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Optimization of Catalytic Naphtha Reforming Process Based on Modified Differential Evolution Algorithm ⋆

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Abstract: Catalytic naphtha reforming is one of the most important processes for high octane gasoline manufacture and aromatic hydrocarbons production. In this article, a modified differential evolution (DE) algorithm is proposed to optimize an actual continuous catalytic naphtha reforming (CCR) process. The optimization problem considers to minimize the energy consumption and maximize the aromatics yield. The CCR process model is established by adopting the 27-lumped kinetics reaction network, and all parameters are adjusted based on the actual process data. The DE algorithm is modified to maintain the diversity of the population. In this mechanism, individuals further from the best individual have larger possibilities to be selected in the mutation operator. The modified DE is evaluated by solving 6 benchmark functions, and the performance is compared with classic DEs. The results demonstrate that the modified DE has better global search ability and higher computation efficiency. Furthermore, the optimization results of catalytic naphtha reforming process indicate that the proposed algorithm has the ability of locating the optimal operating points, in which the aromatics yield is improved, while energy consumption is reduced. Meanwhile, the optimal operating points and results are discussed at the end of the article.

Keywords: Catalytic naphtha reforming process, Energy consumption, Differential evolution, Global search

1. INTRODUCTION

Continuous catalytic reforming of naphtha (CCR) process plays a significant role for high octane gasoline manufacture and aromatic hydrocarbons production. The simplified process flow diagram of this process is shown as Fig.1. In the CCR process, aromatic yield is an important assessment standard of the production quality. However, improving the aromatics yield is often achieved at the cost of larger material and energy consumption. Sometimes, the losses caused by improving the aromatics yield is even larger than the benefits it produced. Therefore, optimization on the CCR process is of important significance.

Differential evolution (DE) is an efficient optimization algorithm, which offers advantages over traditional population-based stochastic algorithm in convergence speed and robustness, Das and Suganthan (2011). In decades, amount of research works on the applications of DE algorithm in chemical processes have been proposed. Angira and Santosh (2007) applied trigonometric mutation operation in the DE algorithm, and the updated algorithm were utilized to solve seven cases of chemical process optimization problems. Xu et al. (2013) proposed an improved the DE algorithm based on self-adaptive strategy. Rahimpour et al. (2010) used the DE method to solve dynamic optimization problem of the naphtha reforming process.

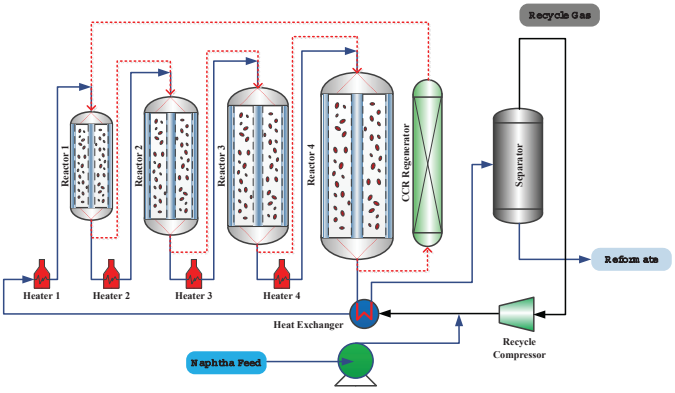

Fig. 1. Simplified process flow diagram of the CCR process

Despite that many research works have been investigated on the applications of modified DEs, most of them mainly focused on the discovery of novel mutation operators or the novel settings of operating parameters. The problem of population diversity decreasing has not been solved effectively. This defect may result in repetitive counting and weak global search ability, which are unacceptable in solving optimization problems of the chemical processes. In this work, a modification strategy on DE algorithm is proposed. This method adopts distance information of the

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population to determine the possibilities that individuals would be chosen in the mutation operator.

This work is organized as follow: Section 2 describes the CCR process in modeling and parameter tunning, and formulates an optimization objective including both aromatic yields and energy consumption. Section 3 introduces the modified DE algorithm in detail, and computational results are listed comparing with several distinguished stochastic optimization algorithms. Section 4 presents the results that the proposed algorithm used to solve optimization problem for the CCR process, and the optimal operating points are discussed. In Section 5, this article is concluded and some lines of future research are mentioned.

