

## Optimization of Al-Doura Catalytic Naphtha Reforming Process Using Genetic Algorithm

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### ABSTRACT

Optimization of Al-Doura catalytic naphtha reforming process was done using genetic algorithm. The objective of optimization is maximization yield of the aromatics in order to increase the octane number of reformat.

One-dimensional steady-state mathematical model was made to study the effect of feedstock composition, feed temperature, total pressure and hydrogen to hydrocarbon feed ratio on the reformat compositions. Detailed kinetic model was developed to describe the reaction kinetic, the model involving 29 components, 1 to 11 carbon atoms for n-paraffins, 5 to 10 carbon atoms for iso-paraffins and 6 to 11 carbon atom for naphthenes and aromatics with 83 reactions. Using Genetic Algorithm, 186 parameters of the proposed kinetic model were predicted depending on plant results collected over two months from Al-Doura reforming process which located in the south of Baghdad. The validity of the kinetic model was approved by comparing the results of developed kinetic model with the actual process results.

Genetic algorithm was used again to optimize the commercial reforming process depending on reformat compositions. Optimization was carried out in temperature range between 450 to 520°C; total pressure range 5 to 35 bar; hydrogen to hydrocarbon ratio 3 to 8 and by varying the percentage of catalyst for each one of four reactors. Optimization results shows that, it's possible to increase the aromatics composition in reformat from 63.42 % in actual unit to 70.89 % by changing the design variables and operating conditions.

**Keywords:** Optimization, Genetic Algorithm, Naphtha Reforming, Reaction Kinetic, MATLAB.

### مفاضلة وحدة تجارية لتهديب النفط باستخدام الخوارزمية الجينية

#### الخلاصة

في هذه الدراسة تم استخدام الخوارزمية الجينية لإيجاد أفضل الظروف التشغيلية لعمل وحدة مصفى الدورة لتحسين النفط. الهدف الرئيسي من عملية التحسين هو تعظيم المواد العطرية الخفيفة ذات العدد الاوكتاني العالي. تم انجاز موديل رياضي لدراسة تأثير تركيب النفط الخام ودرجة حرارة الدخول للمفاعل وضغط الدخول للمفاعل الاول ونسبة الهيدروجين إلى النفط على تركيب المادة المهذبة. وقد تم تطوير نموذج مفصل لوصف حركية التفاعلات لتهديب النفط تحتوي على 29 مادة وهي البارافينات الاعتيادية ذات ذرات الكربون من 1 إلى 11 و البارافينات المتفرعة ذات ذرات الكربون 5 إلى 10 و النفثينات والعطريات ذات 6 إلى 11 ذرة كربون باستخدام حركية تفاعلات من 83 تفاعل. تم حساب 186 ثابت من ثوابت حركية التفاعل باستخدام الخوارزمية الجينية اعتمادا على

النتائج العملية التي تم جمعها على مدى شهرين من وحدة تهذيب النفط الموجودة في مصرفى الدورة بجنوب بغداد . تم اختبار فعالية الموديل الرياضي من خلال مقارنة النتائج المستحصلة من الموديل الرياضي مع نتائج عملية مأخوذة بنفس الظروف .  
تم استخدام الخوارزمية الجينية لمفاضلة عملية تهذيب النفط من خلال اختيار أحسن الظروف من درجات الحرارة من 450 الى 520 درجة مئوية، وضغط بين 10 و 35 بار ونسبة هيدروجين الى النفط بين 3 و 8 وكذلك تغيير نسبة العامل المساعد لكل مفاعل . نتائج الاختيار الافضل اثبتت انه يمكن زيادة كمية المواد العطرية في المادة المهذبة من 63,42% إلى 70,89% من خلال تغيير المتغيرات التصميمية والظروف التشغيلية .

## INTRODUCTION

Catalytic naphtha reforming is very important process for producing high octane gasoline as main products with hydrogen and liquefied petroleum gas as by-products. Generally, naphtha reforming process is carried out in three or four fixed bed reactors which operate adiabatically at temperatures between 450 and 520 °C, total pressures between 10 and 35 bar, and molar hydrogen-to-hydrocarbon ratios between 3 and 8. Usually, the feed to the first reactor is a hydrodesulfurized naphtha cut, composed of normal and branched paraffins, five and six-membered ring naphthenes, and single-ring aromatics.

Catalytic reforming unit's uses industrial catalysts consisted of Gama Alumina support as acid function treated with chlorine in order to increase its surface acidity. The metal function is usually provided by platinum, of very small particles dispersed on the surface of catalyst, and its properties are fine-tuned by the addition of another element such as rhenium, ten, germanium, and iridium<sup>(1)</sup>.

The major chemical reactions during the catalytic reforming are the following<sup>(2)</sup>:

1. Dehydrocyclization of paraffins into aromatics.
2. Isomerization of alkylcyclopentanes into cyclohexanes.
3. Dehydrogenation of cyclohexanes into aromatics.
4. Isomerization of linear paraffins into iso-paraffins.
5. Hydrocracking of naphthenes and paraffins.
6. Hydrodealkylation of aromatics.
7. Coke formation.

Some of these reactions are desired because it increases the octane number of gasoline. Cyclization and aromatization for paraffins are desired reactions because they increasing the number of branches and hence increase of octane number. The dehydrocyclization and dehydrogenation reactions produce hydrogen as by-product. On the other hand, hydrocracking and hydrodealkylation are mostly undesired reactions because they lower reformat and hydrogen yields also coke formation is undesired because its effect on catalyst deactivation<sup>(3)</sup>.

First successful kinetic model for catalytic reforming process is proposed by Smith<sup>(4)</sup>. Smith model divided the naphtha feed into naphthenic, paraffinic and aromatic lumps with average carbon number properties. He also introduced hydrogen, ethane, propane, and butane into the system in addition to these groups. Krane<sup>(5)</sup> developed his model, he assumed that the feed consist of 20 pseudo components and hydrocarbons from 6 to 10 carbon atoms. Moreover, reaction network was contained of 53 reactions. Kmak<sup>(6)</sup> used Langmuir kinetic model for the first time for catalytic reforming process. Taskar and Riggs<sup>(7)</sup> developed a more detailed model of a semiregenerative catalytic naphtha reformer, involving 35

pseudo components. Unmesh and James<sup>(8)</sup> developed a kinetic model included 35 pseudo components in the reaction network, and 36 reactions.

In series of studies, Ancheyta et al.<sup>(9, 10, 11)</sup> extended the work of Krane<sup>(5)</sup> by using a higher number of reactions, taking into account the benzene precursors of the feed, and the effect of pressure and temperature on the rate coefficients. In Ancheyta model, naphtha contained 1:11 paraffinic, 6:11 naphthenic and aromatic hydrocarbons. Also, the reaction of cyclohexane formation from cyclopentane and paraffins isomerization is considered in this model. Hu et al.<sup>(12, 13)</sup> studied of molecular modeling of catalytic reforming. They used molecular type homologous series matrices to represent the naphtha feed compositions. The reaction network involves 21 classes of molecules and 51 reactions. On the basis of the simulation model, they performed a process optimization for feed temperature and pressure under constraints such as benzene content, aromatic content and RON (research octane number) limitations. Mirko et al.<sup>(14)</sup> developed a semi-empirical kinetic model for catalytic reforming using 'lumping' strategy which is based on a paraffins, olefins, naphthalenes, and aromatics (PONA) analysis. They take into account different values of activation energies within specific reaction classes. The parameters of the model have been estimated by bench marking with industrial data.

It is very important to use an appropriate kinetic model capable of predicting the detailed reformate composition in order to use it, in combination with a catalytic reforming reactor model for simulation and optimization purposes, therefore this study had been made to, (1) Describe the reactions kinetic of Al-Doura reforming process located in Baghdad (2) Optimize the existent plant to produce a reformate with maximum amount of aromatics.

### **OPTIMIZATION OF CATALYTIC REFORMING**

Optimization is the third stage in the process of designing a system. The first stage is modeling or simulating the system. The second step is to decide what is to be optimized, that is, to construct the so called objective function. This function may be of single variable or of multi-variables, may be linear or non-linear and may be constrained by certain conditions or unconstrained. Optimization implies either maximizing or minimizing the objective function<sup>(15)</sup>.

Liang et al.<sup>(16)</sup> proved their model assumptions, in which the temperature distribution is assumed only in axial direction in the reactors and all reactions within reforming process are assumed in homogeneous phase.

Hu et al.<sup>(17)</sup> developed a rigorous process model for simulation and optimization of commercial naphtha catalytic reformers. The reaction model is described by Hongen-Watson-type rate equations with catalyst coking kinetics. They used Lagrange-Marquardt composite optimization algorithm to solve the nonlinear optimization.

