Scheduling of cracking production process with feedstocks and energy constraints

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Abstract: This paper addresses the short-term scheduling problem for the ethylene cracking process with feedstocks and energy constraints. The cracking production of ethylene is a process with units that have decaying performance, requiring periodic cleanup to restore their performance. Under the condition of limited feedstocks, the production operating mode of the cracking furnaces is to keep yields constant by continuously increasing the coil temperature. We present a hybrid MINLP/GDP formulation based on continuous-time representation for the scheduling problem over a finite time horizon. In order to solve the proposed model, which is reformulated as an MINLP model, an improved Outer Approximation algorithm with multi-generation cuts and problem-dependent integer cuts are developed to solve real large-scale problems. Numerical examples are presented to illustrate the application of the model. Based on analyzing the optimal solution and sensitivity of the model, some conclusions are obtained to provide useful suggestions for real cracking process production.

Keywords: Scheduling; Continuous Process; MINLP; GDP; Outer Approximation

1. Introduction

Ethylene is one of the most basic chemical products, and the downstream products of ethylene account for more than 70% of total petrochemical products. Until the end of 2014, Chinese ethylene production capacity was the 2nd in the world, and new plants are currently being built. There is a clear need to optimize the operations management for ethylene production processes in order to adapt to the varying market conditions and to save energy for ethylene plants.

The ethylene production is a continuous, multi-stage process that includes cracking, quenching,

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compression and separation sections, with simultaneous production of main products like propylene, hydrogen, and coproduct like hydrogasoline, C4, C9+ etc. Fig. 1 is a simplified flowchart of the ethylene process, which includes the flows of material. The feedstocks include naphtha, hydrogenation tail oils(HTO), light hydrocarbons, liquefied Petroleum Gas(LPG), etc., which also further classified, like light, heavy, sweet, sour etc. naphtha, HTO-A, HTO-B.

The cracking process is the core of the production line because it determines the yields of the final products. It is operated through parallel cracking furnaces, which have decaying performance due to the coking in the inside surface of the tubes. The yield of ethylene decreases nonlinearly, yet the yield of propylene increases with the coking. Cracking furnaces need to be cleaned up periodically in order to efficiently utilize the raw materials.

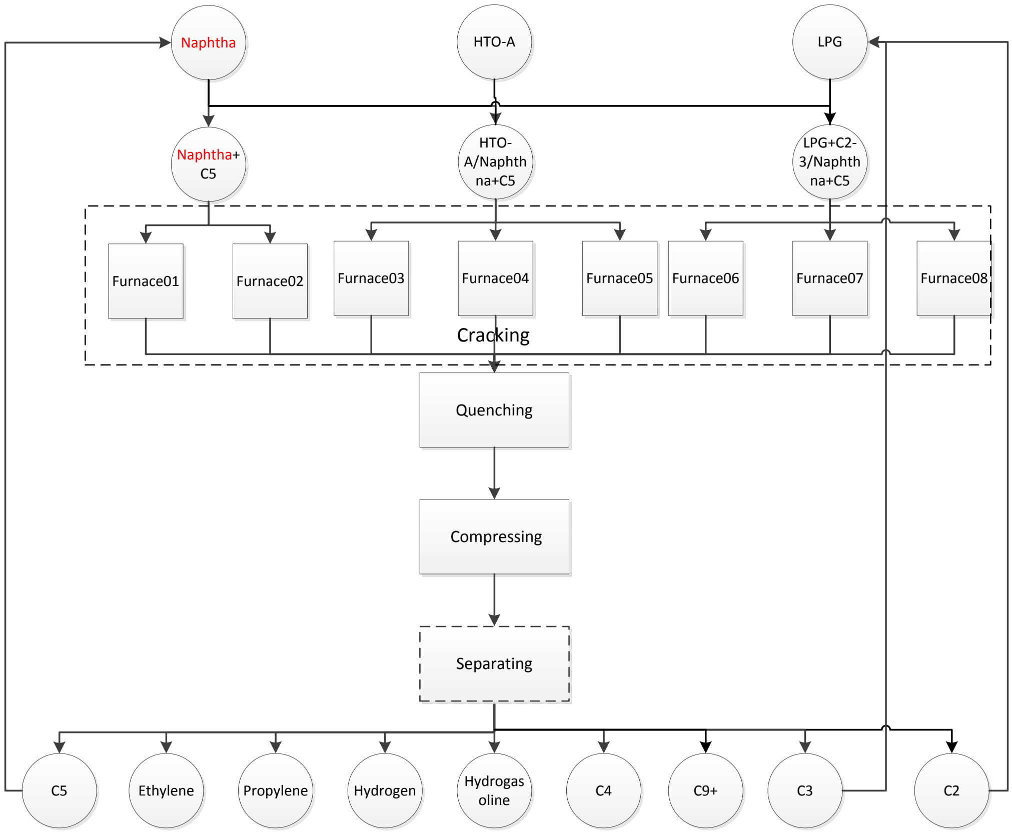

Fig. 1. Flowchart of one ethylene process

Mathematical programming techniques are a major tool for modeling optimization problems in process system engineering, especially Mixed-Integer Linear Programming (MILP) and Mixed-Integer Nonlinear Programming (MINLP) (Méndez et al.[1]).