2. MODELING OF THE CCR PROCESS

The CCR process is shown in Fig.1. In this process, Naphtha is used as catalytic reforming process feed-stock. It usually contains more than 300 chemical compounds. The feed-stock goes through the catalytic reformers combined with a recycle gas stream containing high purity hydrogen. Catalytic reformer is designed as four cascade reactors. Each reformer is equipped with a heater to maintain the reaction temperature at design level. The effluent from the last reactor is cooled and sent to the product separator. The separated hydrogen is sent back to reformers as recycle gas, while liquid product is sent to the distillation unit to obtain aromatic products.

2.1 Lumps kinetic model

As mentioned above, the naphtha feed-stock is of high complexity. For this reason, a detailed kinetic reaction model will be too complicated to be established. In order to reduce the complexity of the kinetic model, components with similar reaction performance will be grouped together as a smaller set of kinetic lumps.

The lump theory is firstly proposed by Smith (1959). It classified naphtha feed-stock as paraffin, naphthene and aromatic, and contained 4 reactions. Based on this theory, amount of researches have been taken in decades. Jenkins and Stephens (1980) proposed 31 lumps kinetic model, Froment (1987) developed a 28 lumps kinetic model. In 2000th, Hongjun et al. (2010) divided the reaction feed-stock and products into 27 lumps, and evaluated the parameters in a method of fractional steps.

In this work, A 27-lumped kinetic model proposed by Hongjun et al. (2010) is adopted. The reaction network is shown in Fig.2. The network takes the following assumption into consideration

- Paraffin cant translate into C6 naphthene and aromatic directly.
- Neglect the reaction that isoparaffin reacts to form C6 naphthene.
- Aromatic is of stability, for this reason, aromatic hydro-cracking reaction only happens on side chain.
- The rate of naphthene isomerization and dehydrocyclization is extremely fast. In consequence, the cracking reaction among naphthene can be neglected.
- Defining isomerization, dehydrocyclization, and aromatization as reversible reaction, while hydrogenolysis and paraffin hydro-cracking are regarded as irreversible reactions.

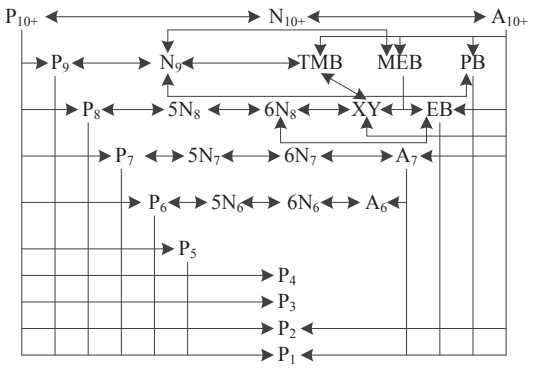

Fig. 2. 27-lumped reaction network of catalytic naphtha reforming

Considering above assumptions, the reaction rate equations can be established as follow

paraffin dehydrocyclization (reversible)

$$r_i = k_i(Y_p - \frac{Y_{5N}}{K_{epi}}) \tag{1}$$

naphthene isomerization (reversible)

$$r_i = k_i(Y_{5N} - \frac{Y_{6N}}{K_{epi}}) \tag{2}$$

naphthene dehydroaromatization (reversible)

$$r_i = k_i(Y_{6N} - \frac{Y_A}{K_{epi}}) \tag{3}$$

paraffin hydrocracking (irreversible)

$$r_i = k_i(Y_{6N} - \frac{Y_A}{K_{epi}}) \tag{4}$$

Where, k_i is reaction rate constant, which can be expressed as

$$k_i = k_{oi} \cdot exp(\frac{-E_i}{RT}) \cdot P_h^{b_i} \cdot \phi_i \tag{5}$$

Where, ϕ_i, $0 < \phi_i < 1$ denotes the catalyst active factor.

Radial-flow reactors are adopted as catalytic reformers in the CCR process. The modeling of the radial-flow reactors is usually assumed that under the normal reformer operating conditions, radial and axial dispersion effects are negligible, Iranshahi et al. (2010), Gyngazova et al. (2011). The global material and the heat balance equations are given as follow

$$\frac{dY}{dR} = \frac{2\pi R \cdot H}{(LHSV \cdot V_c)} \cdot K_r \cdot Y \tag{6}$$

$$\frac{dT}{dR} = \frac{2\pi R \cdot H}{(LHSV \cdot V_c)} \cdot \Sigma \frac{(r_j \cdot \Delta H_j)}{(C_p \cdot Y)} \tag{7}$$

Where, Y is the vector of the molar flow rates including 27 lumps and hydrogen. $LHSV$ denotes the short of liquid hourly space velocity.

