Refinery Optimization Integrated with a Nonlinear Crude Distillation Unit Model

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Abstract: In this paper, the problem of optimal crude oil procurement combined with refinery operations is addressed to obtain an ϵ -global optimal solution. Rather than the traditional planning and scheduling methodologies relying on linear programming (LP), a nonlinear model using Geddes fractional index (FI) is employed to describe the behavior of the crude distillation unit (CDU) and integrated with the entire plant-wide model. Although this representation provides more accurate prediction of the real production of the refinery than the conventional fixed yield approach, its global optimization becomes more difficult owing to the existence of many nonlinear, non-convex terms. To overcome this challenge, advanced interval reduction techniques are developed and combined with state-of-the-art global optimization software to obtain an ϵ -global optimal solution more efficiently. The optimization and comparison are conducted to show the effectiveness of the proposed approach.

Keywords: Global Optimization, Fractional Index Model, Interval Reduction

1. INTRODUCTION

The refining industry is capital intensive such that even one percent improvement can increase the profit significantly. Two important elements that impact profitability of a refinery are crude oil purchases and plant operations. Due to the variation of oil properties, including yields, sulfur concentration and density, the price of crude oils can vary significantly. Usually, low sulfur and low density oil, also called light crude oil, is easier to process and generates more valuable products, but its price is higher compared with the heavy crude oil. Thus, how to design a suitable crude oil procurement recipe according to the crude properties and specific refinery operations to achieve a global optimum is always attractive to academia and the petroleum industry.

Modern refinery optimization schemes rely on an accurate model of the entire plant and efficient mathematical programming technique to achieve a local or global optimal solution. In the early stage, a purely linear model based on material balance is employed to simulate the refinery production process and solved to a global optimal solution nearly instantly. However, with the introduction of more complex units and processes, the inaccuracy of linear model becomes more serious and finally renders this method inappropriate for most real applications. In view of this, it is necessary to develop nonlinear process model based optimization schemes. A common nonlinearity considered in refinery optimization is pooling, which represents multiple flows mixing and distributing to produce several products. Nevertheless, the more important nonlinearity actually lies in the process units. Among all units in the refinery, we are mainly concerned with the crude distillation unit (CDU) because it separates the crude into several fractions and determines the possible

quantities of products directly. Traditionally, a short-cut method is used for distillation column design based on the Fenske-Underwood-Gilliland equations, which are very complex and not suitable for optimization purposes. Lang et al. (1991) combined the bubble-point and sum-rate methods to achieve a good matching between calculations and experimental results. Alhajri et al. (2008) used a high-order polynomial function to represent the volume percent of all fractions based on true boiling point (TBP) temperature. Li et al. (2005) proposed a simplified empirical nonlinear process model for CDUs based on the cut point temperature which takes operating conditions into account. However, this method assumes the CDU can only work in several discrete modes to bypass the difficulty of determining the optimal cut point in the entire temperature domain. Recently, a fractional index (FI) model for CDUs was proposed by Alattas et al. (2011). This model is independent of the crude and enables the solver to decide the cut point temperatures more flexibly, thus obtaining a better solution than other methods. A drawback of this FI model is that it requires the solution of a number of highly nonlinear equations with continuous and integer variables, and thus is computationally intensive. In this paper, we will revisit and simplify this model to make it more practical for real applications.

Since the decision process of crude oil purchase involves integer variables and unit operations incorporate continuous variables, an efficient mixed-integer nonlinear programming (MINLP) algorithm is highly desirable for refinery optimization problems to ensure that a global optimum is obtained with acceptable solution time. Most MINLP algorithms consist of convexification and branch & bound procedures, which generate sequences of lower and upper bounds on the solution values. Once the gap between upper and lower bounds is smaller than a predefined threshold ϵ , then we say an ϵ -global optimal solution is identified. State-of-the-art commercial software, BARON, by Tawarmalani and Sahinidis (2005), is based on the branch-and-reduce method. If the constraints and objective function are convex, the outer approximation method presented by Duran and Grossmann (1986) can reach the global optimum. This has been extended to nonconvex constraints and objective function by Kesavan et al. (2004). Recently developed software, ANTIGONE, by Misener and Floudas (2014), is able to detect special structures of the formulation, such as reformulation-linearization technique (RLT) equations, convexity/concavity, edge-convexity/edge-concavity, αBB relaxations introduced by Androulakis et al. (1995), termspecific under-estimators, and use them in the branchand-cut procedure. Even though these cutting-edge global optimization techniques have already gained great success, we need to point out that a problem specific preprocessing procedure is still often necessary to speed up the solution process. Through case studies, we noticed that the variable bounding step is highly important for global optimization software because the convex relaxation gap is dependent on the size of variable intervals. In fact, by using feasibility and optimality based interval reduction methods proposed in this paper, both the solution gap and solution time can be decreased considerably.

