prior to modelling and simulation of LAB plant of Kaduna refining and petrochemical company (KRPC), existing data were collected from the Flow sheet and operating manuals of the LAB plant of the company. The data were then used for the simulation. Table 8 shows the results of simulation of the LAB plant testing different thermodynamic models. It could be noticed from the table that variation of thermodynamic models had impact on the yield of LAB, which affirm the observation by Abdel-Rahman and [11] who found that using various thermodynamic models affected the results of CHEMCAD simulation of a separation column used in LAB production. Similarly, Abdel-Rahman and Latif [12] observed that use of different thermodynamic models for CHEMCAD simulation of a paraffin separation column of an LAB plant led to variation in results. Also, this was found to align with the results obtained by Abdulla [10] who reported that while four of various thermodynamic models affected the Aspen HYSYS simulation results in the range of 0.1 and 58%, one was observed to give an average value. In this present work, based on the increasing order of the amount of LAB, the performance the models used can be written in the following order SRK<UNIQAC<NRTL<W<PR with the achieved yield in the range of 3666 and 3800 kg/h which compared well with plant LAB yield of 3788 kg/h. Peng-Robison (PR) as a fluid package resulted to 3800 kg of LAB/h which was observed to be higher than LAB yield of KRPC 3788 kg/h as obtained from the data sheet. Comparing the plant yield to the yield obtained from the simulation using each of the fluid packages, it was obvious that only with PR that an improved yield was obtained with 0.316% increment. The performance of this model can be attributed to the fact that PR performs more accurate calculation which leads to prediction of state variables values that are more realistic, thus, PR gives good representation of the system under investigation. This may be the reason why Otaraku et al. [1] used PR as the only fluid package for their work where the effect of the variation of condenser and reboiler temperature on the yield of LAB separation was investigated.

Table 8: Comparison of simulation yield of different thermodynamic models with actual yield in LAB Plant

Thermodynamic Model	Simulation Yield (kg/h)	Actual plant Yield (kg/h)	difference (%)
Peng-Robison	3800	3788	+ 0.32
Wilson	3752	3788	- 0.95
NRTL-Ideal	3700	3788	-2.37
UNIQAC	3698	3788	- 2.44
SRK	3666	3788	-3.22

3.2 Mathematical Model Development

Presented in Table 9 are the various operating conditions used to run the Aspen HYSYS prototype LAB plant and various yield of LAB obtained.

Table 9**:** The Central Composite Design matrix and obtained values of the response

	Factors				Response
Run	**Ptemp, ^oC**	**Ppress, kg/cm^2.g**	**Dtemp, ^oC**	**Dpress, kg/cm^2.g**	**υ_{LAB}, kg/h**
1	457.5	3.125	98.5	3	3799.99
2	405.0	2.750	159.0	3.5	3799.89
3	510.0	2.750	159.0	3.5	3799.8
4	405.0	2.000	159.0	3.5	3799.11
5	405.0	2.750	159.0	3.5	3799.85
6	352.5	3.125	98.5	3.0	3799.32

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	Factors				Response
Run	**Ptemp, ^oC**	**Ppress, kg/cm^2.g**	**Dtemp, ^oC**	**Dpress, kg/cm^2.g**	**υ_{LAB}, kg/h**
7	352.5	2.375	219.5	3.0	3800.49
8	352.5	2.375	219.5	4.0	3800.50
9	457.5	3.125	219.5	3.0	3800.50
10	405.0	2.750	280.0	3.5	3800.59
11	457.5	2.375	219.5	4.0	3800.50
12	405.0	3.500	159.0	3.5	3799.77
13	405.0	2.750	159.0	3.5	3799.82
14	352.5	3.125	219.5	4.0	3800.49
15	352.5	2.375	98.5	3.0	3799.28
16	405.0	2.750	38.0	3.5	3799.12
17	405.0	2.750	159.0	3.5	3799.85
18	457.5	2.375	98.5	3.0	3799.14
19	352.5	3.125	219.5	3.0	3799.49
20	457.5	2.375	98.5	4.0	3799.32
21	352.5	2.375	98.5	4.0	3799.14
22	300.0	2.750	159.0	3.5	3799.06
23	457.5	2.375	219.5	3.0	3800.6
24	405.0	2.750	159.0	3.5	3799.36
25	457.5	3.125	219.5	4.0	3800.52
26	457.5	3.125	98.5	4.0	3799.77
27	405.0	2.750	159.0	3.5	3799.90
28	352.5	3.125	98.5	4.0	3799.34
29	405.0	2.750	159.0	4.5	3799.84
30	405.0	2.750	159.0	2.5	3799.65