2.2 Parameter tunning

In order to adjust the process model to reflect the actual the CCR process accurately, 10 sets of actual operating

Table 1. Operating data from the actual CCR process

	F (t/h)	AP (%)	T1 (°C)	T2 (°C)	T1 (°C)	T4 (°C)	p $(Mpag)$	AY (%)
set 1	198.33	42.43	526.99	526.81	524.98	529.02	1.02	64.02
set 2	198.37	39.98	527.04	527.11	525.08	528.86	1.02	62.48
set 3	198.34	43.85	526.99	527.02	524.99	529.03	1.02	64.27
set 4	198.38	41.18	527.01	527.00	524.71	529.03	1.02	63.54
set 5	198.27	40.85	526.97	527.00	525.00	528.99	1.02	63.54
set 6	198.33	40.34	526.99	527.00	525.05	528.99	1.02	63.21
set 7	198.30	40.10	525.99	525.97	524.00	527.97	1.02	63.92
set 8	198.31	40.08	526.01	525.96	524.04	527.99	1.02	62.75
set 9	198.31	40.10	526.00	525.98	523.95	528.05	1.02	62.50
set 10	198.30	40.13	525.88	526.14	523.88	527.97	1.02	61.69

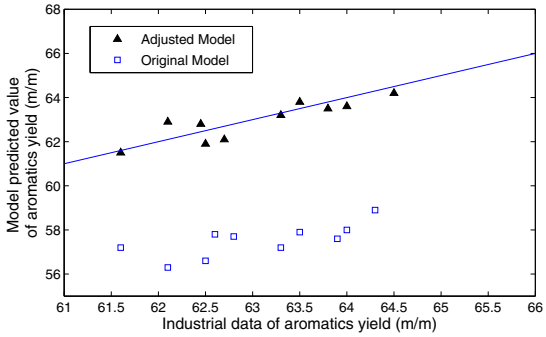

Fig. 3. Comparison between the adjusted kinetic model and the original model on the values of aromatic yields

Table 2. Results of model predict and plant actual data (record main components among set 1 only)

composition	*actual*	*predict*	*difference*
$NP4$	5.09%	5.36%	−0.27%
$NP5$	1.42%	0.00%	1.42%
$SBP6$	3.12%	1.88%	1.23%
$NP6$	1.66%	0.66%	0.99%
$A6$	8.07%	7.11%	−0.04%
$A7$	20.25%	20.31%	−0.06%
EB	5.37%	5.39%	−0.02%
OX	7.88%	7.35%	0.53%
MX	11.78%	11.70%	0.08%
PX	5.61%	5.47%	0.14%
$A9$	20.50%	20.72%	−0.22%

data collected from a certain catalytic reforming unit is used to estimate the reaction parameters. The values of the data are listed in Table.1. Where, F is the mass flow rate of feedstock. AP denotes the aromatic potential content. T_1 T_4 are the values of inlet temperature in each reactor, p denotes the reaction pressure, and AY is the aromatic yields of the products.

In this article, the sum of the squared differences of all components in products is taken as the objective function. Therefore, the parameter estimation problem is converted into an optimization problem. DE is applied to solve this problem. The difference between the adjusted kinetic model and the original model is presented in Fig.3. The data reflect the products aromatic yields of each set.

Table.2 shows the detail result of the parameter tunning. It can be observed that the difference value of main aromatic components are all below 1%. Thus, it could be concluded that the adjusted CCR model is able to reflect the special actual CCR unit accurately.

2.3 Optimization problem for the CCR process

In the CCR process, aromatic yields are important assessment standard of the production quality. Meanwhile, in order to form more $C8-$ aromatic, the yield of heavy aromatic should be limited. Considering the fact that the price of energy is rising and low-carbon is a world-wide issue. In this article, energy consumption is also taken into consideration.

