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A Logarithmic Penalty Function Approach for Enhancing the Alkylation Process in Kaduna and Warri Refineries

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Abstract Petroleum industries play a vital role in the global economy, and research institutions need to focus on optimizing their chemical processes. Achieving the ideal operating conditions for these processes is crucial for effective management decision-making. In the alkylation reaction, isobutane reacts with light olefins, like butylenes, in the presence of a strong acid catalyst to produce high-octane compounds. To optimize the profit function without relying on complex computer programming codes, we utilized a novel logarithmic penalty function (LPF) approach. This approach was specifically designed to handle nonlinear programming problems with irregular features. The approach was implemented using the *fminunc* routine function, employing quasi-Newton methods, and compared it with existing conventional methods (using nonlinear programming system optimization laboratory (NPSOL) code and Hock-Schittkowsky (HS)). The results demonstrated higher efficiency compared to NPSOL and HS approaches as the LPF method yielded a higher objective value, implying a more favorable outcome in terms of maximizing the desired outcome (e.g. profit).

Keywords Logarithmic Penalty Function, Penalized Problem, Alkylation, Isobutyne, Olefin feed.

Mathematics Subject Classification 90C26, 90C30

1 Introduction

Nonlinear functions are commonly used to represent chemical process interactions, and it is important to consider various constraints on the operating ranges of variables, which are known as problem constraints. Each variable plays a role in the interrelationships among them, and changing one variable can affect the others, making the entire model quite complex. The penalty function method is a popular and straightforward approach to handle such complexities without relying on sophisticated computer programming codes. Several types of penalty function methods have been proposed in the literature ([1], [2], [3], [4], [5], [6], [19], [20]). Typically, the penalty function method involves transforming a nonlinear constrained optimization problem into a sequence of unconstrained problems or a single unconstrained problem, and it can be implemented using suitable unconstrained optimization algorithms. The penalty function method has been widely applied to solve practical problems, including electro-optical and spectroscopy intensity [7], power flow [8], and automatic train operation [9].

The structure of this presentation is as follows: Section 2 provides a detailed explanation of the alkylation process, illustrated in Figure 1. This leads to the development of a mathematical model for optimizing the process. In Section 3, the formulation of the process is presented based on the available variables and their relationships in the model, leading to the maximization of an objective function (profit function). Section 4 introduces the Logarithmic Penalty Function and discusses the reformulation of the problem from constrained to unconstrained optimization. The results and general discussion are presented in Section 5, followed by the conclusion in Section 6.

Alkylation Process Optimization

Alkylation refers to the transfer of an alkyl group from one molecule to another. Various entities such as alkyl carbocations, carbanions, free radicals, or carbenes can be utilized for this purpose. The alkylation process is a significant component of managing operations in the petroleum industry. A mathematical model, along with a profit function to be maximized, is employed to determine the optimal operating conditions for the process.

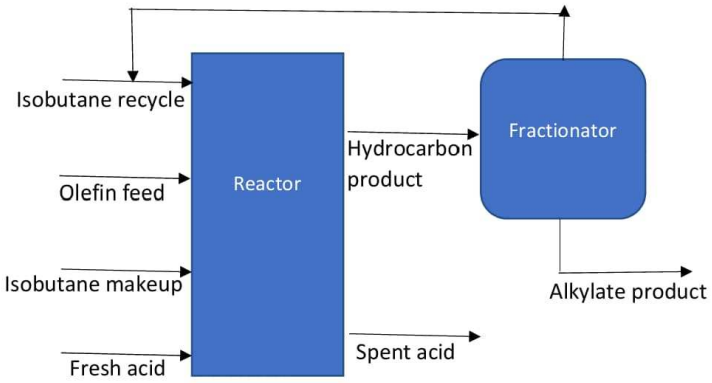

Figure 1: Alkylation Process Diagram

Figure 1 depicts a simplified flow diagram of an alkylation process. The reactor tank receives a mixture of olefin feed and isobutane, along with fresh acid catalyst, while removing used acid from the lower portion of the tank. The hydrocarbon product obtained from the upper part of the reactor tank is directed to a fractionator. Within the fractionator, isobutane is separated from the top and returned to the reactor for recycling, while the alkylate product is extracted from the bottom of the fractionator.