Comparing common continuous processes in petrochemical industries, the literature on scheduling continuous process is not very extensive. For the case of unlimited raw materials and stable market demand, the cyclic scheduling mode is usually adopted to simplify the production management. Sahinidis and Grossmann[2] addressed the optimal cyclic planning for continuous parallel production lines. Pinto and Grossmann[3] addressed the cyclic scheduling problem of multistage continuous process connected by intermediate storage tanks. The two papers were seeking the tradeoff between the costs of inventory and changeover, and formulated the two problems as MINLP models using continuous time-slots, for which the problem-specific General Benders Decomposition (GBD) methods were used to solve these problems. Ierapetritou and Floudas[4] proposed the unit-specific continuous-time modeling method for short-term scheduling of general continuous and semi-continuous process. Méndez and Cerdá[5] addressed the scheduling of resource-constrained multistage parallel continuous process. Based on a predefined set of runs for all products, they optimized the sequence and times of each production run to maximize the economic output. These problems focused on the processes with no decaying performance.

The concept of campaign is used in the scheduling of batch or continuous processes, and can be regarded as the extension of the general lot-sizing problem representing the combination of several tasks and product batches. Papageorgiou and Pantelides[6] formulated the campaign planning and scheduling for general process, which simultaneously determined campaigns and campaign scheduling. The mathematical model is a large-scale MILP, and a problem-specific decomposition method was used. Oh and Karimi[7] decomposed the economic lot scheduling problem with sequence-dependent setups into two problems: campaign sizing and scheduling by defining the lot sizing production of one product as one campaign. The campaign production scheduling is incorporated with the upstream process with a relatively large output. As far as we know, there are no works reported on campaign production scheduling for continuous multi-product processes, like refineries and ethylene processes.

Alle, Papageorgiou and Pinto[8] considered cyclic production scheduling of multistage continuous plants with cleanup operations. The units decaying performance was represented through exponential decay of the product yields. Liza, Pinto and Papageorgiou[9] discussed the economic lot scheduling problem considering units with decaying performance. Those two scheduling problems dealt with single product production assuming sufficient feedstocks, which include no allocation of raw materials to units.

There are several research papers aiming at scheduling problems of real process production, like steel and ethylene. Tang et al.[10-12] focused on the scheduling problems for steelmaking continuous campaigning process for which different mathematical models are formulated, and solved with problem-specific methods for various real cases.

Jain and Grossman[13] presented a pseudo-convex MINLP formulation for cyclic scheduling of continuous parallel-process units with decaying performance. They predefined the number of subcycles for all furnaces, and assumed raw materials based on sufficient feedstocks supplies. They also proved that the length of subcycles for every feedstock on each furnace must be equal. A branch and bound method was developed for solving the model. Based on Jain and Grossman's work, Liu, Xu and Li[14] further considered the non-simultaneous cleanup operations among units with the bounds of subcycle. Schulz, Diaz and Bandoni[15] addressed the maintenance policy for cracking furnaces in an ethylene plant, considering the process operation and unit performance.

The works of Jain and Grossman[13] and Liu, Xu and Li[14] aim at the operating mode of keeping the feed rate and coil temperature constant with which the yield of ethylene continuously decreases over time. This production mode protects the furnace from premature failure, which is based on the assumption that there are sufficient raw materials to operate with high yields. For the case of limited feedstocks, the production mode that is often adopted is that the product yields are kept almost constant by reducing the feed rate and continuously increasing the coil temperature. The latter one maximizes ethylene conversion by raw materials with increasing energy-consumption. To our knowledge, there are no works reported on this operating mode for continuous processes.

In real production processes, the supply of different types of feedstocks may not only be insufficient but also it may be unbalanced. And the continuously production durations of one cracking furnace are usually from 30 to 70 days according to the statistics results. Therefore, several feedstocks are often sequentially combined to be produced between two clean-ups of a furnace in order to improve the utilization of units in the real process and avoid the unnecessary idle times of the units.

Generalized Disjunctive Programming (GDP) is a modelling method based on algebraic constraints and symbolic logic expressions (a review on MINLP and GDP modeling methods is provided by Trespalacios&Grossmann[16]). Most GDP models reported have been for process synthesis and scheduling. Solution methods for GDP include direct solution, like logic-based OA (Türkay&Grossmann[17]), and hull reformulation into MINLP (Lee&Grossmann[18]). Hooker and Osorio[19] proposed the Mixed Logic Linear Programming (MLLP) modeling method combining MILP and GDP.

Outer approximation (OA) is a general algorithm for MINLP problem, which projects the MINLP into discrete space by constructing linear supports on finite vertex points for approximating the nonlinear feasible region, and solving the approximating MILP problem to obtain the optimal solution of the primal problem (Duran&Grossmann[20], Fletcher&Leyffer[21], Grossmann[22], Floudas[23]). The drawback of OA is that with the accumulated constraints, the MILP can become very large leading to long solution times. Based on our numerical experiments of benchmark MINLP cases, obtaining lower bounds from solving the MILP can be computationally expensive. Those two aspects can result in slow convergence of OA (Su, Tang&Grossmann[24]). Su, Tang&Grossmann[24] presented three computational strategies to accelerate the convergence.

Our work aims at the short-term scheduling of parallel cracking decaying process with feedstocks and energy constraints for a fixed time horizon, as opposed to infinite horizon as in cyclic schedule. We consider the operating mode with constant product yield for each type of raw material, and perform serial cracking of different types of raw materials in one production run. We then redefine the scheduling problem, and formulate the corresponding hybrid MINLP and GDP model. The improved OA algorithm proposed in Su, Tang&Grossmann[24] is applied to solve the cases of different problem sizes with real data in efficiency.