As mentioned above, this work considers three optimization factors, which are maximizing aromatic yields, minimizing heavy aromatic yields, and minimizing energy consumption. Due to the fact that the heat duty from heaters is the uppermost energy consumption in the CCR process. In this work, energy consumption is expressed as the fired duty of the four heaters.

The function of optimization problem could be formulated as follow

$$max\ f(x) = \omega_1 AY + \omega_2 HAY - \omega_3 Q \tag{8}$$

where, AY indicates aromatic yield and HAY indicates heavy aromatic yields. Q denotes the fired duty in heaters. $\omega_i, i = 1,2,3$ are weight values. These values are all determined by the actual price of the relevant variable. The decision variable x selected are reactors inlet temperature ($T1$, $T2$, $T3$ and $T4$), reaction pressure (p), and hydrogen-to-oil molar ratio ($nH2/nHC$). According to the actual operation data, the constraint of the decision are presented as

$$510 \leqslant T_1, T_2, T_3, T_4 \leqslant 540 \tag{9}$$
$$0.9 \leqslant p \leqslant 1.1 \tag{10}$$
$$2.5 \leqslant n_{H_2}/n_{HC} \leqslant 540 \tag{11}$$

3. DISTANCE BASED DE

Since an accurately modified CCR model and an optimization problem have been established in section 2. In this section, a modified differential evolution algorithm is proposed to solve this problem.

3.1 Differential evolution

The differential evolution (DE) is a population-based stochastic optimization algorithm, Price (1996). The performance of DE is distinguished, especially in convergence speed and robustness.

In the DE algorithm, mutation and crossover are utilized to generate trial vectors. For the former operation, the classic mutation strategy is presented as follow

$$v_i^t = x_{r_1}^t + F(x_{r_2}^t - x_{r_3}^t) \tag{12}$$

Where $r_i (i = 1,2,3)$ indicates mutually integers selected randomly within $[1, NP]$, and the value of each r_i must be unique. $x_{r_i}^t$ indicates individual selected from the population at generation t, and x_best^t is the best vector among the population. F denotes the scale factor predetermined mutually. The value of F is usually chosen within $(0,1)$.

The strategy that accomplishes the crossover operator is shown as follow

$$u_{i,j}^t = \begin{cases} v_i^t, & if(rand \leqslant CR) \\ x_{i,j}^t, & otherwise \end{cases} \tag{13}$$

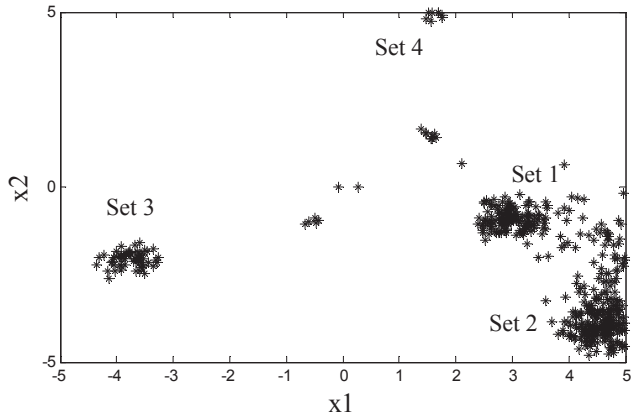

Fig. 4. The illustration of population distance

Where $u_{i,j}^t$ indicates j-th element of i-th new trial vector at generation t.

Finally, offspring can be generated in the use of selection operation which is presented as follows

$$x_i^{t+1} = \begin{cases} u_i^t, & if(f(u_i^t) \leqslant f(x_i^t)) \\ x_i^t, & otherwise \end{cases} \tag{14}$$

3.2 Modified DE based on population distance

Due to the advantage of high convergence and robustness, the DE algorithm is widely used in solving optimization problems. In decades, a number of modified strategies have been proposed to develop the performance of DE, some of which are of high effectivity, such as Fan and Lampinen (2003), Brest et al. (2006), Rahnamayan et al. (2008), and Qin et al. (2009). However, most of these researches mainly focused on the discovery of novel mutation strategies or the setting of operating parameters, such as F and CR mentioned above. The importance of population structure at each generation is always being neglected.

Fig.4 shows a case that the DE algorithm solves a multi-modal optimization problem with 2-dimensional variables at a certain generation. It can be observed that individuals in current population are mainly divided into 4 sets naturally. In fact, each set surrounds a local optimal. It can be found that most individuals located in set 1, and this set also contains the best vector. However, the global optimum is near set 4.