Alkylation Process Formulation

Table 1 simplified the assumptions to be considered for the chemical compounds and their amount in the entire process.

Table 1. Chemical Compound and Their Amount

	Chemical compound	Amount (%)
1	Olefin feed	100% butylenes
2	Isobutane makeup and it recycle	100% isobutene
3	Fresh acid strength	98% by weight

The process variables and their relationships as discussed in Rangaiah [10] are categorized into two groups;

1. Material balances
2. Correlations (linear and nonlinear regressions)

For the material balances, the variables relationships can be described with equality constraints with some specific range in the mathematical programming model, while for the correlations (i.e. linear and nonlinear regressions), the relationships can be represented by inequality constraints.

Further, the variables are subdivided into two kinds: dependent variables and independent variables.

The following are the independent variables:

- Daily olefin feed rate in barrels
- Recycle of isobutane in barrels per day
- Addition of fresh acid at a pace of thousands of pounds each day
- Outside air relative humidity (not in the model)
- The process's cooling water temperature (not in the model)

The dependent variables are categorized into three groups:

a. Variables that are economically significant

b. Indicators of performance and

c. Auxiliary variables

The dependent variables in class (a) include:

- Production of alkylate in barrels per day
- Isobutane makeup per day in barrels
- Motor octane number

The other classes of dependent variables (i.e. b. and c.) are:

- Acid strength expressed as a percentage of total weight
- External isobutane-to-olefin ratio
- Factor of acid dilution and
- F-4 performance rating.

In the mathematical model, there are ten variables, and the variables should be represented by x_i , where $i = 1, \ldots\ldots 10$. Their relationships will be used in determining available constraints to be considered in the model. All the values of x_i are bounded from above and below as summarized in table 2, for instance, because of economic situations, some limitations may be imposed on the affected variable, like in the case of x_1, only 2000 barrels of olefin feed per day may be used in the process. These bounds (upper and lower bound) will be considered as constraints in addition to the other constraints derived from variables relationships, the starting values reviewed by Bracken & Mccormick [11] are included in Table 2.

To define the objective (profit) function, we declare the cost parameters that will be used in the model's profit function. Table 3 outlines the costs parameters and their interpretations.

Table 2: Lower Bound, Upper Bound and Starting Values for The Considered Variables

Variable notation	Variable	Min.	Starting value	Max.
x_1	Olefin feed (barrels/day)	0	1745	2000
x_2	Isobutanes recycle(barrels/day)	0	12000	16000
x_3	Acid addition rate(X1000pounds/day)	0	110	120
x_4	Alkylate yield (barrels/day)	0	3048	5000
x_5	Isobutane makeup (barrels/day)	0	1974	2000
x_6	Acid strength (weight in %)	85	89.2	93
x_7	Motor octane number	90	92.8	95
x_8	External isobutane-to-olefin ratio	3	8	12
x_9	Acid dilution factor	1.2	3.6	4
x_{10}	F-4 performance number	145	145	162

Table 3: Cost Parameters and Their Descriptions

Parameter	Description
c_1	Alkylate product value ($ per octane-barrel)
c_2	Olefin feed cost ($ per barrel)
c_3	Isobutanes recycle cost ($ per barrel)
c_4	Acid addition cost ($ per thousand pounds)
c_5	Isobutane makeup cost ($ per barrel)