The output obtained from running the prototype of LAB production with Aspen HYSYS simulator using the ranges of operating conditions of PACOL and DETAL reactors, were observed to vary as the values of the input variables considered changed according to the RSM design method used (Table 9). The variation in the response values with respect to change in values of the independent variables indicated that the selected factors actually affected the LAB production system. By using the design matrix data given in Table 7, a model relating the LAB yield and the operating conditions of PACOL and DETAL reactors (temperature and pressure) developed was as given in Equation 1.

$$LAB_{Yield} = +3796.53698 + 0.002992\,x_1 + 0.196667\,x_2 + 0.007390\,x_3 + 0.095833\,x_4 \quad (1)$$

where $x_1 = Ptemp$, $x_2 = Ppress$, $x_3 = Dtemp$ and $x_4 = Dpress$

The developed model, which was linear in nature, was analysed, and the results of the statistical analysis were as given in Table 10.

Table 10**:** Results of Analysis of Variance (ANOVA) for LAB yield

Source	**Sum of Squares**	**Df**	**Mean Square**	**F-value**	**p-value**	
Model	5.58	4	1.39	15.12	< 0.0001	Significant
A-Ptemp	0.5922	1	0.5922	6.42	0.0179	
B-Ppress	0.1305	1	0.1305	1.42	0.2453	
C-Dtemp	4.80	1	4.80	52.03	< 0.0001	
D-Dpres	0.0551	1	0.0551	0.5977	0.4467	
Residual	2.30	25	0.0922			
Lack of Fit	2.09	20	0.1045	2.44	0.1638	not significant
Pure Error	0.2143	5	0.0429			
Cor Total	7.88	29				
R-squared: 0.7075 Adjusted R-squared: 0.6607 Predicted R- squared 0.5565, adeq Precision: 14.4266						

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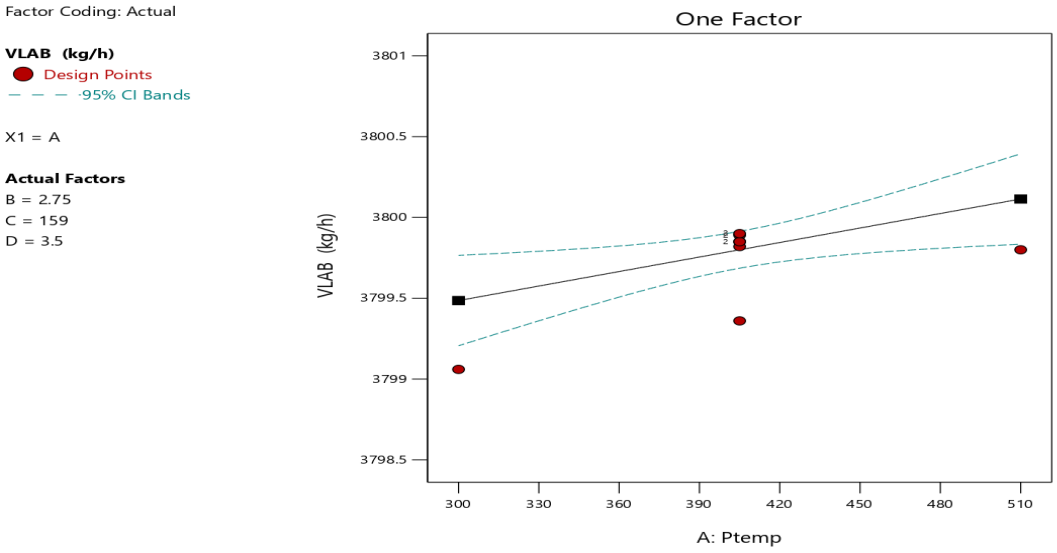
Among the statistical parameters used in evaluating model fitting are probability of error values (p-value) and coefficient of determination (R-squared). P-value is used to ascertain statistical significance of the model and the contribution of various components of the model. Based on 95% confidence interval used for the analysis, p-value must be less than 5% for any model or its terms to be statistically significant. As it can be noticed from Table 10 that the PACOL temperature, A, and DETAL temperature C were the significant terms of the model with p-value of 0.0179 and <0.0001 respectively which were less than 0.05 [8]. Also, the effect of these factor can be noticed in Figure 3, where the sharpest gradient had been observed in 3(c) and sharper one is obvious in 3(a). Also, p-values obtained for B, the PACOL pressure and D, the DETAL pressure corroborate the nature of the slopes of linear graphs in Figure 3(b) and 3(d), hence, the statistical insignificance of these factors on the model. The nature of the slopes of the straight lines in Figure 3(a and c) can be attributed to the fact that increasing temperature of both PACOL and DETAL units significantly improved the yield of LAB. Also, increasing both PACOL and DETAL pressure (Figures 3b and 3d) led to increase in LAB yield, however the increment was not as large as that observed with temperature increase. The results obtained in this work was observed to be in line with the work of Khlebnikova et al. [13] who found that LAB yield increased with increase in temperature and pressure. Also, given in Figure 4 is the contour plot depicting the effect of simultaneous variation of PACOL temperature and pressure on LAB yield, it is noticeable that increasing these two factors had an increasing effect on LAB yield.