The paper is organized as follows. A motivating example is given in Section 2. In Section 3, we describe the scheduling problem by introducing the definition of production run. Section 4 formulates the mathematical model for the problem based on continuous-time representation. Section 5 introduces an efficient improved OA algorithm to optimally solve the different cases with general input data. Comparisons are presented with DICOPT on CPU times and number of iterations. Moreover, the optimal scheduling solution and the sensitivity of the presented model based on one case are analyzed. Finally, some suggestions for real production are discussed in Section 6.

2. Motivating example

For a given ethylene plant, assume that there are 5 cracking furnaces with the supply of 7 types of raw materials. The annual output of ethylene is 120,000 tons. Considering the multiple types and small amount supplying of feedstocks, the design of the unit is fit to simultaneously crack different types of feedstocks in the same production run of one furnace. This makes it possible to allocate multiple types of raw materials in one production run of a furnace.

As the yields of the main supply raw materials are low, and the supply quantity is limited from the upstream refinery, the ethylene plant has to face the situation of insufficient and unbalanced supplies of raw materials. On the other hand, there are strong market demands for ethylene and its derivatives. The business production manager must schedule the process in order to make effective use of feedstocks with limited and unbalanced supply. The yields of ethylene and summation of ethylene and propylene are two important evaluation indictors in SINOPEC and CNPC, which are two main petrochemical corporations in China.

Therefore, most ethylene plants adopt the operating mode keeping almost constant product yields although at the expense of larger energy consumption, which is operated by periodically adjusting the value of Coil Outlet Temperature (COT) (Han&Wang [25]). Fig. 2 shows the statistics for yields of ethylene, propylene and diene of one furnace during a calibrating of COT in the given ethylene plant. By the recalibration of COT, the products yields oscillate in certain ranges until reaching relative stability.

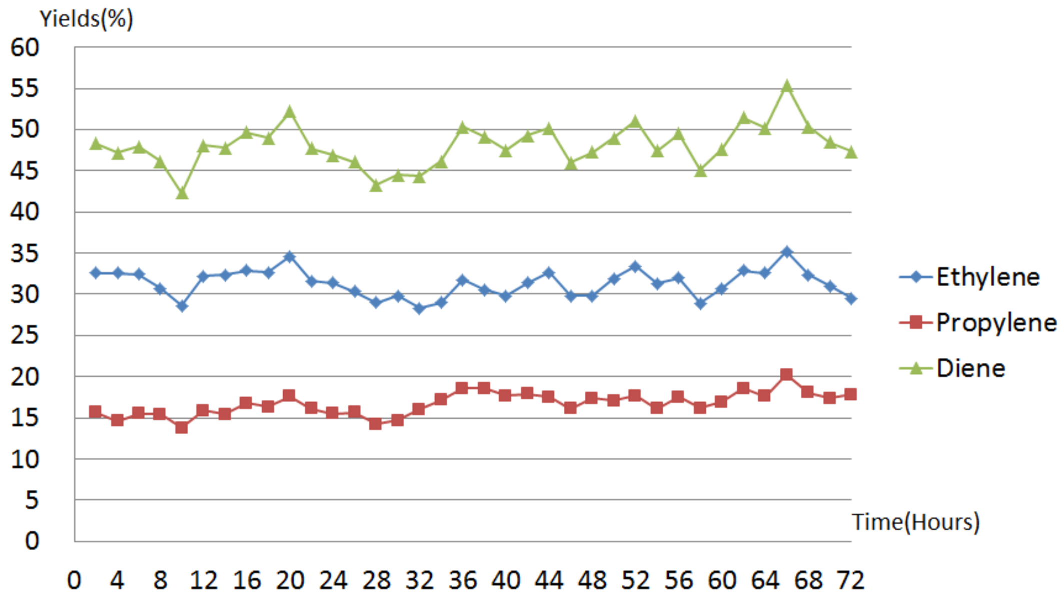

Fig. 2. Yields of ethylene, propylene and diene during calibrating COT

Zhong[26] put forward the simplified computation equation for the unit energy consumption of the ethylene cracking process as follows.

$$E = \frac{1000G + 80S + 9.2W - 92Sh}{Q} \quad (1)$$

Here, E is the unit energy consumption reduced into normal oil, G represents the unit consumption quantity of fuel gas, S is the amount of diluted steam, W is the boiler feed water, Sh is the unit production of high pressure steam, Q is the ethylene yield. The variation curve of unit energy consumption of ethylene during one production run is shown in Fig. 3. The unit energy consumption eq. 1 does not include the unit electricity consumption. Wang[27] gives the total unit energy consumption including the unit electricity consumption for ethylene plant, which ratio is about 5.7%.

Obviously, the energy consumption increases with the accumulated coke inside the furnace. Therefore, the cost of energy consumption must be considered into the ethylene production cost.