The profit function is expressed as follows:

$$f(x) = c_1x_4x_7 - c_2x_1 - c_3x_2 - c_4x_3 - c_5x_5$$

Regression analysis is a statistical tool used to formulate the relationship for x_4, x_7,x_9 and x_{10} in terms of the other variables. The relationships for x_5,x_6 and x_8 were established using the exact models. The alkylate yield represented by x_4, was a function of the external isobutane-to-olefin ratio, x_8, and the olefin feed, x_1.The relationship is governed by a nonlinear regression that operates at reactor temperatures of 80^0F to 90^0F and acid strength of 85 to 93 percent by weight. The equation for regression is

$$x_4 = x_1(1.12 + 0.13167x_8 - 0.0067x_8^2) \tag{1}$$

Volumetric reactor balance was used to determine the isobutane makeup, x_5. The sum of the olefin feed, x_1, and isobutane makeup, x_5, with less shrinkage are equal to alkylate yield. The volumetric shrinkage rate is 0.22 volume percent of alkylate production, which means that

$$\begin{aligned} x_4 &= x_1 + x_5 - 0.22x_4 \quad \text{or} \\ x_5 &= 1.22x_4 - x_1 \end{aligned} \tag{2}$$

The rate of acid addition, x_3, was calculated as a function of the alkylate yield, x_4, the acid dilution factor, x_9, and the acid strength weight percent,x_6, could be used to derive the strength of acid weight percent, x_6 (it is assumed that the acid addition to have a strength of 98%).

$$1000x_3 = \frac{x_3x_9x_6}{98 - x_6} \quad \text{or simply}$$

$$x_6 = \frac{98000x_3}{x_4x_9 + 1000x_3} \tag{3}$$

The external isobutane-to-olefin ratio, x_8, and the acid strength by weight percent, x_6, determine the motor octane number, x_7. The connection, x_4, holds for the same reactor temperatures and acid strengths as for alkylate yield.

$$x_7 = 86.35 + 1.098x_8 - 0.038x_8^2 + 0.325(x_6 - 89) \tag{4}$$

Equation (4) was determined by nonlinear regression.

The total of isobutane recycles x_2 and isobutane makeup $x_5$divided by olefin feed x_1 equals the external isobutane-to-olefin ratio x_8.

$$x_8 = \frac{x_2 + x_5}{x_1} \tag{5}$$

As shown in Equation (6) below, the acid dilution factor, x_9, can be expressed as a linear function of the F-4 performance number, x_{10}, and the motor octane number, x_9.

$$x_9 = 35.82 - 0.222x_{10} \tag{6}$$

As a function of the motor octane number, x_7, the linear regression equation for the last dependent variable, F-4 performance number, x_{10}, can be stated as follows;

$$x_{10} = -133 + x_7 \tag{7}$$

Note that Equations (2), (3) and (5) are equality constraints.

Table 4: Deviation Parameters

Deviation Parameter	Value
d_{4l}	0.99
d_{4u}	100/99
d_{7l}	0.99
d_{7u}	100/99
d_{9l}	0.9
d_{9u}	10/9
d_{10l}	0.99
d_{10u}	100/99

The dependent variables are given in terms of the independent factors and other dependent variables in all of the relationships above. For the process to be balanced, the relationships must also be stable. Furthermore, as shown in Table 2, lower and upper bounds must be set on the variables. The deviations d_l (lower) and d_u (upper) from expected values of the variables are listed in Table 4.

Hence, there are eight inequality constraints in addition to Equations (2), (3) and (5) equality constraints and the lower and upper bounds on all variables can be regarded as inequality constraints. Therefore, the details are as follows;

$$\left[x_1\left(1.12 + 0.13167x_8 - 0.0067x_8^2\right)\right] - d_{4l}x_4 \geq 0 \tag{8}$$

$$-\left[x_1\left(1.12 + 0.13167x_8 - 0.0067x_8^2\right)\right] + d_{4u}x_4 \geq 0 \tag{9}$$

$$\left[86.35 + 1.098x_8 - 0.038x_8^2 + 0.325\left(x_6 - 89\right)\right] - d_{7l}x_7 \geq 0 \tag{10}$$

$$-\left[86.35 + 1.098x_8 - 0.038x_8^2 + 0.325\left(x_6 - 89\right)\right] + d_{7u}x_7 \geq 0 \tag{11}$$

$$\left[35.82 - 0.222x_{10}\right] - d_{9l}x_9 \geq 0 \tag{12}$$

$$-\left[35.82 - 0.222x_{10}\right] + d_{9u}x_9 \geq 0 \tag{13}$$

$$\left[-133 + 3x_7\right] - d_{10l}x_{10} \geq 0 \tag{14}$$

$$-\left[-133 + 3x_7\right] + d_{10u}x_{10} \geq 0 \tag{15}$$

Lower and upper bounds on the variables x_i can be defined as follows;

$$x_i^{(l)} = i\,\text{th variable lower bound}$$
$$x_i^{(u)} = i\,\text{th variable upper bound}$$