In this phenomenon, there is high probability that all $x_{r_i}^t$ would be chosen in set 2. According to the mutation strategy 12 listed above, if $x_{r_i}^t$ are similar with each other, the trial vector could not be much different from the current individuals. That might lead to the deficiencies of population diversity and too much repetitive counting. For the reason that calculating the CCR process model is time consuming, duplicated calculation is unacceptable in the process optimization.

In order to solve this problem, a modified DE algorithm based on distance information (DisDE) is proposed in this work. In this method, individuals at each generation are distributed into S_n sets by the Euclidean distance from individuals to the current best vector. S_n is the number of sets. The equation of counting the Euclidean distance is presented as follow

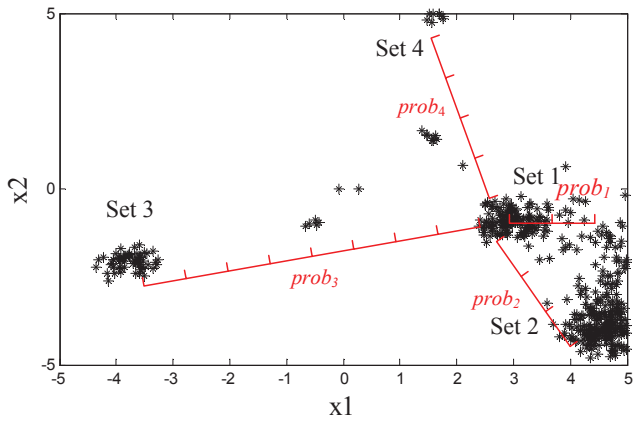

Fig. 5. The illustration of the main idea of the DisDE algorithm

$$d_i^t = \sqrt{\sum_{j=1}^{n} (x_{i,best}^t - x_{i,j}^t)^2} \tag{15}$$

Where d_i^t denotes the distance from i-th vector to the current best vector at generation t. n is dimensionality of variables. According to the distance value of each vector, population could be divided into S_n sets by cluster algorithm, where S_n is an operating parameter predetermined. Thus, the mean distance of each set could be calculated as

$$\bar{d}_{set_k}^t = \sum \frac{d_{set_k}^t}{N_{set_k}} \tag{16}$$

Where $prob_{set}^t$ indicates the number of vectors that belong to set $k, k = 1, ..., S_n$. In the use of mean distance value, selection probability could be obtained as

$$prob_{set_k}^t = \frac{\bar{d}_{set_k}^t}{\sum_{i=1}^{N} \bar{d}_{set_i}^t} \tag{17}$$

Where $prob_{set_k}^t$ is the probability that trial vector is chosen from set k. it is obvious that a set with larger distance value from the best vector might obtain higher probability to be chosen. In this method, the trial vectors chosen to generate offspring would be more different from current individuals. the diversity of population could be kept. The illustration of the main idea of the DisDE algorithm is shown in Fig.5. The flowchart of the proposed algorithm is presented as Fig.6.

3.3 simulation and analysis

In order to demonstrate the performance of the proposed algorithm, DisDE is calculated by solving 6 benchmark functions from CEC 2005. These functions are listed in Table.3. Where D is variable dimensionality, S denotes the range of variables, and f_{min} is the global optimal value of each function. Among the 6 functions, F_1 to F_4 are single-modal functions,which are used to test the convergence speed of algorithms. While F_5 and F_6 are multi-modal functions, and these functions are applied to assess the global search ability.

As comparison, the traditional DE algorithm adopting DE/rand/1 and the TDE, Fan and Lampinen (2003), are