The paper is organized as follows: the nonlinear representation of the refinery consisting of a FI model and a pooling model is built in Section 2; the interval of variables derived from constraint propagation, feasibility based interval reduction (FIR) and optimality based interval reduction (OIR) are presented in Section 3; the optimization results for a simplified refinery with FI model are given in Section 4; the paper ends with conclusions and remarks.

2. REFINERY MODEL





Fig. 1. A simplified refinery model flow chart in Favennec (2001).

A simplified refinery flow chart is used in this paper and shown in Fig. 1. In the refining process, the crude oil flows into the distillation and is separated into several cuts including refinery gas (RG), liquefied gas (LG), light naphtha (LN), heavy naphtha (HN), kerosine (KE), gas oil (GO), vacuum gas oil (VGO) and vacuum residue

(VR) for future processing. A CDU model developed by Alattas et al. (2011) is adopted and revised in this paper to calculate the weight fraction of each cut except LG and RG due to the lack of light end data (Fig. 2). Although there are actually thousands of molecules in the crude oil, we usually group the molecules with similar properties to generate a much smaller number of so-called pseudo-components for design and optimization purposes. In each cut, some pseudo-components will be distributed into distillate and bottoms. The distillate part will go to the higher trays for further separation and the bottoms part is the output of the CDU. Thus, we denote the mole fraction of i^{th} pseudo-component as x_i . Its distribution in the distillate and bottoms are represented by $x_{dis,i}$ and $x_{bot,i}$, respectively.



Fig. 2. The separation process.

Geddes (1958) derived the relationship between component composition ratio versus relative volatility on a logarithmic scale as straight lines and the slope of these lines is named the fractionation index (FI), which can be calculated from column tests. Moreover, the TBP data analysis for FI evaluation was conducted on the performance data from three commercial units, Gilbert et al. (1966). The resulting Thiele Geddes method for component i is

$$\frac{x_{dis,i}}{x_{bot,i}} = (\alpha_{i,o})^{FI} \frac{x_{dis,o}}{x_{bot,o}},\tag{1}$$

where subscript o represents the reference component and $\alpha_{i,o}$ is the relative volatility. Further assume that in cut j, we have cut point temperature T_j , relative volatility $\alpha_{j,i,o}(T_j)$ and equilibrium constant $K_{j,i}(T_j)$, then according to Jakob (1971), we can replace the relative volatility in (1) by equilibrium constant for simplification. As a result, the FI equation is:

$$\frac{x_{dis,j,i}}{x_{bot,j,i}} = \left(K_{j,i}(T_j)\right)^{FI}.$$
(2)

It is worthwhile to note that the FI of a pseudo-component may change if the cut point temperature varies. Specifically, we have

$$FI = \begin{cases} FI_{r,j} & \text{if } IT_j \leq Tb_i < T_j \\ FI_{s,j} & \text{if } ET_j \geq Tb_i \geq T_j \end{cases}$$

where $FI_{r,j}$ and $FI_{s,j}$ are two different FI parameters for the cut j; Tb_i is the true boiling point temperature of that pseudo-component; IT_j and ET_j are initial and end boiling points for the cut j. If the true boiling point of a pseudo-component is smaller than IT_j , then this component will only exist in the overhead and if the true boiling point of a pseudo-component is larger than ET_j ,