Weifeng et al.<sup>(18)</sup> developed a rigorous process model for analysis and optimization of commercial catalytic reforming process using simple kinetic model involving 17 lumps and 17 reactions. They revealed that operating conditions of reforming process remarkably affect the aromatics yield and catalyst coking.

Jin Li et al.<sup>(19)</sup> developed a rigorous mathematical model of a Semi-regenerative catalytic naphtha reformer employing a detailed kinetic scheme involving 28 pseudo-components connected by a network of 68 reactions. The kinetic model was parameterized by benchmarking against industrial plant data.

Weifeng et al. <sup>(20)</sup> studied simulation and optimization of industrial continuous catalytic reforming using 18-lump kinetic model. The simulation was done using Aspen plus platform. Weifeng et al. <sup>(21)</sup> proposed neighborhood and genetic algorithm for multi-objective optimization of industrial naphtha continuous catalytic reforming process that aims to obtain aromatic products. Their model based on a 20-lumped kinetics reaction network. Their primary objectives was maximization of yield of the light aromatics and minimization of the yield of heavy aromatics and their decision variables were, four reactor inlet temperatures, reaction pressure, and hydrogen-to-oil molar ratio.

Reza et al. <sup>(22)</sup> simulated semi-regenerative catalytic reforming process of Tehran refinery by Hysys-Refinery Simulator. Simulation was used for optimization and prediction of operating parameters. They studied the effect of catalyst distribution on the octane number of produced gasoline while all other operating parameters were held constant.

Arani et al. <sup>(23)</sup> studied dynamic modeling of catalytic naphtha reforming process using MATLAB software in SIMULINK mode. They used Hougen-Watson Langmuir-Hinshelwood type reaction rate expressions to represent rate of each reaction.

Ali et al. <sup>(24)</sup> make a parametric study of catalytic reforming process in a pilot plant by varying the pressure, H<sub>2</sub>/HC ratio, and space velocity. Their results show that lower aromatics and higher hydrogen yields can be accomplished by increasing the space velocity in existing reformers, which will also result in better C<sub>5</sub> + yield.

The parameters of reaction kinetic are depends absolutely on naphtha composition, catalyst type, and catalyst activity and process operating condition. All of published kinetic models couldn't capable to predict Iraqi reformate composition of alkylcyclopentanes, n-paraffins and i-paraffins. This study came to describe precisely the kinetic model of Iraqi heavy naphtha reforming process by fine tuning of the model parameters.

## **GENETIC ALGORITHM**

Genetic Algorithm is powerful and widely applicable stochastic search and optimization methods based on the concepts of natural selection and natural evaluation. The genetic algorithm was first introduced in 1975 by Holland <sup>(25)</sup>. Genetic Algorithm work on a population of individuals represents candidate solutions to the optimization problem. These individual are consists of a strings (called chromosomes) of genes. The genes are a practical allele (gene could be a bit, an integer number, a real value or an alphabet character,...,etc depending on the nature of the problem). Genetic Algorithm applying the principles of survival of the fittest, selection, reproduction, crossover, and mutation on these individuals to get, hopefully, new better individuals (new solutions). Genetic Algorithm generates new population of chromosomes by selecting the better fit solutions from existing population and applying genetic operators to produce new offspring of the solutions. The process is repeated successively to generate new population iteratively. Figure (1) shows the flowchart of the main steps of Genetic Algorithm.

## **MATHEMATICAL MODEL**

### **Model assumptions**

The following assumptions were considered in mathematical modeling:

1. The system at steady state.

2. The variation in the radial direction is negligible. Therefore, the compositions, temperature and pressure are only functions of axial direction <sup>(16)</sup>.
3. All reactions are in homogenous phase <sup>(16)</sup>.
4. All reactions are pseudo first order with respect to hydrocarbon <sup>(9, 10, 11)</sup>.
5. Plug flow in reactor.

**Model equations**

The equations of mathematical model results from application of material and energy balance principles in a differential volume <sup>(26)</sup>.

$$-\frac{dC_i}{dZ} = \sum_{i=1}^m \frac{Mwt}{Z \times WHSV} (r_i) \quad \dots (1)$$

$$\frac{dT}{dZ} = \frac{S \sum_{i=1}^m (r_i)(-\Delta H_{Ri})}{\sum_{i=1}^m F_i C_{p_i}} \quad \dots (2)$$

Where: m represent the number of component in the mixtures.

Ergun equation was used for computing total differential pressure drop in axial flow reactor;

$$-\frac{dP_t}{dZ} = 1.7 \times 10^{-5} \frac{1-e}{e^3 \rho d_p} G^2 + 1.5 \times 10^{-3} \frac{(1-e)^2 m}{e^3 \rho d_p^2} G \quad \dots (3)$$

The heat capacity was evaluated using third order polynomial;

$$C_{p_i} = A_i + B_i T + C_i T^2 + D_i T^3 \quad \dots(4)$$

The coefficients of heat capacity polynomial were taken from Reid et al. <sup>(27)</sup>.

Equation (5) was used to change the way of result displaying from reactor length to catalyst weight.

$$dw = S \rho_{cat} (1 - e) dZ \quad \dots(5)$$

For each individual reactor within the process, numerical integration method was used to integrate the component mass balance, energy balance and pressure drop differential equations (1, 2 and 3) to obtain concentrations, temperature and pressure drop profiles. All computations and evaluations within this study were coding using MATLAB 7 software. Fourth order Runge-Kutta integration command named ode15s was used to integrate twenty-nine stiff ordinary differential equations for mass balance and two equations for heat and pressure drop equations.

**Proposed Kinetic Model**

According to Ancheyta et al. <sup>(9, 10,11)</sup> model, the naphtha feed to reforming process contain 1 to 11 carbon atoms paraffin's (P<sub>1</sub>-P<sub>11</sub>) and 6 to 11 carbon atoms for naphthenes (N<sub>6</sub>-N<sub>11</sub>) and aromatics (A<sub>6</sub>-A<sub>11</sub>). Their kinetic model employs a lumped mathematical representation of the seventy-one chemical reactions for all 24 lumps within the reaction network as can be shown in table (1). The effect of temperature

and pressure on the 71 original kinetic constants was expressed using equation (6) (28).

$$k_i = k_i^o \left[ \frac{E_{Aj}}{R} \left( \frac{1}{T_o} - \frac{1}{T} \right) \right] \left( \frac{p_i}{p_o} \right)^{ak} \quad \dots(6)$$

The values of pressure effect factors (*ak*) are given in table (2).

In this study paraffin isomerization (n-P<sub>i</sub> ↔ iso-P<sub>i</sub>) reactions for 5 to 10 carbon atom was taken into account in the kinetic model. The total number of reactions is 71 for the original kinetic model plus 12 reactions (6 forward and 6 equilibrium) for paraffin isomerization reactions in our extended model. The reactions kinetic were expressed by 83 first order reaction steps. All reaction steps within the reaction network are combined into twenty-nine rate reaction equations (*r<sub>i</sub>*), one for each component. Each reaction rate equation is a function of the kinetic constant (*k<sub>i</sub>*) and the component concentration (*C<sub>i</sub>*). Each one of these 83 reaction rate constants (*k<sub>i</sub>*) has two unknown variables which are the activation energy and pre-exponential factor. The 186 (2×83) kinetic parameter of the proposed kinetic model were estimated by using genetic optimization method.

**Simulation condition**

The derived model was tested comparing it results with the results of Al-doura catalytic reforming unit composed of four reactors in series with inter-stage heater. Figure (2) shows the schematic diagram of Al-Doura naphtha reforming process. The same operating conditions of the actual reforming unit were taken into account in simulation. The operating condition of this unit were as follows: 470 °C inlet temperature, 27.5 bar reactor pressure, hydrogen to oil ratio of 7 mol/mol, and feedstock flow rate of 30 m<sup>3</sup>/hr. The length, diameter, and catalyst-bed weight for each one of these four reactors are given in Table (3). To overcome the effect of deactivation of the catalyst, several sets of data results for actual plant was taken into consideration. The samples taken from the feed and four reactors products were determined by GC analysis to calculate their compositions.