In addition, in order to know how well the experimental data fitted the proposed linear model for LAB yield as a function of PACOL and DETAL temperature and pressure, the R-squared value was used. Usually, the closer the value of R-squared to unity, the better the model represent the experimental data. The obtained R-squared value of model was 0.7075 which mean that the model was able to explain more than 70% of the variations in LAB yield which occurred as a result of change in the value of considered independent variables. Also, the predicted and adjusted R-squared values were observed to differ by less than 0.2 which also affirmed the good representation of the experimental data by the model.



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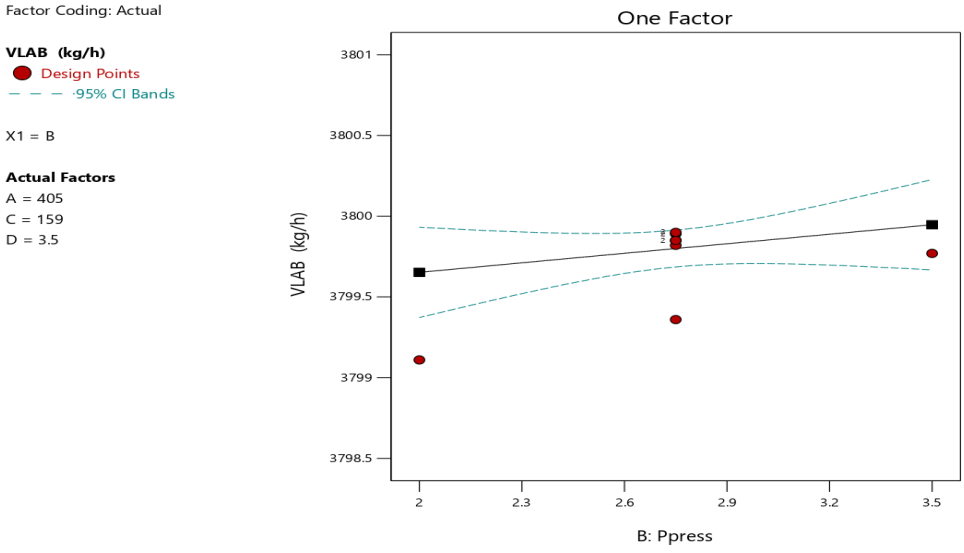