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then this component will only exist in the bottoms. Here we assume that the interval $U_j := [IT_j, ET_j]$ does not overlap between the cuts. This implies that a pseudocomponent will only distribute into bottoms and distillate at one cut and it will be solely gas or liquid at other cuts. Moreover, we restrict the cut point temperature within a sub-domain of U_j , namely, $T_j \in \Omega_j := [\underline{T}_j, \overline{T}_j] \subset U_j$, such that there is only one pseudo-component for each cut whose FI parameter cannot be determined in advance. In order to model the switching of the FI parameter, we introduce the binary variable v_i for pseudo-component i if $Tb_i \in \Omega_j$:

$$v_i(ET_j - IT_j) \ge T_j - Tb_i,\tag{3}$$

$$(v_i - 1)(ET_j - IT_j) < T_j - Tb_i.$$
 (4)

Then FI equation (2) for these components becomes:

$$\frac{x_{dis,j,i}}{x_{bot,j,i}} = \left(K_{j,i}(T_j)\right)^{FI_{r,j}} v_i + \left(K_{j,i}(T_j)\right)^{FI_{s,j}} (1-v_i).$$
(5)

Based on the FI equations (5), (3) and (4), we can formulate the mole balance for the pseudo-component. For cut j and pseudo-component i satisfying $Tb_i \in U_j$, we have

$$N_i = P_{dis,j} x_{dis,j,i} + P_{bot,j} x_{bot,j,i}, \tag{6}$$

$$P_{bot,j} = \sum_{i:Tb_i \in U_j} P_{bot,j} x_{bot,j,i} + \sum_{i:Tb_i \in U_{j-1}} P_{dis,j-1} x_{dis,j-1,i},$$

$$P_{dis,j} = \sum_{i:Tb_i \in U_j} P_{dis,j} x_{dis,j,i} + \sum_{i:Tb_i < IT_j} N_i,$$
(8)

$$\sum_{i} N_i = 1, \tag{9}$$

where N_i is the mole number of the pseudo-component iin the feed and we can only consider 1 mole crude input for modeling purposes. $P_{dis,j}$ and $P_{bot,j}$ are the total mole number of cut j in distillate and bottoms, respectively. Given the mole fraction, we can calculate the weight W_j of each cut:

$$W_{j} = \sum_{i:Tb_{i} \in U_{j}} P_{bot,j} x_{bot,j,i} M_{i} + \sum_{i':Tb_{i'} \in U_{j-1}} P_{dis,j-1} x_{dis,j-1,i'} M_{i'},$$

where $j \in \text{Cut} = \{LN, HN, KE, GO, VGO, VR\}$ and the yield weight fraction Y_j is:

$$Y_j = W_j / \sum_i N_i M_i \tag{10}$$

where M_i is the molecular weight of pseudo-component *i*. The remainder work of CDU modeling is to write equations for the equilibrium constant $K_{j,i}$. Assuming ideal behavior and according to Raoult's law:

$$K_{j,i} = \frac{VP_i(T_j)}{P} \tag{11}$$

where $VP_i(T_j)$ is the vapor pressure which can be calculated according to the state equation proposed by Twu et al. (1994) and P is the column's pressure. However, note that this state equation is an exponential function with high order signomial terms, which is very difficult to handle with current global optimization software, thus we use the quadratic function in (12) to approximate the original state equation. The parameters $\gamma_0, \gamma_1, \gamma_2$ are estimated by using least squares to fit the data generated by the state equation. This approximation is accurate enough because the decision variable T_j is only within a small interval instead of the entire temperature domain. The approximation can be verified by Fig. 3.

$$VP_i(Tr_{j,i}) = \gamma_2(Tr_{j,i})^2 + \gamma_1 Tr_{j,i} + \gamma_0$$
 (12)

where $Tr_{j,i}$ is the reduced temperature defined by the ratio of cut point temperature and critical temperature of pseudo-component $i: T_j/Tc_i$. When modeling, the true



Fig. 3. The comparison of state equation data and its quadratic function approximation for different pseudo-components.

boiling point (TBP) data from the crude oil assay is used as the input to ASPEN to generate the pseudo-components and their parameters Tc_i , M_i , Tb_i and N_i .

2.2 Pooling Process

(7)

Once the yield fractions are obtained, we can follow Favennec (2001) to write linear equations for mass balance, capacity limitation, demand, importation, quality constraints and so on. However, we notice that at least two factors will make the problem more complex. First, the LG produced from the CDU, reformer and cracker are mixed in the pipeline and distributed to the different gasoline tanks PG98 and ES95. Second, the cracker can work in two production modes: Mogas and AGO. The products of these two modes are mixed and distributed to the desulfurization unit, HGO and HF tanks. This mixing and distributing of flows is called pooling in the refinery model and this process will introduce bilinear terms in the final quality expressions even under linear mixing rules.