**Process Optimization**

All optimization steps within this study were done using Genetic Algorithm. Genetic Algorithm was used to predict the parameters of kinetic model by minimizing the objective function *J* in equation 7, which is the sum of squares of errors between the predicted and measured values for all of the state variables.

$$J = \frac{1}{n_{exp}} \sum_{i=1}^{nr} \left( \sum_{j=1}^{nc} (y_{i,j}^{pred} - y_{i,j}^{exp})^2 + \left( \frac{T_i^{pred} - T_i^{exp}}{T_i^{exp}} \right)^2 \right) \quad \dots (7)$$

The goal of optimization of naphtha reforming process is to maximize the hydrogen and aromatic production which leads to the maximum consumption of the paraffins and naphthenes. In order to reach this end, the inlet temperature of the gas at the entrance of each reactor (T1, T2, T3, T4), the total pressure of the process (pr), the hydrogen to naphtha feed ratio (H2 /HC), as well as the catalyst distribution in each reactor (w1%, w1%, w3%, w4%) have been optimized using the differential evolution (DE) method. The objective function of maximization the aromatics composition in reformat (A%) is formulated mathematically as follows:

Maximize A% (T1, T2, T3, T4, w1%, w1%, w3%, w4%, pr, H2 / HC)

## RESULTS AND DISCUSSION

### Kinetic model

Using the differential evolution-optimization algorithm to optimize the system through a sequence of optimization-evaluation, the objective function (Eq. (7)) was minimized and the global optimum set of kinetic parameters was found out. Values of the Frequency factors (A1 to A83), Activation Energies (E1 to E83) were found by minimization of the sum of the squares of the deviations between the plant and the calculated results of the key variables (the compositions and temperature of effluent from each one of the four reactors). Figure (3) shows a plot of the best and mean fitness (J) with respect to generation number. Table (4) contains the parameters used in Genetic Algorithm. The kinetic parameters of obtained reaction rate are presented in the Tables (5 and 6).

Genetic Algorithm has one disadvantage which is a huge computation time in the case of complex systems. In the present study a PC with 4.12 GHz and 4GB RAM runs take about 133 hr to reach produced results.

### Validity of Predictive Kinetic Model

To approve the validity of the predicted kinetic model, the simulation model results using the predicted kinetic model were compared with actual results collected from al-doura reforming process. Figure (4) shows the comparison between actual and simulated reformate compositions for four reactors. It can be observed that the calculated compositions agree very well with actual process with average deviation less than 2%.

Figures (5, 6, 7, 8, and 9) represent a plot of comparison between the actual and predictive results for reformate, n-paraffins, i-paraffins, naphthenes and aromatics respectively. Predicted and actual reformate composition profiles of total (n- and iso-) paraffins, naphthenes and aromatics are presented in Figure (4).

From Figures (6) and (7) it can be seen, that the percentage of light paraffins (n-, and iso- P<sub>5</sub>, and P<sub>6</sub>) increased, because they are produced by hydrocracking or hydrogenolysis and the n-P<sub>7</sub> and iso-P<sub>7</sub> slightly decreases but heavier paraffins P<sub>8</sub>-P<sub>11</sub> (n-, and iso-) exhibited high levels of conversion especially in the 3<sup>rd</sup> and 4<sup>th</sup> reactor.

Figure (8) show that the naphthenes (N<sub>5</sub>-N<sub>11</sub>) as well as MCP essentially react to completion. The concentrations of (N<sub>5</sub>-N<sub>11</sub>) decreases as they undergo conversion. A high rate of conversion of naphthenes was found in the first and second reactors (N<sub>6</sub> and N<sub>7</sub>) are almost totally converted. After third reactor, naphthenes compositions approach very low values. The dehydrogenation of naphthenes and production of aromatics and hydrogen was the fastest among reforming reactions, therefore it nearly took place in 1<sup>st</sup> reactor and the variation of aromatics and naphthenes concentration were very significant. The increase in concentration of aromatics in the 2<sup>nd</sup> and 3<sup>rd</sup> reactors was basically due to the disappearance of paraffins. Hydrocracking of naphthenes and paraffins were slow and exothermic reactions, so these reactions take place often in 3<sup>rd</sup> reactor.

From Figure (9) it can be observed that as the feedstock pass through the unit the content of aromatic hydrocarbons are increased, also the increasing of light aromatics contents ( A<sub>7</sub>, A<sub>8</sub>, A<sub>9</sub> and A<sub>10</sub>), are faster than in heavier aromatics (A<sub>6</sub>, and A<sub>11</sub>).

Table (7) shows the difference between the reformate composition obtained by simulation and Al-Doura reforming unit. It can be observed from this table that there are very good agreement between the simulated and reported values.

Figures (10) show both the simulated and actual pressure drop with respect to accumulative catalyst weight within the Al-Doura reforming process. It can be observed from this figure, that the total pressure drop within the four reactors is about 18.1 %. Also there is a proportional relation between the drop in pressure and the reactor length or accumulated catalyst weight. The actual final pressure is lower than the predictive pressure because of the effect of catalyst plugging.

Figure (11) shows the predicted and actual temperature distribution along the reforming process. The major reforming reactions are highly endothermic producing a decrease in the temperature of the reaction stream and catalyst along the reactor. For this reason, commercial catalytic reformers are designed with multiple reactors and with heaters between the reactors to maintain reaction temperature at operable levels. As the feedstock passes through the sequence of heating and reacting, the reactions become less endothermic and temperature difference across the reactors decrease. In the first reactor, the major reactions are endothermic and very fast, such as dehydrogenation of paraffins and naphthenes to aromatics as can be seen in Figure (11), while in second reactor isomerization take place, the remaining naphthenes are dehydroisomerized and temperature drop is observed. The temperature drop through the third and fourth reactors were low compared to first two reactors, which is due to the exothermic of hydrocracking and dehydrocyclization reaction of paraffins.

Table (7) shows the comparison between the actual and simulated temperature drop within the four reactors. It can be observed from this table, the present model prediction match very well with the information reported in the commercial reforming unit <sup>(10)</sup>. The maximum absolute difference between predicted and actual reactor temperatures is (7.66 °C) in fourth reactor while the minimum absolute difference between predicted and actual reactor temperatures is (3.56 °C) in first reactor. One can observe from actual results of the last reactor, the temperature is increased about 2°C due hydrocracking reactions were taking place.

For a good model, the kinetic parameters (i.e. frequency factors and activation energies) for a specific reactor must be determined accurately. The experimental validation revealed that the new predictive kinetic model has high prediction capabilities.

### **Optimization Results**

The performances of Al-Doura naphtha reforming process were investigated under the following operating condition: reaction temperature in the range 450-520 °C, pressure at 10 to 35 bars, hydrogen to hydrocarbon ratio from 3 to 8 and using different percentage catalyst weight from 0 to 100 % for each one of process reactors. Figure (12) shows a plot of the best and mean objective function with respect to generation number.

Table (9) contain a comparison between actual plant reformate composition comparing with six randomly selected generations from genetic algorithms. Absolutely, the last generation (number 500) represents the best one. By comparing the reformate composition resulted from actual design with the resulted from the best design (generation 500), it's clear that the aromatic content in reformate could be increase from 63.42 % in actual unit to 70.89 % by changing the design variables and operating conditions. From table (9), it's clear that the distribution of the catalyst in the reactors is the most important parameter in increasing the performance of the Al-Doura reforming plant. According to the results presented in table (9) it was observed that increasing the pressure does not change the reformate

composition seriously. Increasing the pressure has a small effect on decreasing of aromatics and hydrogen content in reformate, because the dehydrogenation of naphthenes and dehydrocyclization of paraffins and reducing hydrocracking favored lower.

Also, the H<sub>2</sub>/HC ratio has little effect on the aromatics yield as shown in Table (9), while reducing H<sub>2</sub>/HC ratio is useful in reducing energy costs for corresponding and circulating hydrogen and favors dehydrogenation of naphthenes and dehydrocyclization of paraffins. Unfortunately reducing H<sub>2</sub>/HC ratio can also increase catalyst coking and decrease catalyst activity and increase hydrocracking reaction. Figure (13) represent the composition profile of reformate in four reactors depending on optimum design representing in generation 500.

## CONCLUSIONS

The following conclusions can be pointed out from this study:

- The predicted kinetic model agrees very well with experimental data of Al-Doura naphtha reforming unit.
- The proposed mathematical model is suitable to study the effect of the reactors feed temperature, total pressure and hydrogen to hydrocarbon feed ratio on the reformate compositions. The calculated reformate composition agrees very well with experimental plant data.
- Genetic Algorithm can be used effectively in for parameters estimation and processes optimization.
- Optimization results shows that, it's possible to increase the aromatics composition in reformate from 63.42 % in actual unit to 70.89 % by changing the design variables and operating conditions.