To reformulate the mathematical programming model into an unconstrained problem, from each lower and upper bound for the variable, we generate another two inequality constraints below;

$$x_i^{(l)} \leq x_i \leq x_i^{(u)}, \text{ this implies } -x_i + x_i^{(l)} \leq 0, \text{ and } x_i - x_i^{(u)} \leq 0.$$

2 Logarithmic Penalty Function Approach to Alkylation Process Optimization

Since the inceptions of the penalty function approach a few decades ago, penalty function approaches are of tremendous interest to practitioners and theorists because they provide a basic and straightforward technique for dealing with constrained optimization issues that may be easily performed even without usage of advanced computer programming codes.

In a quest to overcome its naturally sluggish convergence, it is useful to employ almost all components of optimization theory, such as required conditions, Lagrange multipliers, and many other forms of optimization, Hassan and Baharum [12] proposed a new logarithmic penalty function (LPF), which was tested on some simple theoretical problems from the Hock-Schittkowsky [13] collection of test problems, it was then harmonized with modified Courant-Beltrami [14], [15] and extended to a more general form [16], [18] that is capable of dealing with both equality and inequality constraints.

Considering the great importance of petroleum industries to global economy, the alkylation reaction optimization is chosen to test the LPF applicability to practical (chemical process) problems and compare its optimal values to those of earlier techniques as in [11], [17]. The following form is the new logarithmic penalty function.

$$p_1(x) = \sum_{j=1}^{m} \ln\left[\left(h_j(x)\right)^2 + 1^j\right] \tag{16}$$

The new LPF in Equation (16) is specifically designed to handle equality constraints, a hybridization of Equation (16) and a modified Courant-Beltrami penalty function (17) below;

$$p_2(x) = \sum_{q=1}^{s} \ln\left[\left(g_q^+(x)\right)^2 + 1^q\right] \tag{17}$$

As a result, the general form of the logarithmic penalty function proposed by Hassan and Baharum [16] is as follows: -

$$p(x) = \sum_{q=1}^{s} \ln\left[\left(g_q^+(x)\right)^2 + 1^q\right] + \sum_{j=1}^{m} \ln\left[\left(h_j(x)\right)^2 + 1^j\right] \tag{18}$$

Note that $g_q^+(x) = \max\{0, g_q(x)\}$.

When Equation (18) is added to the objective function, it imposes a significant cost for violating the constraints for any infeasible point x, whereas Equation (18) is zero for every feasible point.

If the chemical process in the previous section is considered, ten variables (dependent and independent) involved, there were three equality and eight inequality constraints; others were obtained from the variables' upper and lower boundaries. Considering the structure of the modified Courant-Beltrami penalty function, the problem is required to be converted into the minimization problem, so, there is a need to reverse the inequalities of Equations (8) - (15) into $\leq$, these will enable the transformation of the process into a single unconstrained optimization problem via Equation (18).

$$\text{Min } P(x,c) = f(x) + c\sum_{q=1}^{s} \ln\left[\left(g_q^+(x)\right)^2 + 1^j\right] + c\sum_{j=1}^{m} \ln\left[\left(h_j(x)\right)^2 + 1^j\right] \;,\quad q \in q = \{1,2,\ldots..s\}\,,\; j \in J = \{1,2,\ldots\ldots,m\} \tag{19}$$

where c is the penalty parameter, it is positive number (i.e. $c > 0$).