Let H denote the flow, f denote the flow fraction, \tilde{q} denote the known property of inflow and q denote the unknown property of outflow. Here we employ the classical pq-formulation proposed by Tawarmalani and Sahinidis (2002) to model this pooling process. Suppose that there are \mathcal{I} inflows, then we have

$$\sum_{n=1}^{L} f_n = 1,$$
(13)

$$\sum_{n=1}^{L} H_m f_n \tilde{q}_n = q_m H_m, \quad \forall m$$
(14)

$$\sum_{n=1}^{\mathcal{I}} H_m f_n = H_m, \quad \forall m \tag{15}$$

where n is the subscript of inflow and m is the subscript of outflow. Even though (15) is redundant in the nonlinear model, it is very useful to tighten the convex relaxation of the model.

2.3 Sulfur Model for Fluid Catalytic Cracker

One of the most important qualities of refinery products is the sulfur concentration. Hence, it is worth constructing a more accurate sulfur model to characterize the impact of sulfur in the crude on the final products. Here we further consider the sulfur in the Fluid Catalytic Cracker (FCC) because one of its outputs, catalytic cracked gasoline (CN), is the major source of sulfur for gasoline95 (ES95) and gasoline98 (PG98).

According to Sadeghbeigi (2000), sulfur in CN is approximately an affine function of the feed sulfur content in VGO:

$$s_{CN} = 0.054 \left(\sum_{i} f_{VGO_i} \tilde{s}_{VGO_i} \right) - 0.0024$$
 (16)

where s_{CN} is the unknown sulfur fraction of CN; \tilde{s}_{VGO_i} is the known sulfur fraction in VGO of crude i; f_{VGO_i} is the flow fraction of VGO from crude i. Parameters 0.054 and 0.0024 are identified from the figure on page 193, Sadeghbeigi (2000). Let the maximum permissible sulfur fraction in gasoline to be 0.025 and assume that the sulfur fraction in the imported high quality gasoline is negligible. Then the equations for sulfur in the produced gasoline are:

$$\begin{aligned} H_{CN,95}s_{CN} \leqslant & 0.025(H_{CN,95} + H_{LN,95} + H_{ISO,95} + H_{ISO,95} + H_{LG,95} + H_{R95,95} + H_{100,95} + H_{imp,95}) \\ H_{CN,98}s_{CN} \leqslant & 0.025(H_{CN,98} + H_{LN,98} + H_{ISO,98} + (18)) \end{aligned}$$

$$H_{LG,98} + H_{R95,98} + H_{100,98} + H_{imp,98})$$

where the subscript imp denotes the importation.

2.4 Objective Function

The aim of the refinery optimization is to maximize the economic return from crude purchase and refinery operations. Thus the objective function incorporates the crude purchase cost, operation cost, importation expense and final products sales. The price of the crude is mainly determined by its API gravity, but also related to the sulfur concentration and yield. In order to address situations in which the production of the refinery cannot meet market demands or quality specs, we allow the refinery to import high quality products by paying a higher price than its sales. A linear form of the objective function is:

$$obj = C_{sale}H_{products} - C_{crude}H_{crude}$$
(19)
$$- C_{operation}\sum H - C_{imp}H_{imp}$$

where C represents the price and H represents the flow. In the optimization, we need to \max_H obj, subject to the refinery model.

3. GLOBAL OPTIMIZATION

Even though several global optimization software packages can be used for models containing continuous variables, integer variables and non-convex terms, a well-designed pre-processing procedure is still the key step to obtain the ϵ -global optimum in a short time. Considering that the convex relaxation is one of the most important parts of global optimization and its relaxation gap is highly dependent on the variable intervals, ways to reduce the variable bounds attract considerable attentions in global optimization research. Given the refinery model, the variable interval derived from the physical limitations such as unit capacity may not be tight enough to yield a tight relaxation. Thus, in this paper, we mainly consider three approaches for interval reduction, including interval analysis (IA), feasibility-based interval reduction and optimalitybased interval reduction, to speed up the algorithm.