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**NOMENCLATURE**

A	Aromatics	( - )
C <sub>i</sub>	Concentration of species i	mole/cm <sup>3</sup>
C <sub>p</sub>	Specific heat	J/mole.K
DE	Differential Evaluation	( - )
d <sub>p</sub>	Equivalent diameter of a catalyst particle	m
e	Void fraction of reactor bed	m <sup>3</sup> /m <sup>3</sup>
E <sub>A</sub>	Activation energy	kcal/mole
F <sub>i</sub>	Molar flow rate of species i	mole/hr
G	Total mass flux of fluid	kg.s/m <sup>2</sup>
HC	Hydrocarbons	( - )
iso-P	Iso Paraffin	( - )
k <sub>i</sub> <sup>o</sup>	Pre-exponential factor	( - )
k <sub>i</sub>	Reaction rate constant	hr <sup>-1</sup>
m	Viscosity	pa.s
Mwt	Molecular weight	g/gmole
MCP	Methylcyclopentane	( - )
N	Naphthene	( - )
nr	Reactor number	( - )
nc	Component number	( - )
n-P	Normal Paraffin	( - )
P	Paraffin	( - )
P <sup>o</sup>	Partial pressure	bar
P <sub>t</sub>	Total pressure	bar
R	Gas constant	J/mole.K
r <sub>i</sub>	Reaction rate of species i	mole/gcat. Hr
S	Cross sectional area of reactor	m <sup>2</sup>
T	Reaction temperature	K
T <sup>o</sup>	Initial temperature	K
w	Catalyst weight	k
WHSV	Weight hour space velocity	hr <sup>-1</sup>
y	Mole fraction	(-)
Z	Length of reactor	m
ΔH <sub>Ri</sub>	Heat of i <sup>th</sup> reaction	J/ mole
αk	Pressure effect	( - )
ρ	Reformate density	Kg/m <sup>3</sup>
ρ <sub>cat</sub>	Catalyst density	Kg/m <sup>3</sup>

**Table (1) Reactions of the kinetic model <sup>(10)</sup>.**

Number of Reactions					
Paraffin's		Naphthenes		Aromatics	
$P_n \rightarrow N_n$	6	$N_n \rightarrow A_n$	6	$A_n \rightarrow A_{n-j} + P_j$	7
$P_n \rightarrow P_{n-j} + P_j$	26	$N_n \rightarrow N_{n-j} + P_j$	11	$A_n \rightarrow P_n$	5
subtotal	32	$N_n \rightarrow P_n$	7	$A_n \rightarrow N_n$	1
		subtotal	24	subtotal	13
Total			71		
n: Number of atoms of carbon ( $1 \leq I \leq 5$ )					

**Table (2) values of pressure effect reaction rate <sup>(28)</sup>.**

Reactions	$a_k$
isomerization	0.37
dehydrocyclization	-0.7
hydrocracking	0.433
hydrodealkylation	0.5
dehydrogenation	0.0

**Table (3) Operating conditions of heavy naphtha reforming process.**

Reactor number	1	2	3	4
Catalyst weight kg	2700	4500	4750	5875
Inlet Temperature C	470	470	470	470
Reactor Length m	6	6	6	6
Reactor Diameter m	2.4	2.4	2.4	2.4

**Table (4) Genetic algorithm parameters.**

Population size	20
Maximum generation	500
Crossover probability	0.8
Mutation probability	0.02
Neighborhood size	0.05

**Table (5) Kinetic constants of the kinetic model.**

Reaction Step	K <sub>o</sub>	E <sub>A</sub> (cal/mol)	Reaction Step	K <sub>o</sub>	E <sub>A</sub> (cal/mol)	Reaction Step	K <sub>o</sub>	E <sub>A</sub> (cal/mol)
P <sub>11</sub> → N <sub>11</sub>	0.035245	395276.3	P <sub>8</sub> → 2P <sub>4</sub>	0.005289	1380792.1	N <sub>8</sub> → N <sub>7</sub> +P <sub>1</sub>	0.002424	371403.8
P <sub>10</sub> → N <sub>10</sub>	0.241102	12571.5	P <sub>7</sub> → P <sub>6</sub> +P <sub>1</sub>	0.008641	94594.4	N <sub>11</sub> → A <sub>11</sub>	3.348710	144406.1
P <sub>9</sub> → N <sub>9</sub>	0.290453	30913.4	P <sub>7</sub> → P <sub>5</sub> +P <sub>2</sub>	0.000299	16285.9	N <sub>10</sub> → A <sub>10</sub>	3.038205	6884.6
P <sub>8</sub> → N <sub>8</sub>	0.175516	158287.1	P <sub>7</sub> → P <sub>4</sub> +P <sub>3</sub>	0.001681	527194.7	N <sub>9</sub> → A <sub>9</sub>	0.861510	30772.9
P <sub>7</sub> → N <sub>7</sub>	0.057523	191369.1	P <sub>6</sub> → P <sub>5</sub> +P <sub>1</sub>	0.009588	8913.1	N <sub>8</sub> → A <sub>8</sub>	0.878139	60476.8
P <sub>6</sub> → N <sub>6</sub>	0.000059	192859.3	P <sub>6</sub> → P <sub>4</sub> +P <sub>2</sub>	0.001313	415920.4	N <sub>7</sub> → A <sub>7</sub>	0.700312	62857.3
P <sub>11</sub> → MCP	0.036723	355184.0	P <sub>6</sub> → 2P <sub>5</sub>	0.005137	507601.3	N <sub>6</sub> → A <sub>6</sub>	0.780104	235830.4
P <sub>11</sub> → P <sub>10</sub> +P <sub>1</sub>	0.002968	522203.6	P <sub>5</sub> → P <sub>4</sub> +P <sub>1</sub>	0.002226	401961.2	A <sub>11</sub> → P <sub>11</sub>	0.013169	158262.4
P <sub>11</sub> → P <sub>9</sub> +P <sub>2</sub>	0.002368	511721.9	P <sub>8</sub> → P <sub>3</sub> +P <sub>2</sub>	0.010772	309494.9	A <sub>10</sub> → P <sub>10</sub>	0.009227	63877.0
P <sub>11</sub> → P <sub>8</sub> +P <sub>3</sub>	0.006108	611515.3	N <sub>11</sub> → P <sub>11</sub>	0.019734	251645.9	A <sub>9</sub> → P <sub>9</sub>	0.015866	24716.6
P <sub>11</sub> → P <sub>7</sub> +P <sub>4</sub>	0.007452	482015.1	N <sub>10</sub> → P <sub>10</sub>	0.015486	217366.5	A <sub>8</sub> → P <sub>8</sub>	0.006085	190006.3
P <sub>11</sub> → P <sub>6</sub> +P <sub>5</sub>	0.005719	451844.4	N <sub>9</sub> → P <sub>9</sub>	0.049227	93506.0	A <sub>7</sub> → P <sub>7</sub>	0.004767	65813.8
P <sub>10</sub> → P <sub>9</sub> +P <sub>1</sub>	0.010474	299602.9	N <sub>8</sub> → P <sub>8</sub>	0.024536	9238.9	A <sub>11</sub> → A <sub>10</sub> +P <sub>1</sub>	0.000257	269271.0
P <sub>10</sub> → P <sub>8</sub> +P <sub>2</sub>	0.005233	342144.2	N <sub>7</sub> → P <sub>7</sub>	0.018438	25427.7	A <sub>11</sub> → A <sub>9</sub> +P <sub>2</sub>	0.001533	180996.3
P <sub>10</sub> → P <sub>7</sub> +P <sub>3</sub>	0.010343	320263.7	N <sub>6</sub> → P <sub>6</sub>	0.188152	35330.5	A <sub>10</sub> → A <sub>9</sub> +P <sub>1</sub>	0.004166	183215.0
P <sub>10</sub> → P <sub>6</sub> +P <sub>4</sub>	0.001905	411541.4	MCP → P <sub>6</sub>	0.004166	258539.6	A <sub>10</sub> → A <sub>8</sub> +P <sub>2</sub>	0.002375	358128.6
P <sub>10</sub> → 2P <sub>5</sub>	0.002494	415569.4	N <sub>11</sub> → N <sub>10</sub> +P <sub>1</sub>	0.051563	182029.9	A <sub>10</sub> → A <sub>7</sub> +P <sub>3</sub>	0.000015	279077.2
P <sub>9</sub> → P <sub>8</sub> +P <sub>1</sub>	0.029129	12375.4	N <sub>11</sub> → N <sub>9</sub> +P <sub>2</sub>	0.068256	492859.0	A <sub>9</sub> → A <sub>8</sub> +P <sub>1</sub>	0.003869	66711.0
P <sub>9</sub> → P <sub>7</sub> +P <sub>2</sub>	0.003438	538520.9	N <sub>11</sub> → N <sub>8</sub> +P <sub>3</sub>	0.020517	426514.3	A <sub>9</sub> → A <sub>7</sub> +P <sub>2</sub>	0.002181	214672.7
P <sub>9</sub> → P <sub>6</sub> +P <sub>3</sub>	0.006675	571163.5	N <sub>10</sub> → N <sub>9</sub> +P <sub>1</sub>	0.006209	481410.6	A <sub>8</sub> → A <sub>7</sub> +P <sub>1</sub>	0.000853	198549.3
P <sub>9</sub> → P <sub>5</sub> +P <sub>4</sub>	0.001055	894217.5	N <sub>10</sub> → N <sub>8</sub> +P <sub>2</sub>	0.015040	338830.2	A <sub>6</sub> → N <sub>6</sub>	0.011706	94161.1
P <sub>8</sub> → P <sub>7</sub> +P <sub>1</sub>	0.002730	434829.9	N <sub>10</sub> → N <sub>7</sub> +P <sub>3</sub>	0.003359	287185.9	MCP → N <sub>6</sub>	0.116207	103435.9
P <sub>8</sub> → P <sub>6</sub> +P <sub>2</sub>	0.019787	508944.7	N <sub>9</sub> → N <sub>8</sub> +P <sub>1</sub>	0.101649	149915.7	N <sub>6</sub> → MCP	0.037806	13742.9
P <sub>8</sub> → P <sub>5</sub> +P <sub>3</sub>	0.004421	513079.2	N <sub>9</sub> → N <sub>7</sub> +P <sub>2</sub>	0.007559	286681.6			