Substituting the profit function and the constraints into Equation (19), the Equation (20) is obtained.

$$\begin{aligned}
\text{Min } f(x) = {} & 0.063\; x_4x_7 - 5.04x_1 - 0.035x_2 - 10.00x_3 - 3.36x_5 \\
& + \ln((\max\{0, \left[x_1\left(-1.12 - 0.13167x_8 + 0.0067x_8^2\right)\right] + 0.99x_4\})^2 + 1\,) \\
& + \ln((\max\{0, \left[x_1\left(+1.12 + 0.13167x_8 - 0.0067x_8^2\right)\right] - 0.99x_4\})^2 + 1\,) \\
& + \ln((\max\{0, \left[-86.35 - 1.098x_8 + 0.038x_8^2 - 0.325\,(x_6 - 89)\right] + 0.99x_7\})^2 + 1\,) \\
& + \ln((\max\{0, \left[86.35 + 1.098x_8 - 0.038x_8^2 + 0.325\,(x_6 - 89)\right] - 0.99x_7\})^2 + 1\,) \\
& + \ln((\max\{0, [-35.82 + 0.222x_{10}] + 0.9x_9\})^2 + 1\,) \\
& + \ln((\max\{0, [35.82 - 0.222x_{10}] - 0.9x_9\})^2 + 1\,) \\
& + \ln((\max\{0, [133 - 3x_7] + 0.99x_{10}\})^2 + 1\,) \\
& + \ln(\left(\max\{0, [-133 + 3x_7] - 0.99x_{10}\}\right)^2 + 1\,) \\
& + \ln(\left(\max\{0, x_1 - 2000\}\right)^2 + 1\,) \\
& + +\ln((\max\{0, x_2 - 16000\})^2 + 1\,) \\
& + \ln(\left(\max\{0, x_3 - 120\}\right)^2 + 1\,) \\
& + +\ln(\left(\max\{0, x_4 - 5000\}\right)^2 + 1\,) \\
& + \ln(\left(\max\{0, x_5 - 2000\}\right)^2 + 1\,) + \ln((\max\{0, x_6 - 93\})^2 + 1\,) + \ln((\max\{0, -x_6 + 85\})^2 + 1\,) \\
& + \ln((\max\{0, x_7 - 95\})^2 + 1\,) \\
& + \ln((\max\{0, -x_7 + 90\})^2 + 1\,) \\
& + \ln(\left(\max\{0, x_8 - 12\}\right)^2 + 1\,) \\
& + \ln((\max\{0, -x_8 + 3\})^2 + 1\,) \\
& + \ln(\left(\max\{0, x_9 - 4\}\right)^2 + 1\,) + +\ln(\left(\max\{0, -x_9 + 1.2\}\right)^2 + 1) + \ln((\max\{0, x_{10} - 162\})^2 + 1\,) \\
& + \ln((\max\{0, -x_{10} + 145\})^2 + 1\,)
\end{aligned} \tag{20}$$

Many unconstrained optimization algorithms could be used to deal with the transformed Problem (20). The quasi-newton algorithm is among the most sophisticated method to handle such a problem. The Problem (20) was solved using the *fminunc* routine function. The optimal values were summarized in Table 6, and it was compared with the results obtained using nonlinear programming system optimization laboratory (NPSOL) code and differential evolution [17], [13], and alkylation process optimization [11].

Table 5: Profit and Cost Parameters' Values

Profit and Cost Parameter	Value
c_1	\$0.063 per octane-barrel
c_2	\$5.04 per barrel
c_3	\$0.035 per barrel
c_4	\$10.00 per thousand pounds
c_5	\$3.36 per barrel

3 Result and Discussion

Generally, in all the penalty function approaches, the parameter c plays a dominant role in prescribing a massive penalty if any of the constraints is violated. Ideally, the larger the value of the parameter c, the closer the optimal solution is expected, increasing the penalty parameter will forces the minimizer toward the feasible region. The suitable threshold for the considered chemical process optimization is $c = 433$, so, for any value $c \geq 433$, the optimal solution can be obtained. Based on the comparison with conventional approach in (HS) and (OS) from [13] and [11] respectively, and Non-Linear Programming System Optimization Laboratory (NPSOL). However, the objective value obtained via minimization problem of LPF is -2415.42 which were later, converted back to maximization problem as in Table 6.