3.1 Forward/Reverse Interval Analysis

Given an equation F(x) = 0, forward interval analysis derives its interval $[\underline{F}, \overline{F}]$ bounds based on the initial range for each variable. Then by setting the equation interval as [0,0], the reverse interval analysis will contract the domain for each variable sequentially, Jaulin et al. (2001). Similarly, we can also set interval as $[0, +\infty]$ or $[-\infty, 0]$ for inequalities. Here this methodology is implemented by using the interval analysis package MC++ and directed acyclic graph (DAG) representation from Schichl and Neumaier (2005) to reduce the range for variables in the refinery model. The interval analysis takes very short processing time without solving an optimization problem. But its drawback is that the resulting bounds may not be tight enough.

3.2 Feasibility based interval reduction (FIR)

The FIR method is a pre-processing step for global optimization. To acquire a tighter bound on a variable, say x, the direct way is to solve the optimization problem: min / max x, subject to the refinery model. This method does not exclude any feasible points of the original problem and can be very effective when the initial interval is much larger than the feasible region according to Balendra and Bogle (2009).

However, solving such an optimization problem subject to the refinery model actually has the same computational burden as the original problem, thus also slow. One way to address this issue is to limit the solving time of the software and employ its best estimation as the variable bound. An alternative way is to construct convex and concave relaxations of the original problem and solve the relaxed formulation to get the variable bounds. In this paper, we utilize the second way because it provides more flexible and faster solution. Generally, this refinery model contains four kinds of non-convex terms which should be relaxed: bilinear terms, trilinear terms, signomial terms, and integer variables.

Bilinear term For bilinear terms, the McCormick relaxation proposed by McCormick (1976) is the best way to construct its convex and concave hulls.

Trilinear term It has been shown by Rikun (1997) that the convex and concave envelopes of a trilinear term are still the polyhedral and we employ the procedure provided by Myer and Floudas (2003) to construct such polyhedron.

Signomial term Since the FI parameter can be an arbitrary real positive number derived from the column test, $(K_{j,i})^{FI}$ is a signomial term. According to Lundell et al. (2009), the power transformation and piecewise linear functions can be used to convexify signomial terms. However, this scheme will introduce more binary variables and render the entire formulation more complex. Note that

 $(K_{j,i})^{FI}$ is either convex or concave and the bound on $K_{j,i}$ is known, its convex and concave relaxation can be built by using an affine function:

If
$$FI > 1$$
: Convex: $(K_{j,i})^{FI}$
Concave: $\frac{(\overline{K}_{j,i})^{FI} - (\underline{K}_{j,i})^{FI}}{\overline{K}_{j,i} - \underline{K}_{j,i}}(K_{j,i} - \underline{K}_{j,i})$
If $FI \leq 1$: Concave: $(K_{j,i})^{FI}$
Convex: $\frac{(\overline{K}_{j,i})^{FI} - (\underline{K}_{j,i})^{FI}}{\overline{K}_{j,i} - \underline{K}_{j,i}}(K_{j,i} - \underline{K}_{j,i})$

Integer variables The integer variables v_i are introduced to model due to the switching of the FI parameter. Given the assumptions made before, only one pseudo-component for each cut should be decided by optimization solver. In this paper, we simply relax the integer requirement to obtain a nonlinear convex problem for FIR.

After relaxation, the resulting nonlinear convex problem can be solved by the software CONOPT to obtain the upper and lower bounds of variables quickly. It is worthwhile to note that the convex and concave relaxation is based on the interval of variables involving in the bilinear or trilinear terms. The initial guess for these variable intervals can be obtained by using forward/reverse interval analysis. Once the variable interval is contracted by solving the convex optimization, the relaxation also becomes tighter and we may repeat this optimization procedure to generate stronger bounds.

3.3 Optimality based interval reduction (OIR)

Different from the FIR, the OIR method cuts off part of the feasible region of the original formulation but still retains the global optimum. By solving OIR, we expect to obtain much tighter bounds for variables, thereby accelerating the branch & bound procedure. The prerequisite of OIR is a feasible solution, say obj' found by local optimization software. Then it is clear that the global optimum obj* should be no smaller than the current feasible solution, namely, obj* \geq obj'. This cut can be integrated into the optimization formulation of FIR to yield the OIR formulation, which is still convex and can be solved by CONOPT to get tighter interval for the variables. The OIR is triggered when the incumbent solution is updated significantly and can be combined with the FIR in the optimization algorithm.