**Table (6) Kinetic constants of the kinetic model.**

Reaction Step	K <sub>r</sub> <sub>o</sub>	E (cal/mol)	K <sub>e</sub> <sub>o</sub>	E <sub>c</sub> (cal/mol)
n-P <sub>5</sub> ↔ i-P <sub>5</sub>	0.082534	47594.43	1.760852	32849.74
n-P <sub>6</sub> ↔ i-P <sub>6</sub>	1.000953	54892.38	4.520159	30526.59
n-P <sub>7</sub> ↔ i-P <sub>7</sub>	0.745269	54432.3	2.762023	30129.55
n-P <sub>8</sub> ↔ i-P <sub>8</sub>	3.97936	54311.55	3.660238	30097.75
n-P <sub>9</sub> ↔ i-P <sub>9</sub>	0.423443	48212.04	6.542571	48093.3
n-P <sub>10</sub> ↔ i-P <sub>10</sub>	0.316826	54574.42	6.71224	30139.25
-r <sub>A</sub> = Kr(C <sub>a</sub> - C <sub>b</sub> / K <sub>e</sub> );    Kr = K <sub>r</sub> <sub>o</sub> * exp(-E / RT);    K <sub>e</sub> = K <sub>e</sub> <sub>o</sub> * exp(-E <sub>c</sub> / RT)				

**Table (7) Actual and simulated reformate compositions.**

	Composition												
	Feed	Reactor 1			Reactor 2			Reactor 3			Reactor 4		
		Exp.	Pred.	Abs. diff.									
<b>n-P1</b>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<b>n-P2</b>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<b>n-P3</b>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<b>n-P4</b>	0.0036	0.0023	0.0000	0.0023	0.0014	0.0000	0.0014	0.0026	0.0000	0.0026	0.0014	0.0000	0.0014
<b>n-P<sub>5</sub></b>	0.0045	0.0047	0.0080	0.0033	0.0064	0.0086	0.0022	0.0086	0.0088	0.0002	0.0084	0.0098	0.0014
<b>n-P<sub>6</sub></b>	0.0430	0.0261	0.0385	0.0124	0.0272	0.0240	0.0032	0.0265	0.0202	0.0063	0.0242	0.0184	0.0058
<b>n-P<sub>7</sub></b>	0.0751	0.0521	0.0663	0.0142	0.0464	0.0410	0.0054	0.0352	0.0306	0.0046	0.0289	0.0240	0.0049
<b>n-P<sub>8</sub></b>	0.0834	0.0523	0.0559	0.0036	0.0387	0.0289	0.0098	0.0234	0.0179	0.0055	0.0161	0.0121	0.0040
<b>n-P<sub>9</sub></b>	0.0676	0.0343	0.0396	0.0053	0.0200	0.0136	0.0064	0.0092	0.0090	0.0002	0.0050	0.0070	0.0020
<b>n-P<sub>10</sub></b>	0.0225	0.0038	0.0141	0.0103	0.0054	0.0077	0.0023	0.0073	0.0057	0.0016	0.0069	0.0044	0.0025
<b>n-P<sub>11</sub></b>	0.0020	0.0040	0.0020	0.0020	0.0043	0.0020	0.0023	0.0064	0.0016	0.0048	0.0063	0.0011	0.0052
<b>i-P<sub>5</sub></b>	0.0061	0.0081	0.0051	0.0030	0.0071	0.0080	0.0009	0.0114	0.0111	0.0003	0.0093	0.0139	0.0046
<b>i-P<sub>6</sub></b>	0.0373	0.0536	0.0489	0.0047	0.0607	0.0677	0.0070	0.0704	0.0722	0.0018	0.0666	0.0720	0.0054
<b>i-P<sub>7</sub></b>	0.0492	0.0680	0.0596	0.0084	0.0675	0.0777	0.0102	0.0688	0.0739	0.0051	0.0605	0.0633	0.0028
<b>i-P<sub>8</sub></b>	0.0189	0.0671	0.0578	0.0093	0.0616	0.0714	0.0098	0.0522	0.0573	0.0051	0.0387	0.0422	0.0035
<b>i-P<sub>9</sub></b>	0.1106	0.0787	0.0892	0.0105	0.0713	0.0692	0.0021	0.0574	0.0544	0.0030	0.0402	0.0438	0.0036
<b>i-P<sub>10</sub></b>	0.0989	0.0890	0.0878	0.0012	0.0700	0.0658	0.0042	0.0496	0.0494	0.0002	0.0355	0.0367	0.0012
<b>MCP</b>	0.0033	0.0021	0.0049	0.0028	0.0005	0.0038	0.0033	0.0005	0.0032	0.0027	0.0036	0.0038	0.0002
<b>N<sub>6</sub></b>	0.0214	0.0000	0.0097	0.0097	0.0000	0.0008	0.0008	0.0000	0.0006	0.0006	0.0000	0.0006	0.0006
<b>N<sub>7</sub></b>	0.0554	0.0046	0.0173	0.0127	0.0035	0.0005	0.0030	0.0036	0.0009	0.0027	0.0032	0.0011	0.0021
<b>N<sub>8</sub></b>	0.0699	0.0078	0.0148	0.0070	0.0076	0.0016	0.0060	0.0072	0.0019	0.0053	0.0055	0.0016	0.0039
<b>N<sub>9</sub></b>	0.0406	0.0183	0.0118	0.0065	0.0152	0.0040	0.0112	0.0098	0.0026	0.0072	0.0055	0.0020	0.0035
<b>N<sub>10</sub></b>	0.0542	0.0000	0.0009	0.0009	0.0000	0.0006	0.0006	0.0000	0.0004	0.0004	0.0000	0.0003	0.0003
<b>N<sub>11</sub></b>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<b>A<sub>6</sub></b>	0.0035	0.0080	0.0052	0.0028	0.0106	0.0116	0.0010	0.0135	0.0149	0.0014	0.0161	0.0202	0.0041
<b>A<sub>7</sub></b>	0.0255	0.0632	0.0622	0.0010	0.0812	0.0853	0.0041	0.1001	0.1018	0.0017	0.1215	0.1243	0.0028
<b>A<sub>8</sub></b>	0.0762	0.1379	0.1304	0.0075	0.1707	0.1700	0.0007	0.2059	0.2112	0.0053	0.2478	0.2544	0.0066
<b>A<sub>9</sub></b>	0.0136	0.1070	0.0831	0.0239	0.1114	0.1230	0.0117	0.1152	0.1274	0.0122	0.1244	0.1209	0.0035
<b>A<sub>10</sub></b>	0.0136	0.1070	0.0868	0.0202	0.1114	0.1132	0.0018	0.1152	0.1228	0.0076	0.1244	0.1217	0.0027
<b>A<sub>11</sub></b>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000	0.0004	0.0004
<b>n-Paraffin</b>	0.30162	0.1796	0.22724	0.04764	0.1498	0.12923	0.02057	0.1192	0.09814	0.02106	0.0972	0.0826	0.0146
<b>i-Paraffins</b>	0.32102	0.3645	0.34716	0.01734	0.3382	0.35841	0.02021	0.3098	0.31671	0.00691	0.2508	0.27019	0.01939
<b>Napthenes</b>	0.24487	0.0328	0.05929	0.02649	0.0268	0.01122	0.01558	0.0211	0.00964	0.01146	0.0178	0.00937	0.00843
<b>Aromatics</b>	0.13249	0.4231	0.36631	0.05679	0.4852	0.50114	0.01594	0.5499	0.57551	0.02561	0.6342	0.63784	0.00364
<b>Teamperature</b>	743.15	698.15	694.594	3.55626	732.15	725.604	6.5456	738.15	734.216	3.93388	745.15	737.487	7.66286

Table (9) Comparison between actual and optimized design.