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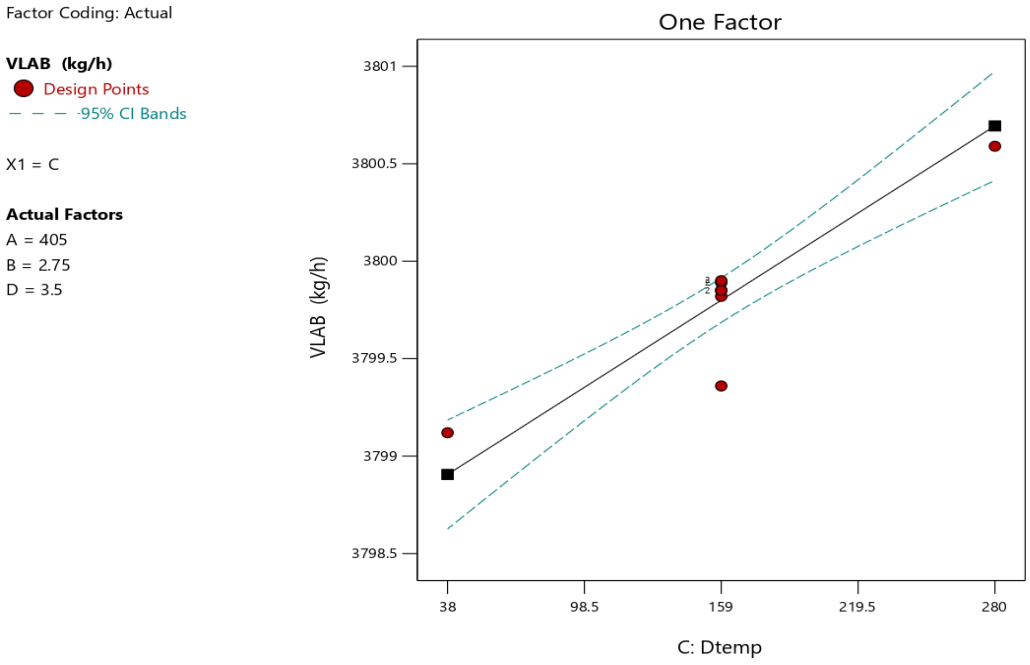
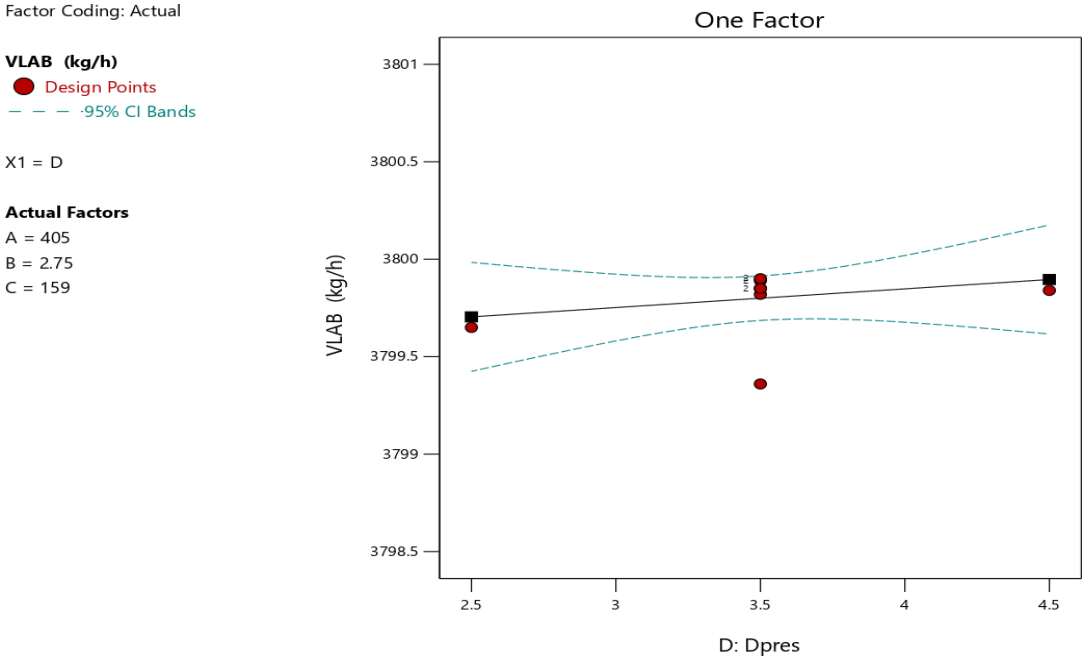


(c)



(d)

Figure 3: The Effects of (a) PACOL temperature, (b) PACOL Pressure (c) DETAL temperature and (d) DETAL pressure on LAB yield