4. OPTMIZATION STUDY

Based on the refinery model proposed in this paper, we optimize the refinery profits with four sources of crude using an Intel Xeon CPU 3.07GHZ with 4GB memory assigned for Ubuntu-64 bit operating system. All algorithms in this study are implemented in GAMS 24.2.1 with LP solver CPLEX, NLP solver CONOPT and MINLP solver ANTIGONE. In order to make the optimization study more practical, we limit the crude purchase either to be zero or within the interval [40, 200]. In such setting, integer decision variables should be introduced for each crude. The price of crude, importation and products are shown in Tables 1-3 and we use the approximate conversion 1 tonne = 7.14 barrels of crude oil for objective

function calculation. The sulfur fraction data from the crude oil assay are shown in Table 4. Other parameters can be found in Favennec (2001). The suggested model includes 687 continuous variables, 10 binary variables, 91 inequalities and 693 equalities before pre-processing. There are 303 bilinear terms and 204 signomial/trilinear terms. The solution time is limited as 24 hours to obtain an ϵ -global optimal solution, where the relative gap is $\epsilon = 1\%$. The resulting profit is 31.8 million \$/month and the purchase amounts of each crude are shown in the Table 5. The purchase recipe indicates that the high sulfur crude oil is not favorable to the profitability because the sulfur constraints may be violated and high quality products should be purchased to recover the sulfur spec. The resulting cut point temperatures are shown in the Table 6. It is not surprising that the importation is zero because the optimal solution always guarantees the market demands and quality of products due to the high penalty of importation price and hard constraints on quality indexes.

We also test different interval reduction techniques and evaluate their impacts on the solution time. Although solving the FIR and OIR for a single variable is cheap, there are a number of variables involved in the nonlinear terms and bounding all of them will be time consuming. Therefore, we only use OIR and FIR to calculate the bounds of selected variables: $x_{bot,j,i}, x_{dis,j,i}, P_{bot,j}, W_j, Y_j$, crude purchase and all flow variables related to bilinear terms. The parameter used for cut $obj^* \ge obj'$ is set as obj' = -1\$ because the refinery should make profits and then obj' = 29.86 million \$ by solving the problem and obtaining a feasible solution within 120s. Even though the same optimal feasible solution is obtained based on these approaches, the solution times are very different. The results are shown in Fig. 4 and Table 7 for comparison. It is clear that the OIR and FIR combined methodology is superior because it only takes 347s for range reduction and totally 2340s to obtain the solution with relative gap 1% whereas the pure interval analysis method takes 24 hours to reach the gap 3%. In fact, the OIR and FIR combined method is also the fastest way to find the optimal feasible solution in 1261s. The FIR based method finds this solution in 2440s and the interval analysis (IA) based method takes 6544s. It is also worthwhile to note that the ANTIGONE also does the variable bounding without using $obj^* \ge obj'$, at nodes of the branch & bound tree.

Table	1.	Crude	price	\$	/barrel
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	Crude_1	Crude ₂	Cruc	le ₃	$Crude_4$				
_	112.85	103.19	99.5	58	98.18	_			
Table 2. Product price \$/tonne									
ES95	6 PG98	JET	HGO	$_{\rm HF}$	LG	LN			
1120	1216	923	921	397	860	914			
Table 3. Importation price $f/tonne$									
S95	PG98	JET	HGO	HF	LG	LN			
240	2432	1846	1842	794	946	1005.4			

5. CONCLUSION

A simplified crude distillation unit model is developed based on the fractional index theory and embedded into a

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Table 4. Crude sulfur wt%

Fig. 4. The comparison of relative gap based on different interval reduction techniques

simplified refinery model to determine the optimal crude purchase and plant operations. Due to the existence of many non-convex terms and integer variables, the resulting mixed-integer nonlinear programming problem should be solved by integrating specific interval reduction techniques with state-of-the-art commercial software to achieve an ϵ -global optimum within a short time. An optimization study is conducted to show the effectiveness of the proposed global optimization scheme.

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