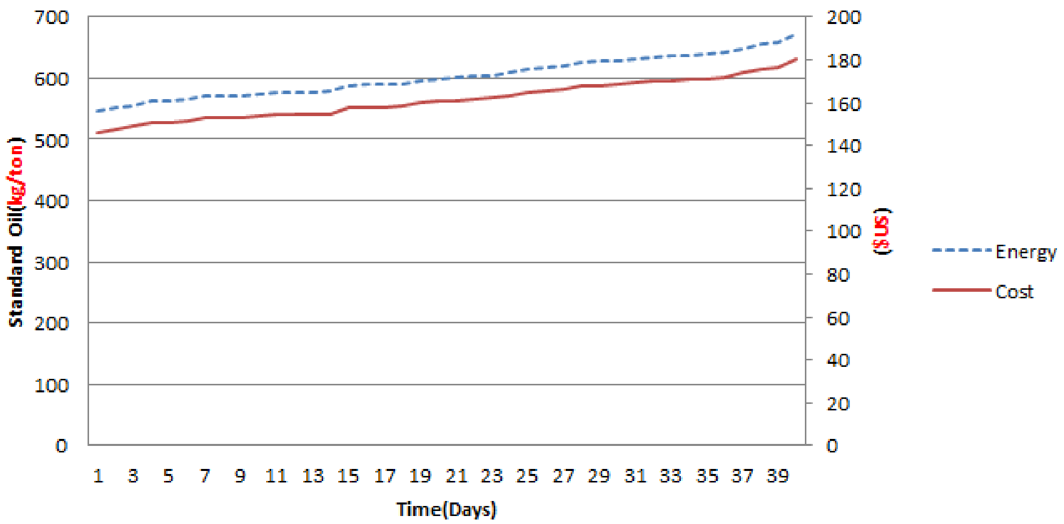

Fig. 3. Unit energy consumption statistics for ethylene production of one furnace

With the cracking process, the temperature of the tube wall rises over 1000°C. Therefore, cracking furnaces need to be cleaned periodically to remove the coke in order to fully utilize the energy, and protect the furnace. The operations of cleanup also need additional and centralized energy consumption.

Facing the situation of limited feedstock for one type of raw material, or unbalanced supplies among different types of feedstocks, scheduling of production runs is often adopted. Here, one production run consists of cracking different types of raw materials, with only one cleanup operation between adjacent production runs. The advantages of this scheduling mode are to reduce the times of unnecessary cleanup, and the feasibility to allocate the available inventory of feedstocks to each furnace. The definition of the types for raw materials is based on the yields, coking velocities and operational conditions. Therefore, the different quality of naphtha is regard as different types of feedstocks.

There are multiple tradeoffs in the production run scheduling for cracking process between the production run length and energy consumption, feedstocks supplying and production run composition, cracking operations and clean-ups. Optimization of the production run scheduling requires determining the production runs of each unit, including the start and end times, production run composition of serially cracking raw materials, and decoking sequence among units. The schedule should satisfy the mass balance of the feedstocks, non-simultaneous decoking for units, safe operation based on considering the thickness of coke and final products demand. The objective is to maximize the net profit of the cracking process over the production horizon.

3. Problem statement

In order to describe the short-term scheduling problem for parallel cracking process with multiple types of feedstocks, we first provide the definition of a production run.

We define the continuous production composed of a subsequence of operations in which no clean-up takes place for one cracking furnace as one production run. The simplest production run is continuously cracking one type of raw material during the whole production run. This case must be based on the sufficient feedstocks since the lengths of one production run vary typically from 30 to 70 days, and the cracking production is continuously operating with typically a flowrate of 100~200 ton/d. For the case of limited raw materials, different types of feedstocks are sequentially cracked in one production run. This production run scheduling is shown in Fig. 4 with almost constant product yield for one raw material. Fig. 5 shows the inventory variations of feedstocks for different production runs. Obviously, the flexible operation can decrease the supply and storage level of the feedstocks, and reduce the pressure of feedstocks shortage. In this paper, we assume that the general production run consists of cracking few types of feedstocks as shown in Fig. 4.

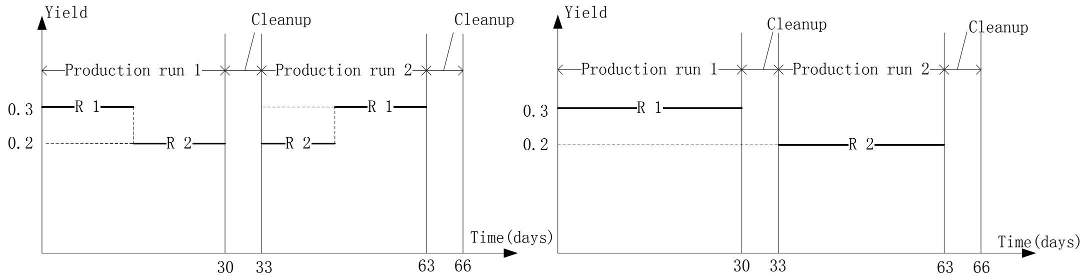

Fig. 4. Scheduling of two production-runs for one furnace

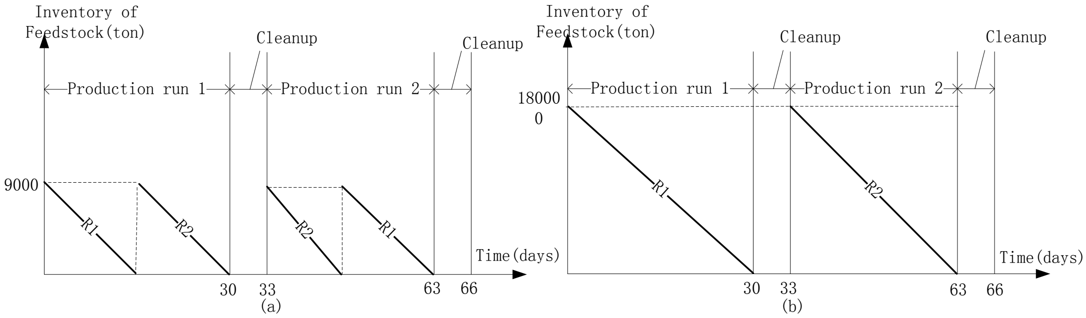

Fig. 5. Inventory curves of the raw materials for scheduling of different type of production runs

The scheduling for cracking process with feedstocks and energy constraints is described as follows.