	Actual	Generation No.					
		1	100	200	300	400	500
T1 (C°)	743.25	726.40	741.83	742.32	742.32	742.32	742.32
T2 (C°)	741.25	728.02	742.55	742.55	742.55	742.55	742.55
T3 (C°)	741.25	738.73	742.29	742.29	742.41	742.41	742.41
T4 (C°)	741.25	741.42	742.18	742.73	742.73	742.73	742.73
W1 (Kg)	2700.00	3175.81	4852.37	4852.37	4852.37	4917.63	4852.37
W2 (Kg)	4500.00	8944.27	2306.84	2306.84	2306.84	2098.14	2306.84
W3 (Kg)	4750.00	1071.67	1975.20	1975.20	1975.20	2001.77	1975.20
W4 (Kg)	5875.00	4633.25	8690.58	8690.58	8690.58	8807.46	8690.58
P (Pa)	2350000	1576220	1505316	1505316	1505316	1505316	1505316
H2/Hc	7.000	6.556	7.933	7.933	7.933	7.933	7.933
n-Paraffins	0.0972	0.1229	0.0726	0.0706	0.0704	0.0704	0.0704
Iso-Paraffins	0.2508	0.2959	0.2155	0.2133	0.2132	0.2132	0.2132
Naphthenes	0.0178	0.0067	0.0073	0.0075	0.0075	0.0075	0.0075
Aromatics	0.6342	0.5745	0.7047	0.7086	0.7089	0.7089	0.7089

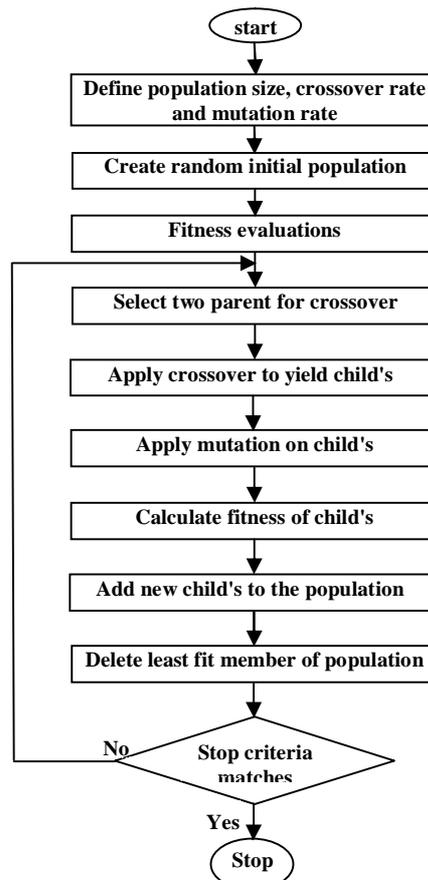


Figure (1) Flowchart of Genetic Algorithm.

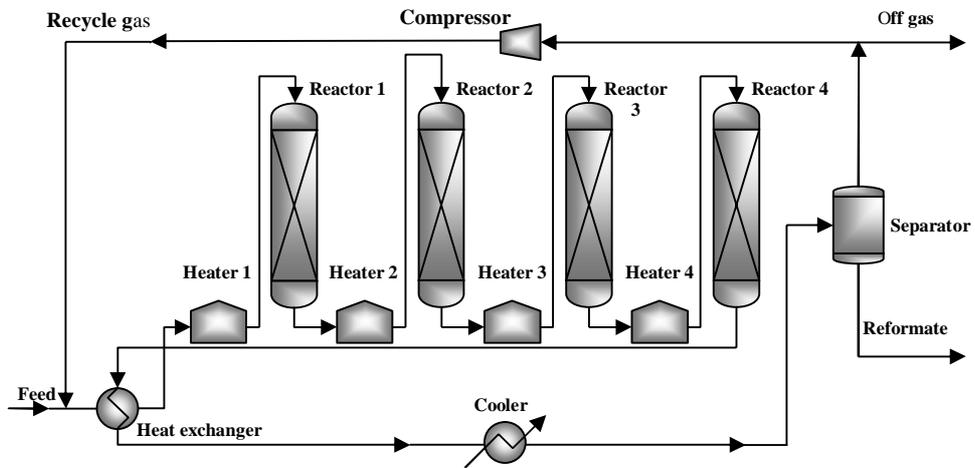


Figure (2) Schematic diagram of Al-Doura naphtha reforming process

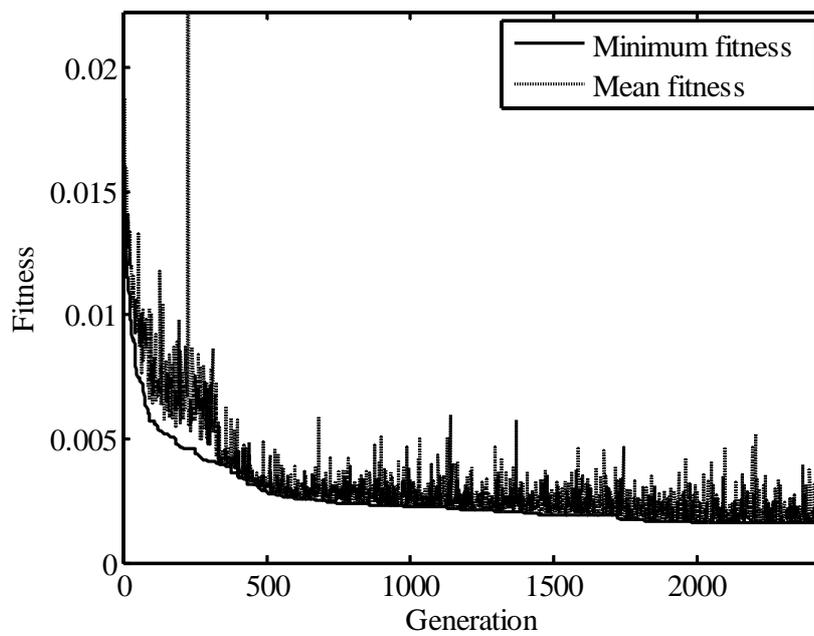


Figure (3) Minimum and mean fitness with respect to generation number.

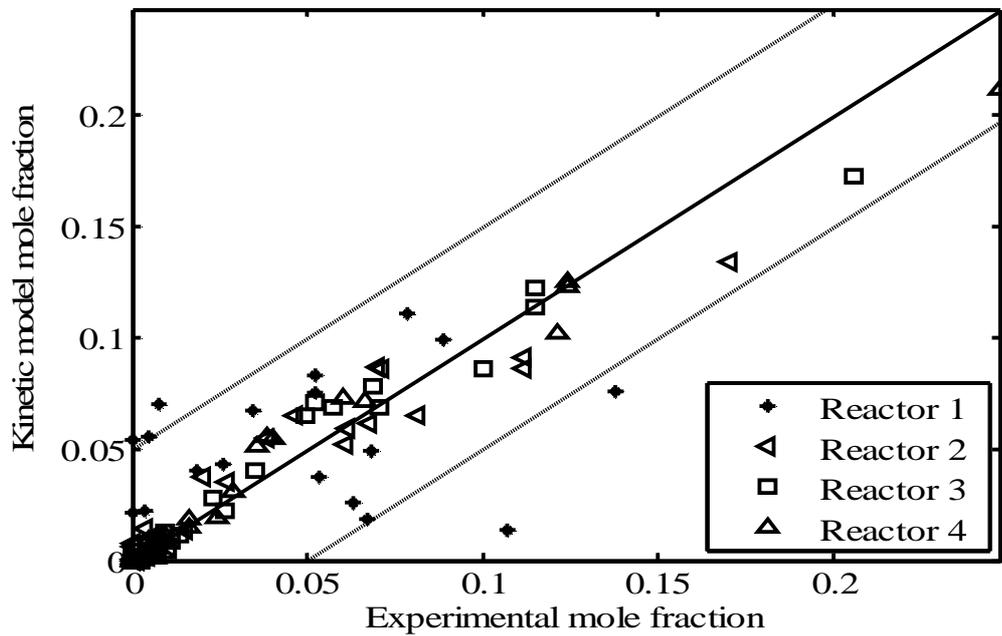


Figure (4) Comparison between actual and simulated reformate compositions.