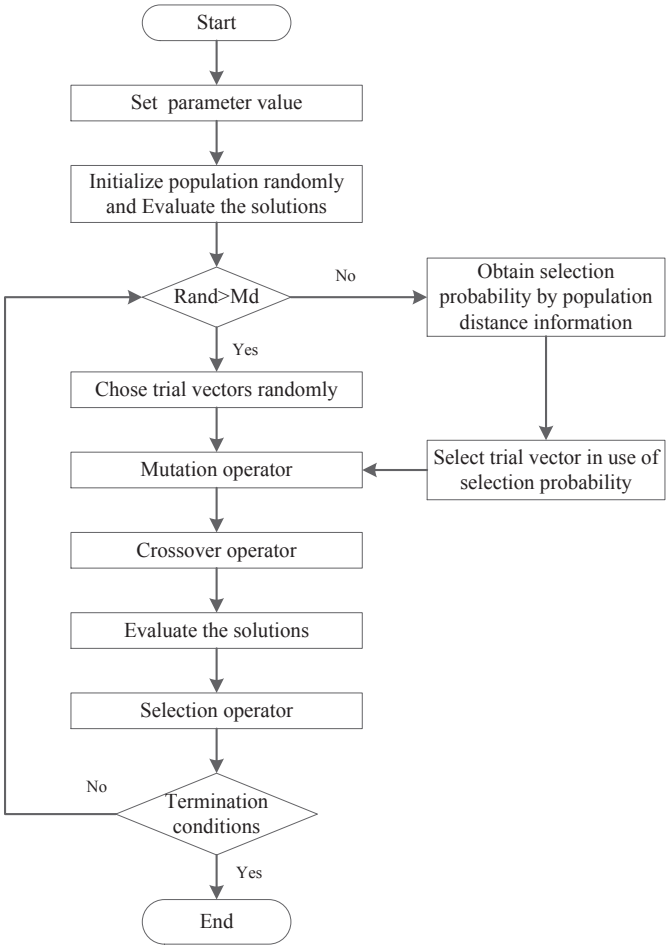

Fig. 6. Flowchart of modified DE algorithm

Table 3. Benchmark functions from CEC 2005

$Benchmark function$	D	S	f_{min}
$F_1(x)$: Shifted Sphere Function	30	$[-100,100]^D$	0
$F_2(x)$: Shifted Schwefel's Probblem 1.2	30	$[-100,100]^D$	0
$F_3(x)$: Shifted Schwefel's Probblem 1.2 with Noise in Fitness	30	$[-100,100]^D$	0
$F_4(x)$: Schwefel's Problem 2.6 with Global Optimum on Bounds	30	$[-100,100]^D$	0
$F_5(x)$: Rotated Hybrid Composition Function	2	$[-5,5]^D$	0
$F_6(x)$: Rotated Hybrid Composition Function with Global Optimum on the Bounds	2	$[-5,5]^D$	0

selected to make experimentations. All the algorithms are predetermined the same operating parameter and maximum generation, as $F = 0.4$, $CR = 0.9$, $Gm = 3000$, $Pop = 200$, and calculated 30 times for each function. Where G_m denotes the maximum generation and Pop indicates the population size. And $Mt = 0.15$ for TDE, $Md = 0.2$ for DisDE.

The results of each algorithm solving the mentioned functions are listed in Table.4. In each function, the best result is in bold type. For the functions F_1 to F_4, the DisDE performs the bestin F_2 and F_4, and the results of DisDE in F_1 and F_3 is still much better than the original DE algorithm.

Table 4. Results of 6 benchmark functions

		$DisDE$	DE	TDE
$F_1(x)$	min	$7.25E-18$	$2.53E-15$	**1.88E-22**
	$mean$	$1.19E-17$	$2.28E-14$	**5.64E-21**
	std	$1.90E-18$	$1.71E-14$	**1.23E-20**
$F_2(x)$	min	**2.79E-09**	$2.35E-07$	$3.76E-08$
	$mean$	**4.98E-08**	$7.78E-07$	$2.10E-07$
	std	**6.60E-08**	$4.33E-07$	$2.83E-07$
$F_3(x)$	min	$4.85E-05$	$7.49E-05$	**1.15E-07**
	$mean$	$1.30E-04$	$2.03E-04$	**4.72E-07**
	std	$1.75E-04$	$1.71E-04$	**5.36E-06**
$F_4(x)$	min	**3.14E-01**	$2.58E+01$	$1.30E+00$
	$mean$	**3.86E-01**	$3.84E+01$	$6.24E+00$
	std	**7.17E-02**	$2.64E+01$	$2.69E+00$
$F_5(x)$	min	**0**	0	0
	$mean$	**200**	300	300
	$prob$	**0.8**	0.63	0.5
$F_6(x)$	min	**0**	0	200
	$mean$	**200**	300	300
	$prob$	**0.73**	0.27	0.10