Given:

(1) a fixed time horizon of production operation H

(2) a set of feedstocks $i \in I$ with initial inventory quantity at the beginning of the horizon and average supply rates during the horizon

(3) a set of cracking furnaces $j \in J$

(4) a set of yield parameters c_{ijl} of each feedstock i for main final products l on each cracking furnace j

(5) a set of demands Q_l for the final products $l \in L$

(6) a set of prices P_l for main final products, costs for feedstocks Cr_i and inventory Cv_i, costs of energy consumption Ce_j

(7) a set of decoking parameters γ_{ij} for each raw material on every cracking furnace

(8) operation constraints on the length of production runs, continuously cracking duration for one type of feedstock, limitation on coking thickness, non-simultaneously decoking operations among

furnaces.

Determine:

(1) active production runs for each furnace

(2) active sequence of cracking feedstocks in each active production run

(3) composition and duration of each active production run on every unit

(3) coking thickness of each production run and cleanup times

(4) inventory quantity of each feedstock at the end of each production run for all units

The objective is to maximize the net profit over the fixed production horizon *H*, which is the income of the total final products minus the cost of cracking total feedstocks, inventory, energy consumption on cracking and decoking operations.

This optimization problem involves a complex tradeoff between production and cleanup operations for continuous production process with multiple types of input flows, meeting the mass balance of feedstocks, the decoking limitations and the demand of final products.

The following assumptions are made:

(A1) If one type of feedstock is allocated to one production run, its cracking process is continuous in the production run.

(A2) There is only one type of feedstock flowing into one furnace at one time, and the flowrate of one feed stocks to one furnace is constant.

(A3) According to the statistic coking periods of all types of feedstocks, we estimate the average coking rate of each feedstock. The coke thickness is a linear function of processing time, which equals to the product of the coking rate and processing time.

(A4) Decoking duration is fixed for one furnace, which is much less than the duration of one production run. Therefore, the decoking operations for one production run of any furnace must be completed before the cleanup of the next production run. There is no crossover among decoking operations of different furnace production runs.

4. Mathematical formulation

Considering the independent operations of the units and the operational continuity of each unit, the unit-specific event-based continuous-time representation is adopted to formulate the timings and compositions of production runs, cleaning operations for each furnace (Janak, Lin&Floudas[28]). Here, we define the event as the beginning of cracking one type of feedstock in one active production run. According to the length of production horizon and limitation on production run length, we prespecify the number of cracking production runs for each furnace.

The model involves allocation and sequencing variables, and relationships among the production runs of different furnaces. Therefore, we adopt the hybrid MINLP and GDP modeling methods to describe the production run scheduling problem, and formulate some constraints of the mathematical model by introducing necessary logic variables.

In particular, the inventory quantity of feedstocks is specified at the end time of each production run for every furnace in order to accurately satisfy mass balance during whole production horizon.

Nomenclature

Indices and sets

$i = 1, \cdots, I$ feedstocks/raw materials

$j = 1, \cdots, J$ furnaces

$k = 1, \cdots, K$ production runs

$l = 1, \cdots, L$ final products

$s = 1, \cdots, S$ event points in production runs

Parameters

c_{ijl} yield factor of product *l* for feedstock *i* cracked in furnace *j*

Cc_j unit decoking cost of furnace *j*

Ce_j unit energy consuming of the furnace *j*

$Cg_{ii'}$ changeover cost between the feed *i* and feed *i'*

Cr_i cost of the raw material *i*

Cv_i unit inventory cost of raw material *i*

Cy_l unit inventory cost of the final product *l*

F_{ij} processing rate of the feed *i* cracked in the furnace *j*

H time horizon for scheduling

$I0_i$ initial inventory quantity of the raw material *i*

Is_{ik} safe inventory quantity of the raw material *i* in the *kth* production run

P_l price of the product *l*

Q_l demand quantity of final product *l*

R_{ij} average coefficient of coking rate of the feed *i* cracked in the furnace *j*

Sf_i average supply rate of the raw material *i*

T_j^L lower bound of feedstock changeover in the furnace *j*

T_j^U upper bound of one production run in the furnace *j*

TH_j thickness limitation of coking for furnace *j*

β_{ij} cracking cost coefficient of raw material *i* in furnace *j*

γ_{ij} decoking cost coefficient of raw material *i* in furnace *j*

$\lambda_{ii'}$ dependent coking factor between the feed *i* and feed *i'*

τ_j decoking duration of furnace *j*

Binary/Boolean Variables

x_{ijks} binary variable: 1 if feed *i* is processed at the *sth* event point of *kth* production run in furnace *j*, else 0