Table 6: Comparison of Optimization Methods: HS, OS, NPSOL and LPF

Variable	Optimal value (HS)	Optimal value (OS)	Optimal value (NPSOL)	Optimal value(LPF)
x_1	1,698.096	1,698	1,698.1	1,737
x_2	15,818.73	15,818	15,819	12,000
x_3	54.10228	54.1	54.107	0
x_4	3,031.226	3,031	3,131.2	3,052
x_5	2,000	2,000	2,000	1,987
x_6	90.11537	90.1	90.115	93
x_7	95.0	95.0	95.0	95
x_8	10.49336	10.5	10.49	8
x_9	1.561636	1.6	1.56	2
x_{10}	153.53535	154	153.54	153

The solutions yielded by solving the problem using the four methods are given in Table 6. The values of HS, OS, and NPSOL are obtained from [13], [11] and [17], respectively. Observe that, the profit function (Objective value) via LPF method happens to be better than the conventional approach used in (HS) and (OS) from [13] and [11] respectively. However, evolutionary computational strategy using NPSOL is a little bit better than LPF in terms of their objective values.

Penalty function approaches are commonly used in optimization problems to enforce constraints. The parameter c in these approaches plays a crucial role in determining the magnitude of the penalty imposed when any of the constraints is violated. A larger value of c indicates a more severe penalty, which pushes the minimizer towards the feasible region and increases the likelihood of obtaining an optimal solution. In other words, as the penalty parameter increases, the optimal solution is expected to be closer to the true optimal solution.

In the context of the considered chemical process optimization, the suitable threshold value was identified for the parameter c as 433. It was concluded that for any value of $c \geq 433$, the optimal solution can be obtained. This threshold value ensures that the constraints are strongly enforced, leading to a solution that is closer to the optimal one.

To evaluate the performance of their proposed method, it was compared with conventional approaches referred to as (HS) and (OS) from references [13] and [11], respectively. Additionally, their methods were compared with the Non-Linear Programming System Optimization Laboratory (NPSOL), which is known for its effectiveness in solving optimization problems. By solving the minimization problem using the new LPF method, the objective value of -2415.42 was obtained. It should be noted that this objective value was later converted back to a maximization problem as indicated in Table 6.

Table 6 presents the solutions obtained using the four different methods: HS, OS, NPSOL, and LPF. The values for HS and OS were obtained from references [13] and [11], while the value for NPSOL was obtained from [17]. Notably, the profit function, represented by the objective value, obtained through the LPF method outperformed the conventional approaches (HS and OS) from references [13] and [11], respectively. This indicates that the LPF method yielded a higher objective value, implying a more favorable outcome in terms of maximizing the desired outcome (e.g. profit).

However, it is worth mentioning that the evolutionary computational strategy implemented in NPSOL demonstrated a slight advantage over the LPF method in terms of achieving better objective values. Although LPF outperformed the conventional approaches, NPSOL showed a slightly higher objective value, suggesting a potentially more optimal solution.

In summary, the parameter c plays a critical role in penalty function approaches, and a suitable threshold value of $c = 433$ was determined for the considered chemical process optimization problem. The LPF method showed superior performance compared to the conventional approaches (HS and OS) in terms of the objective value. However, the evolutionary computational strategy employed in NPSOL exhibited a slight advantage over LPF in terms of achieving even better objective values.

Nonetheless, from the comparison as presented in Table 6, it indicates that, the increase of olefin feed (barrel/day) from 1698 to 1737 will cut down acid addition rate (X1000 pounds/day) to 0, which is its lower bound. On the other hand, isobutane makeup which was uniformly 2000 (barrel/day) from other methods will as well be trimmed to 1987 (barrel/day). Same thing goes to isobutane recycle. Moreover, there was a little increase in alkylate yield and acid strength. These shows how good is the new LPF is in chemical process optimization and it will be more economical to decision makers in petroleum industries.

Conclusion

The new LPF approach was explicitly designed to handle the problems with irregular features. However, the chemical process is chosen to identify the best set of operational conditions. The results obtained turns out to be more economical to be considered in taking the managerial decision concerning the entire alkylation process. The comparison with some of the existing methods has been presented in Table 6.

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