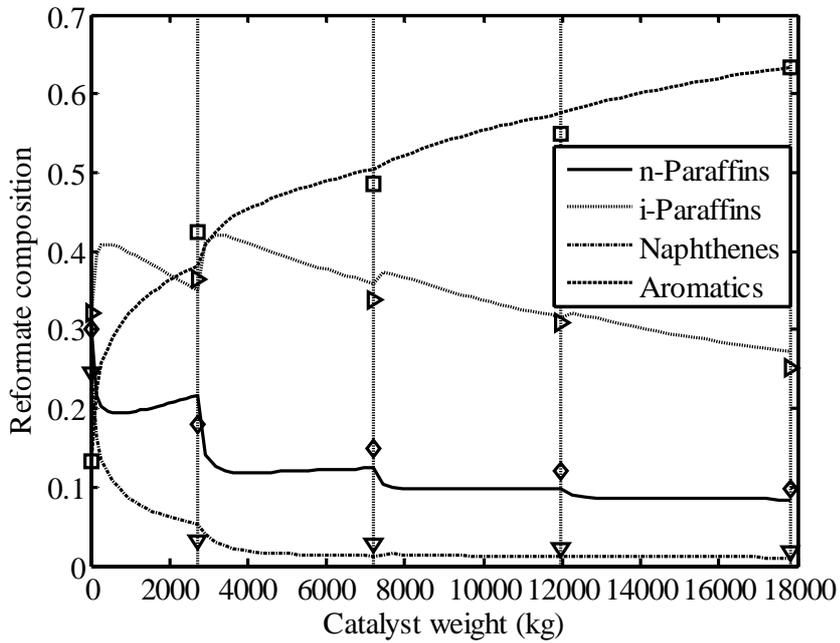


Figure (5) Comparison between actual and simulated n-paraffins, i-Paraffins, naphthenes, and aromatics (Symbols actual, lines predicted).

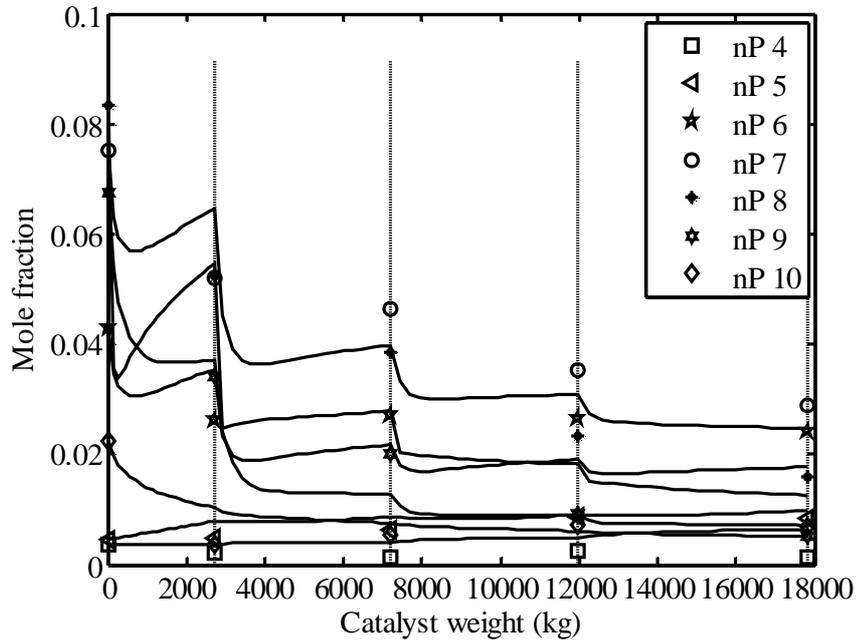


Figure (6) Comparison between actual and simulated n-paraffins composition(symbols actual, lines predicted).

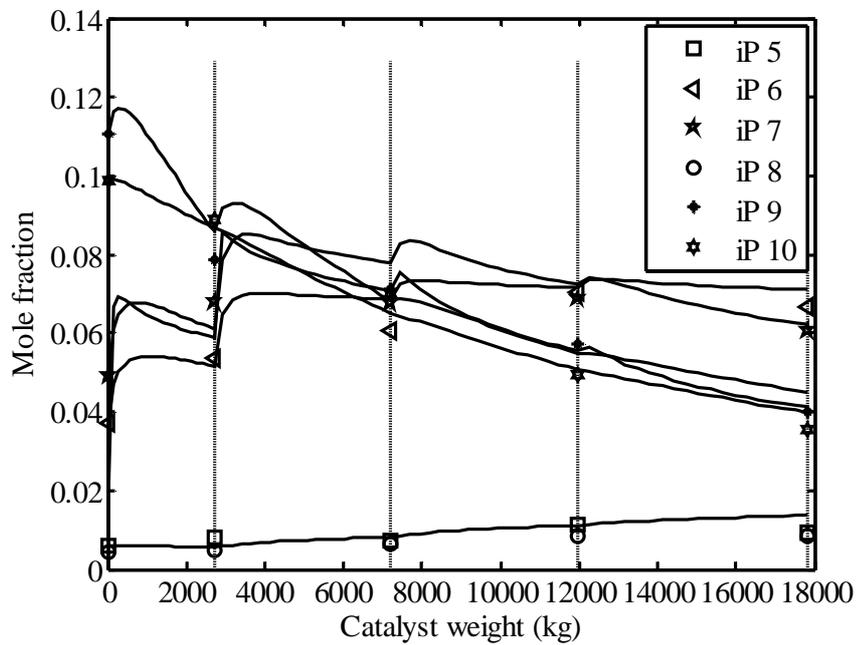


Figure (7) Comparison between actual and simulated i-paraffins composition(Symbols actual, lines predicted).

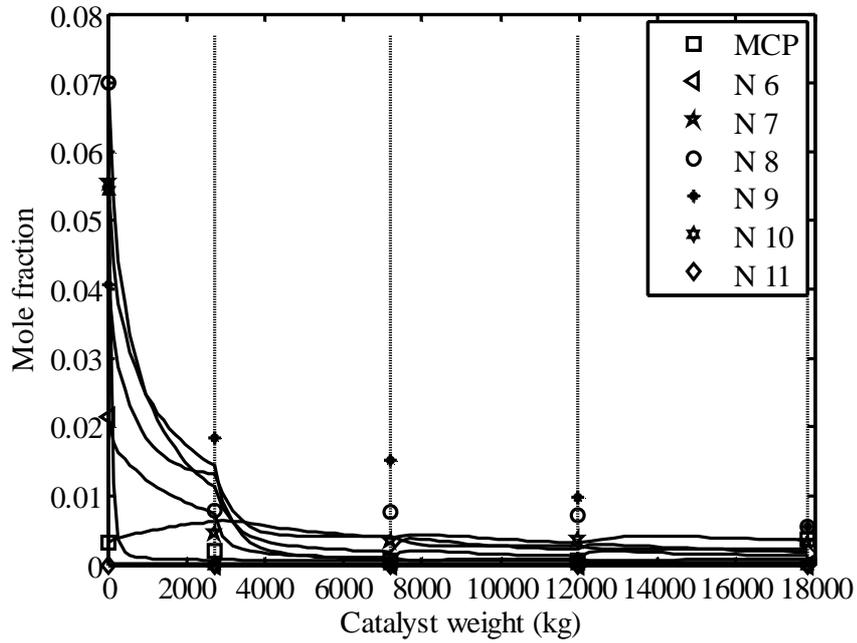


Figure (8) Comparison between actual and simulated naphthenes composition(Symbols actual, lines predicted).

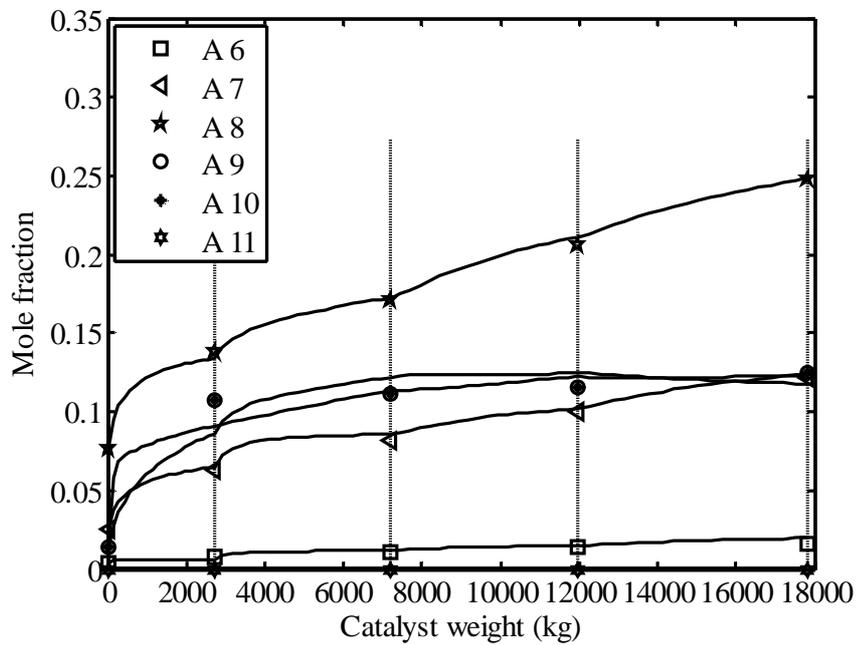


Figure (9) Comparison between actual and simulated aromatics composition(Symbols actual, lines predicted).