$\tilde{x}_{ijk}$ binary variable: 1 if feed *i* is processed at the *kth* production run in furnace *j*, else 0

$\hat{x}_{jk}$ binary variable: 1 if the *kth* production run in furnace *j* is active, else 0

$\tilde{X}_{ijk}$ boolean variable: true if feed *i* is processed at the *kth* production run in furnace *j*, else false

$\hat{X}_{jk}$ boolean variable: true if the *kth* production run in furnace *j* is active, else false

$y_{ii'jk}$ binary variable: 1 if feed *i* is processed just before feed *i'* at the *kth* production run in furnace *j*, else 0

$Y_{ii'jk}$ boolean variable: true if feed *i* is processed just before feed *i'* at the *kth* production run in furnace *j*, else false

$z_{jj'k}$ binary variable: 1 if the *kth* decoking of furnace *j* is before the *kth* decoking of furnace *j'*, else 0 if the *kth* decoking of furnace *j* is behind the *kth* decoking of furnace *j'*

$Z_{jj'k}$ boolean variable: true if the *kth* decoking of furnace *j* is before the *kth* decoking of furnace *j'*, else false, if the *kth* decoking of furnace *j* is behind the *kth* decoking of furnace *j'*

Continuous Variables

$Cg_{ii'jk}$ semicontinuous variable, changeover cost between the feed *i* and feed *i'* in the *kth* production run of furnace *j*

I_{ijk} continuous variable, inventory amount of feed *i* at the ending time of production run *k* for furnace *j*

Ip_{lk} continuous variable, inventory amount of final product *l* at the average time of production run *k*

p_{jk} continuous variable, processing duration of the *kth* production run of furnace *j*

ps_{ijk} continuous variable, processing duration of feed *i* in the *kth* production run of furnace *j*

ts_{jk} continuous variable, beginning time of the *kth* production run of furnace *j*

$\lambda_{ii'jk}$ semicontinuous variable, dependent coking factor between the feed *i* and feed *i'* in the *kth* production run of furnace *j*

τ_{jk} continuous variable, decoking duration of *kth* production run of furnace *j*

Objective function（maximize net profit）

The objective of the short-term scheduling problem for a given time horizon is to maximize the net profit, which is defined as the total income from the values of final products, minus the cost of raw materials, inventory of feedstock and final products, changeover of feedstocks, energy consumption of production and decoking.

$$
\begin{aligned}
Max\ w = & \sum_{l=1}^{L}\left(P_l \cdot Ip_{lK} - \sum_{k=1}^{K} Cy_l \cdot Ip_{lk} \right) - \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}(Cr_i \cdot F_{ij} \cdot ps_{ijk} + \sum_{i' \neq i}^{I} Cg_{ii'jk}) \\
& - \sum_{i=1}^{I}\sum_{k=1}^{K} Cv_i \cdot I_{ijk}\Big|_{j=1} - \sum_{j=1}^{J}\sum_{k=1}^{K}(Ce_j \cdot e^{\sum_i^I \beta_{ij} \cdot ps_{ijk}} + Cc_j \cdot \sum_i^I \left(R_{ij} \cdot ps_{ijk} \right)^{\gamma_{ij}})
\end{aligned} \tag{2}
$$

Here, the first term in the sum represents the total products value minus the inventory cost of final products, the second term in the sum represents the cost of processed feedstocks plus the changeover cost in one production run, the third term represents the inventory cost of feedstock, the last term in the sum includes the energy consumption cost of cracking process and the decoking cost, which are the nonlinear exponential functions of processing durations according to the fitted curves of real data. The inventory of the feedstocks is specified with one of the units, like furnace 1.

Allocation constraints

At most one kind of feedstock *i* is allocated to one event point *s* one production run *k* for one furnace *j*.

$$\sum_{i=1}^{I} x_{ijks} \leq 1 \quad \forall j,k,s \tag{3}$$

The feedstock *i* must be either processed continuously in the *kth* production run of furnace *j* an event in *S*, or otherwise, it is not processed.

$$\sum_{s=1}^{S} x_{ijks} \leq 1 \quad \forall i,j,k \tag{4}$$

The active number of production runs for each furnace is same in order to balance the working load among units.

$$\sum_{i=1}^{I}\sum_{k=1}^{K} x_{ijks} = \sum_{i=1}^{I}\sum_{k=1}^{K} x_{ij+1ks} \quad \forall j < J, s=1 \tag{5}$$

The active events are always adjacent and in the front of the set of events for one active production run. Similarly, the active production run is always adjacent, which also means the idle production runs are adjacent and in the end of the production run sequence.

$$\sum_{i=1}^{I} x_{ijks} \geq \sum_{i=1}^{I} x_{ijks+1} \quad \forall j,k,s < S \tag{6}$$

$$\sum_{i=1}^{I} x_{ijks} \geq \sum_{i=1}^{I} x_{ijk+1s} \quad \forall j, k < K, s = 1 \tag{7}$$

All the types of feedstocks must be processed at least once during the whole time horizon.

$$\sum_{j=1}^{J} \sum_{k=1}^{K} \sum_{s=1}^{S} x_{ijks} \geq 1 \quad \forall i \tag{8}$$

The relationship equations between the allocation and sequence variables for one production run of one furnace are as follows.