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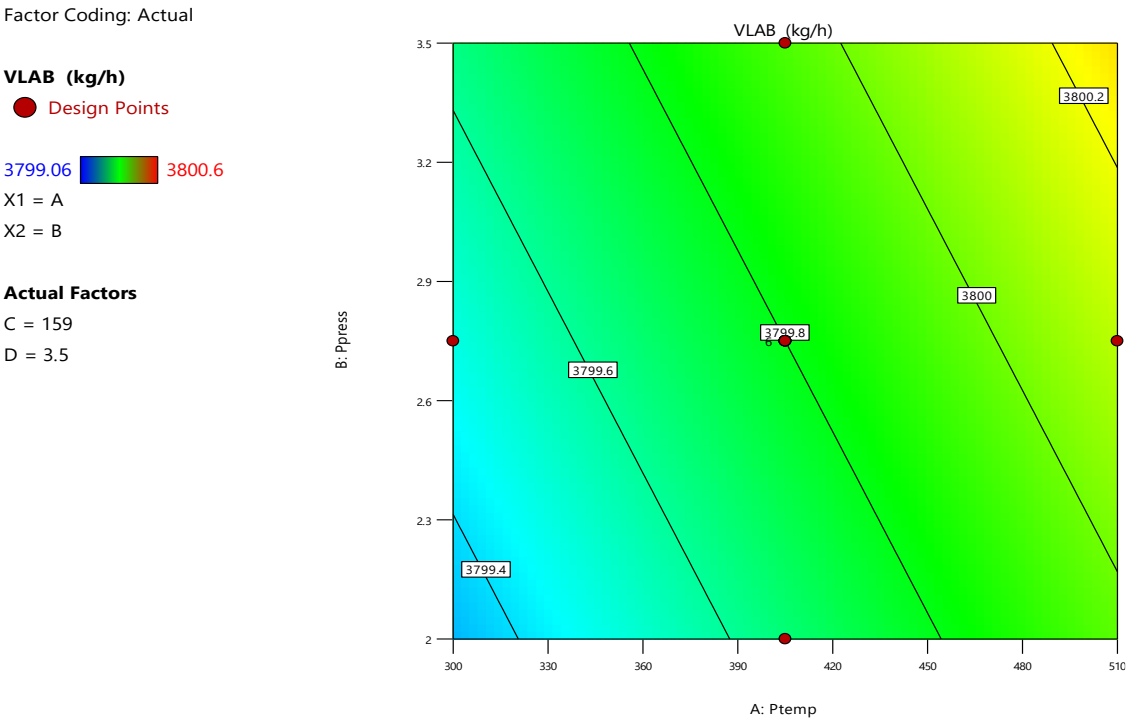

Figure 4**:** Graph of PACOL operating conditions against LAB yield

3.3 Optimization and Validation

3.3.1 RSM Optimization

Numerical optimization of the RSM carried out using Design Expert V.13 results revealed that 457.349 ºC, 2.3203 kg/cm^2.g, 275.692 ºC and 2.815 kg/cm^2.g respectively for PACOL temperature, PACOL pressure, DETAL temperature and DETAL pressure were the optimum conditions for the improved LAB yield. Under these conditions, the model suggested LAB yield of 3800.669 kg/h with desirability of 1. The graphical representation for the selected optimum conditions is given in Figure 5. The predicted LAB yield was noticed to compare well with the actual plant LAB yield of 3788 kg/h. Validating these conditions in the Aspen HYSYS plant model gave LAB yield of 3868 kg/h.