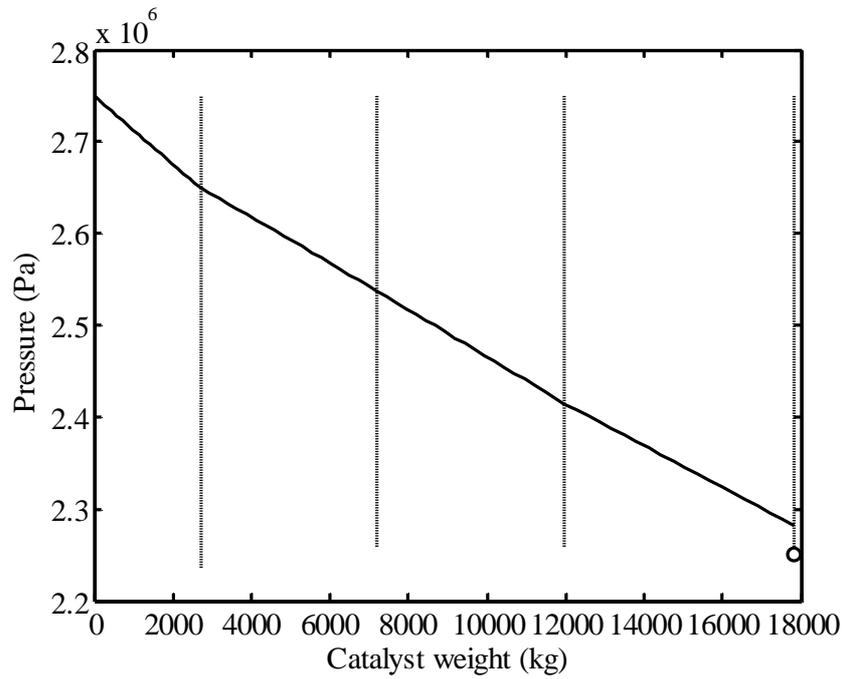


Figure (10) Comparison between actual and simulated pressure drop (Symbols actual, lines predicted).

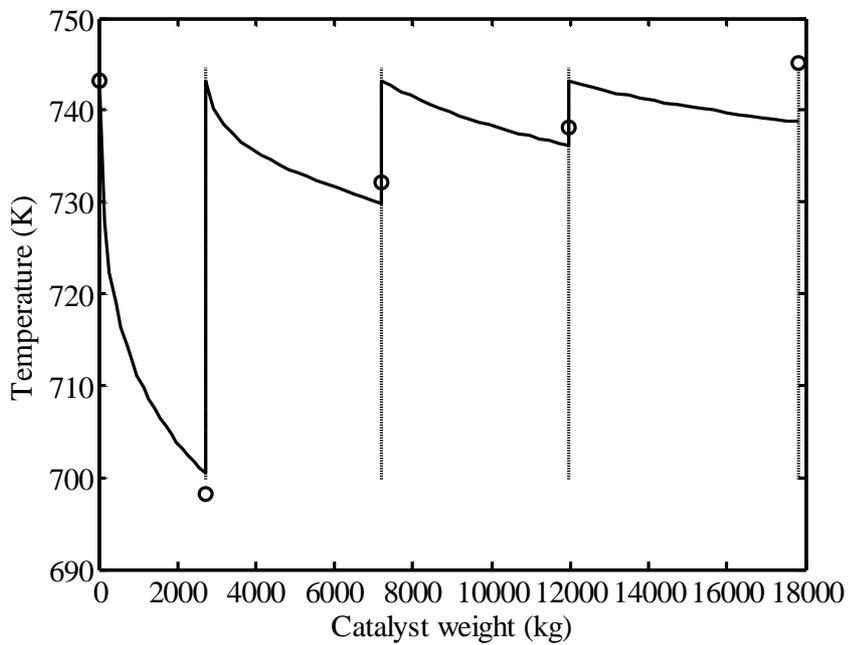


Figure (11) Comparison between actual and simulated temperature profile(Symbols actual, lines predicted).

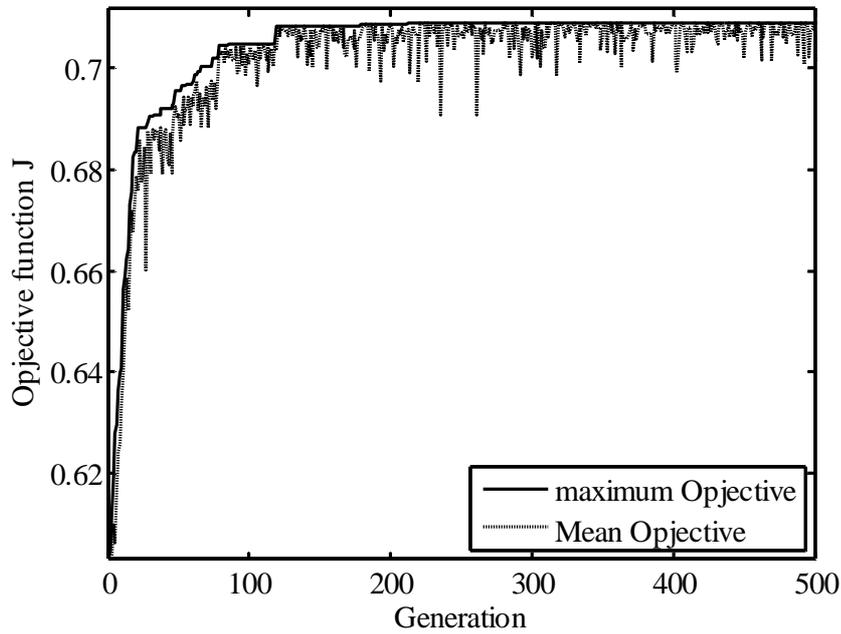


Figure (12) optimization objective Function with respect to generation number.

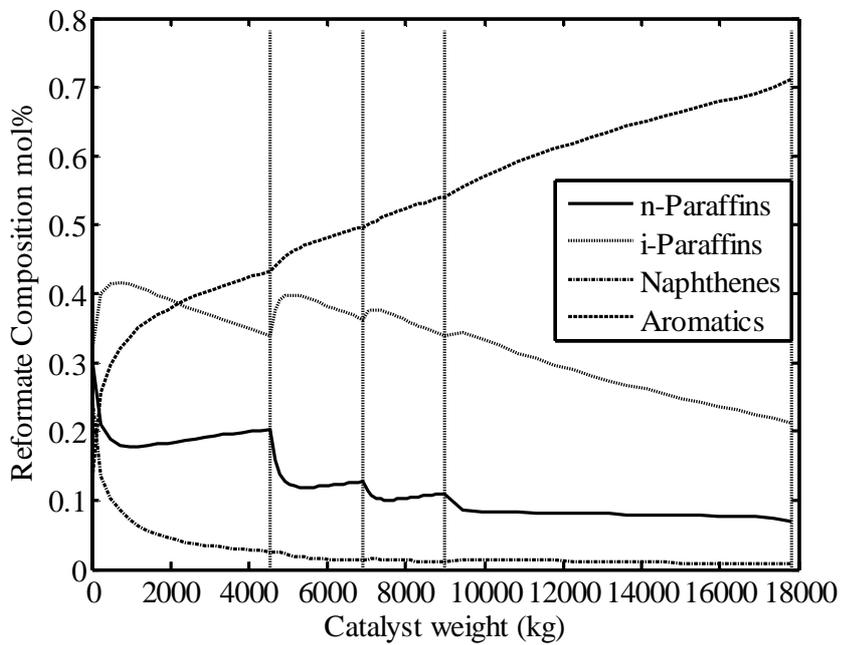


Figure (13) Simulation results for n-paraffins, i-Paraffins, naphthenes, and aromatics depending on optimum design.