$$y_{ii'jk} \leq x_{ijks} \quad \forall i \neq i', j, k, s < S \tag{9}$$

$$y_{ii'jk} \leq x_{i'jks+1} \quad \forall i \neq i', j, k, s < S \tag{10}$$

$$y_{ii'jk} \geq x_{ijks} + x_{i'jks+1} - 1 \quad \forall i \neq i', j, k, s < S \tag{11}$$

We further introduce two tighter constraints for the allocation and sequence variables in one production run instead of the constraints eq. (9) and (10) (Sahinidis and Grossmann[2]).

$$\sum_{i' \neq i}^{I} y_{ii'jk} \leq x_{ijks} \quad \forall i, j, k, s < S \tag{9'}$$

$$\sum_{i \neq i'}^{I} y_{ii'jk} = x_{i'jks+1} \quad \forall i', j, k, s < S \tag{10'}$$

The decoking sequence constraint of the furnaces is as follows. For one production run $k < K$, the decoking operation of furnace *j* is either before one of furnace *j'*, or behind of it.

$$z_{jj'k} + z_{j'jk} \leq 1 \quad \forall j \neq j', k < K \tag{12}$$

Timing constraints

The continuous processing time of feed *i* lies within practically allowable minimum and maximum values from the viewpoint of management and operation. If the feed *i* is not allocated to the *kth* production run of furnace *j*, the processing time is zero. Here, we assume the processing time of one feed does not exceed the upper bound of continuous processing time of furnace, and must be greater or equal to the shortest operating time to avoid frequent changeovers.

$$\tilde{x}_{ijk} = \sum_{s=1}^{S} x_{ijks} \quad \forall i, j, k \tag{13}$$

$$\begin{bmatrix} \tilde{X}_{ijk} \\ T_j^L \le ps_{ijk} \le T_j^U \end{bmatrix} \vee \begin{bmatrix} \neg\tilde{X}_{ijk} \\ ps_{ijk} = 0 \end{bmatrix} \quad \forall i, j, k \tag{14}$$

The sum of processing times for the allocated feedstocks in each production run equals to the total length of production run for one furnace *j*:

$$\sum_{i=1}^{I} ps_{ijk} = p_{jk} \quad \forall j, k \tag{15}$$

If one production run is active on one furnace, the length of the production run is within the upper bound, which is set based on operating limits. We determine whether one production run is active or not through whether the first event of the production run is active or not. The following beginning time of production run is longer than the completion time of forward production run, which is the beginning time plus processing time and decoking time.

$$\hat{x}_{jk} = \sum_{i}^{I} x_{ijks} \quad \forall j, k, s = 1 \tag{16}$$

$$\begin{bmatrix} \hat{X}_{jk} \\ p_{jk} \le T_j^U \\ \tau_{jk} = \tau_j \\ ts_{jk} + p_{jk} + \tau_{jk} \le ts_{jk+1} \end{bmatrix} \vee \begin{bmatrix} \neg\hat{X}_{jk} \\ p_{jk} = 0 \\ \tau_{jk} = 0 \\ ts_{jk} \le ts_{jk+1} \end{bmatrix} \quad \forall j, k < K \tag{17}$$

The bounds of the start times ts_{jk} and the end times for all furnaces are defined. Assume that all cracking units are clean at the beginning of the time horizon, and simultaneous decoking at the last production run for all units is feasible.

$$ts_{j1} = 0 \quad \forall j \tag{18}$$

$$\begin{bmatrix} \hat{X}_{jk} \\ p_{jk} \le T_j^U \\ \tau_{jk} = \tau_j \\ ts_{jk} + p_{jk} + \tau_{jk} \le H \end{bmatrix} \vee \begin{bmatrix} \neg\hat{X}_{jk} \\ p_{jk} = 0 \\ \tau_{jk} = 0 \\ ts_{jk} \le H \end{bmatrix} \quad \forall j, k = K \tag{19}$$

There is no crossover between different production runs for any furnace. That is, the beginning time of the *kth* production run for one unit must be earlier than the beginning time of the *k+1th* production run for any units. Similarly, the same applies to the end times of production runs.

$$ts_{jk} \le ts_{j'k+1} \quad \forall j \ne j', k < K \tag{20}$$

$$ts_{jk} + p_{jk} \le ts_{j'k+1} + p_{j'k+1} \quad \forall j \ne j', k < K \tag{21}$$

Decoking constraints

If there are feedstocks changeovers in one production run, this would influence the accumulated coke thickness, and increase the changeover cost of production.

$$\begin{bmatrix} Y_{ii'jk} \\ \lambda_{ii'jk} = \lambda_{ii'} \\ Cg_{ii'jk} = Cg_{ii'} \end{bmatrix} \vee \begin{bmatrix} \neg Y_{ii'jk} \\ \lambda_{ii'jk} = 0 \\ Cg_{ii'jk} = 0 \end{bmatrix} \quad \forall i \neq i', j, k \tag{22}$$

The accumulated coke thickness of one production run for one furnace should not exceed the maximum limitation to protect the equipment.

$$\sum_{i=1}^{I} (R_{ij} \cdot ps_{ijk} + \sum_{i' \neq i}^{I} \lambda_{ii'jk}) \leq TH_j \quad \forall j, k \tag{23}$$

The non-simultaneous decoking constraints for all furnaces are presented as follows except for the last time of decoking.

$$\begin{bmatrix} Z_{jj'k} \\ ts_{jk+1} + \tau_{j'k} \leq ts_{j'k+1} \end{bmatrix} \vee \begin{bmatrix} \neg Z_{jj'k} \\ ts_{j'k+1} + \tau_{jk} \leq ts_{jk+1} \end{bmatrix} \quad \forall j \neq j', k < K \tag{24}$$

Inventory balances and demand constraints

The inventory of raw material *i* at the end time of production run *k* for unit *j* is equal to the quantity of initial stock adding the supplying quantity minus the total processing quantity of all processing units until this time, which is the inventory balance constraint of the feedstocks.