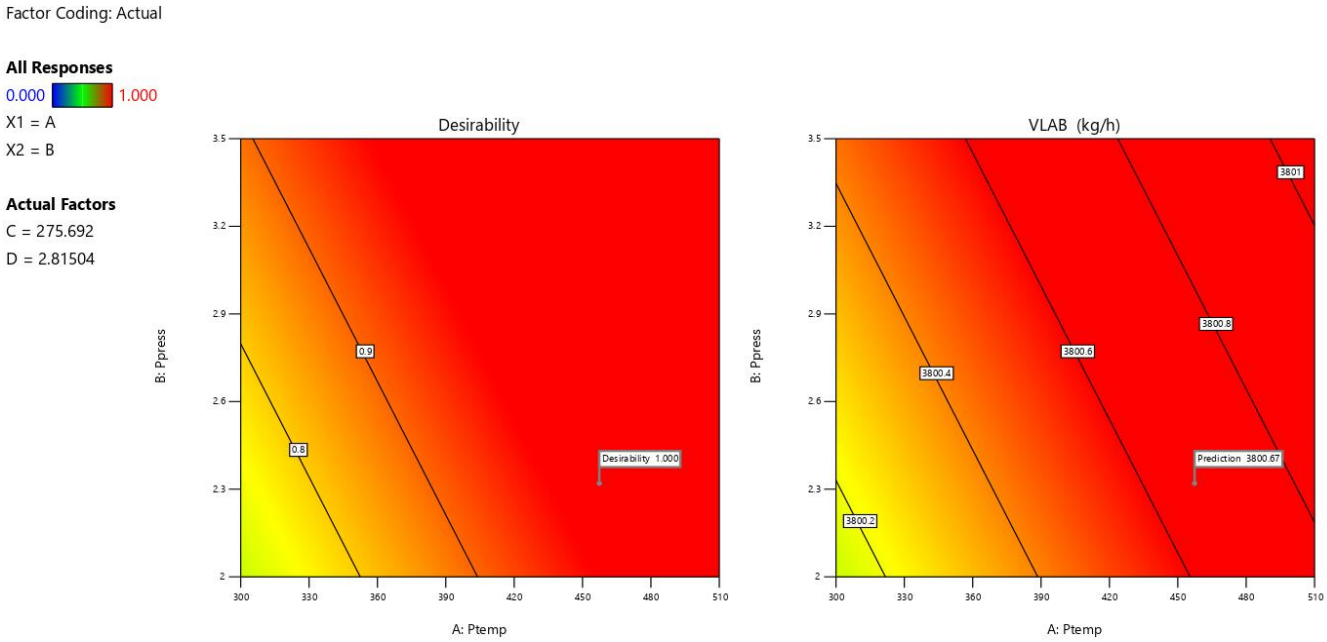

Figure 5**:** Graph of desirability and LAB yield against operating conditions

3.3.2 Particle Swarm Optimization

The particle swarm optimization results revealed 500 ℃, 3.5 kg/cm^2.g, 280 ℃, and 4.5 kg/cm^2 respectively as the optimum operating conditions of the PACOL temperature, PACOL pressure DETAL temperature and DETAL pressure with the LAB

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yield of 3800.12 kg/h. Presented in Figure 6 is the screen shot of the linear model coded in *mfile* and maximized using particle swarm method. The result of the optimization displayed in the Command Window was as shown in Figure 6. Validating the particle swarm predicted optimum conditions in Aspen HYSYS model resulted to LAB yield of 3857.837 kg/h.