Table 5. Price of aromatics

	Ben	Tol	A8	A9	A10
$\$/t$	1548	1389	1683	1270	1222
mass frac	0.11	0.37	0.52	0.58	0.42

It can be observed from the results of F_5 and F_6 that DisDE both performs best. Especially in solving F_6, due to the global optimum is located on the bounds, it is very difficult for algorithms to discover the global optimum. This feature can be reflected from the results. It is obvious that the probability of DE and TDE locating the global optimum in F_6 is low, the value of which are below 30%. While, the proposed algorithm located the global optimum more in 30 calculation times. Thus, it can be concluded that the modification strategy that we adopt in the DE algorithm is able to improve the global search ability and promote the computation efficiency.

4. OPTIMIZATION OF CCR PROCESS BY DISDE

As the optimization objective function established in 8, it can be observed that the function is composed of AY, HAY, Q, and their weight values. AY and HAY can be estimated as follow

$$AY = \frac{(F_{A6} + F_{A7} + F_{A8})}{F_{inlet}} \tag{18}$$

$$HAY = \frac{(F_{A9} + F_{A10})}{F_{inlet}} \tag{19}$$

Where $F_{Ai}, i = 6,7,8,9,10+$ denotes the mass flow rate of structure of aromatic. F_{inlet} is the mass flow rate of naphtha feedstock. The value of $\omega_1, i = 1,2,3$ is determined by actual price of the relevant variable, which is listed in Table.5.

In addition to the aromatic price and mass flow rate, energy consumption data is also available as

$$1kg\ oil = 41.868MJ$$

$$oil\ price = \$770/t$$

According to all data listed above, values of $\omega_1, i = 1,2,3$ can be estimated as

$$\omega_1 = 3$$

$$\omega_2 = 2.5$$

$$\omega_3 = 1.8 \times 10^{-10}$$

Table 6. Results of optimization for the CCR process

	actual	optimal	effect
$F(t/h)$		*198.333*	
$AP(\%)$		*42.425*	
$T_1()$	525.882	522.307	-3.575
$T_2()$	526.137	522.586	-3.551
$T_3()$	523.877	525.368	1.491
$T_4()$	527.967	533.07	5.103
$p(MPag)$	1.020	0.962	-0.058
$n_{H_2}/n_{HC}(mol/mol)$	3.07	2.78	-0.29
$AY(\%)$	61.68	64.02	2.34
$HAY(\%)$	20.63	17.60	-3.03
$Q(kJ/h)$	$3.16E+08$	$3.09E+08$	$-7.00E+06$

The result of solving this objective function problem applying the proposed algorithm is shown in Table.6. From the optimization, it can be observed that the increasing of T_1, T_2, p, and *hydrogen-to-oil molar ratio* might lead to both decreasing of the aromatic yields and heavy aromatic yields. With the temperature increasing, more energy would be consumed in vain. An increasing in T_3 could obtain higher aromatic yields, but the effect is slight. Meanwhile, a larger value of T_4 could result in significant increase in aromatic yields, while decreasing in heavy aromatic yields. Despite that higher temperature means more energy consumption, in the mean of increasing T_4, the benefits from higher aromatic yields would be much larger.

In Table.6, actual denotes the normal operating point in the CCR process, optimal lists the suggestion operating points, and effect records the difference value between actual and optimal. It can be observed that the aromatic yields are increased by 2.34% by optimization. Such improvement is remarkable. Meanwhile, the heavy aromatic yields decreased by 3.03%, which means more heavy aromatic is formed $A6$ to $A8$. Additionally, the total heat duty decreased by $7.00E+06kj/h$. The reason is that the modified algorithm decreased the temperature which has slight effort to obtain more aromatic, while increased the effective ones. Based on such result, it can be concluded that in the way of redistributing the operating points, including $heatertemperature$, $pressure$ and $hydrogen-to-oilmolarratio$, the efficiency of the CCR process could be promoted, while more energy is economized.

5. CONCLUSION

In this article, a modified DE algorithm is proposed. The validity of modification is verified by solving 6 benchmark functions, and the proposed algorithm is applied to the optimization of the continuous catalytic naphtha reforming (CCR) process successfully.

The future work will pay attention focus on the investigation of classification method used to distribute individuals, and attempt to make the individuals distribution more reasonable.

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