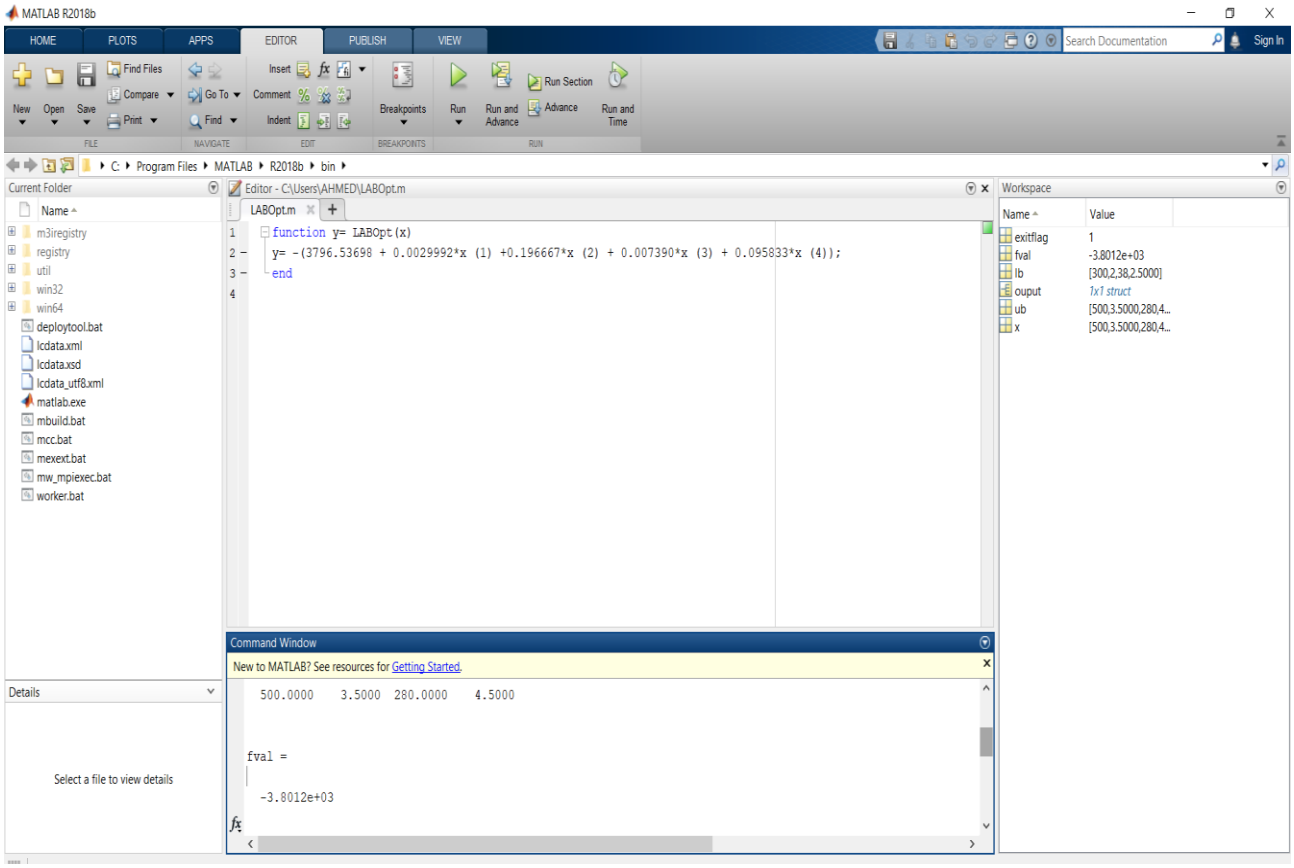

Figure 6: Particle swarm optimization from MATLAB File

3.4 Optimization Results Evaluation

Table 11 shows the summary of the results for RSM and particle swarm optimization of LAB yield. It was clear from the results shown in the table that RSM optimization of the process was able to achieve 2.10 % improvement in LAB yield compared to the particle swarm optimization which led to 1.85 % increase in the yield of LAB when the actual KRPC LAB yield was used as a basis. Furthermore, the RSM optimum conditions obtained (457.349 ℃, 2.320 kg/cm^2.g , 275.692 ℃, and 2.815 kg/cm^2.g,) were observed to be lower than those (500 ℃, 3.5 kg/cm^2.g 280℃, and 4.5 kg/cm^2) given by particle swarm. This can translate to lower energy consumption and lesser operating cost.). Based on total feed rate (without recycle), at various optimum operating conditions stated earlier, 100.10 % and 99.9 5% yields were achieved with RSM and particle swarm respectively.

Table 11: Comparison of numerical and Particle Swarm Optimization results with KRPC Plant LAB yield

Optimization method	PACOL Reactor Temperature, ºC	PACOL Reactor Pressure, kg/cm^2.g	DETAL Reactor Temperature, ºC	DETAL Reactor Pressure, kg/cm^2.g	LAB Yield kg/h	KRPC LAB yield kg/h	(%) Gain
RSM	457.349	2.320	270.692	2.815	3868	3788	2.10
Particle swarm	500.000	3.500	280.000	4.500	3862	3788	1.85

4. CONCLUSION

The results obtained from the Aspen HYSYS modelling and simulation of the LAB production process revealed that the developed model was successful and was able to converge when simulated with Peng-Robison as fluid package to give the yield of LAB as 3800 kg/h. which, is very close to the actual LAB plant yield of 3788 kg/h at the same feed rate. Moreover, the linear model equation developed for the LAB yield using Design-Expert 13.0.0 can be used to represent the behaviour of the KRPC LAB plant satisfactorily since the model was found to be statistically significant and the R-squared value was high (70.75%), in addition there was a close agreement between the predicted and adjusted R-squared values (difference of

0.151). Furthermore, RSM optimization approach gave optimum condition that can lead to reduced energy consumption with yield improvement of 2.10 % at the optimum PACOL temperature, PACOL pressure, DETAL temperature and DETAL pressure of 457.35 ^{o}C, 2.320 kg/cm^2.g, 275.692 ^{o}C and 2.815 kg/cm^2.g respectively. On the other hand, particle swarm optimization improved the plant yield by 1.85 % at optimum operating conditions of temperature (500 ^{o}C and 280 ^{o}C) and pressure (3.5 kg/cm^2.g and 4.8 kg/cm^2.g) for PACOL and DETAL reactors respectively. Finally, the optimisation study showed improvement in the production yield which means that when the plant is operated at these conditions, an improved profit can be obtained.

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