As the end times of one production run for each unit are different, the variable I_{ijk} is introduced to describe the inventory at the different end times of the units for one type of feedstock.

$$I_{ijk} = I0_i + Sf_i \cdot \left(ts_{jk} + p_{jk}\right) - \sum_{j'}^{J} \sum_{k'}^{k} F_{ij'} \cdot ps_{ij'k'} \quad \forall i, j, k \tag{25}$$

In order to ensure continuous operation of the cracking units, the safety inventory constraint must be obeyed.

$$I_{ijk} \geq Is_{ik} \quad \forall i, j, k \tag{26}$$

The inventory quantity of the final products is computed as follows.

$$Ip_{lk} = \sum_{i}^{I} \sum_{j}^{J} \sum_{k'}^{k} c_{ijl} \cdot F_{ij} \cdot ps_{ijk} \quad \forall l, k \tag{27}$$

The demands of the final products l must be satisfied at the end of the time horizon.

$$\sum_{k=1}^{K} Ip_{lk} \geq Q_l \quad \forall l \tag{28}$$

In general, the proposed mathematical formulation corresponds to a hybrid MINLP/GDP model with nonconvex objective function and linear constraints. However, the hybrid formulation is convex under some conditions, specifically when the power parameters of decoking cost γ_{ij} are not less than 1. Otherwise, the formulation of production run scheduling for cracking process is nonconvex.

5. Solution method and numerical experiments

In this section, we firstly transform the proposed hybrid MINLP/GDP into an MINLP, and introduce the improved OA solution method with modified integer cuts. The 12 numerical examples are then solved with DICOPT and improved OA. Finally, the optimal scheduling and the sensitivity of the proposed model based on one example are analyzed.

5.1. Reformulation and solution method

The disjunctive constraints eq. 14, 17, 19, 22 and 24 are reformulated using convex-hull reformulations by introducing disaggregated variables (Lee&Grossmann[18]) as shown in the Appendix. Therefore, the proposed model is reformulated into an MINLP model, which can in principle be solved directly by MINLP solvers.

Considering the nature of the proposed model with many discrete variables, we introduce the improved strategy of Multi-generation Cuts for OA (MC-OA) aiming at addressing MINLP solution difficulties (Su, Tang&Grossmann[24]). The reformulated MINLP is decomposed into the subproblems of NLPs with fixed allocation and sequence variables (x, y, z) and the master problem of MILP linearizing cumulative hyperplanes of nonlinear objective function obtained at the optimal solutions of subproblems. By the parallel solution of a specified number |M| of NLPs in one iteration of MC-OA, we obtain multiple feasible production run schedules with the lower bounds of the total income. The master problem of MILP is updated by adding the multiple linear cuts on those solutions of NLPs, which solution is to get a set of new allocation and sequence variables, and a new upper bound of the primal objective function.

Moreover, considering the separable nature of the discrete variables in the proposed model, integer cuts are modified as follows

$$\sum_{(i,j,k,s)\in B^{xit}} x_{ijks} - \sum_{(i,j,k,s)\in N^{xit}} x_{ijks} \le \left|B^{xit}\right| - 1 \quad \forall it \tag{29}$$

$$\sum_{(j,j',k)\in B^{zit}} z_{jj'k} - \sum_{(j,j',k)\in N^{zit}} z_{jj'k} \le \left|B^{zit}\right| - 1 \quad \forall it \tag{30}$$

Here *it* means the it^{th} iteration of the OA method, B^{*it} means the set in which the binary variables equal to 1, and N^{*it} means the set in which the binary variables equal to 0 in the it^{th} iteration.

The modified integer cuts reduce the feasible space of the discrete variables to accelerate the convergence of MC-OA.

The procedure of MC-OA with the modified integer cuts for the reformulated MINLP model is as follows.

Initialization: set $n = 0, UBD = \infty$, / specify |M|

(1) Solve the relaxed MINLP without integer limitation, let the solution of the continuous variables in nonlinear terms be $\left(ps^n\right)$.

(2) Linearize the nonlinear terms about $\left(ps_{ijk}^n\right)$ for the MINLP. Solve the relaxed MILP. Let the multiple solutions be $\left(x^{n+1,m}, y^{n+1,m}, z^{n+1,m}\right), m \in M$.

Repeat

(1) Solve the parallel subproblem NLPs($x^{n+1,m}, y^{n+1,m}, z^{n+1,m}$), or the feasible problem F($x^{n+1,m}, y^{n+1,m}, z^{n+1,m}$), and let the solutions be $ps^{n,m}$.

(2) IF (NLP is feasible and $w^{n,m} < UBD$) THEN

Update current best solution by setting $UBD = w^{n,m}$.

(3) Derive the multiple linear supporting cuts about $\left(ps^{n,m}\right)$, also derive the separable integer cuts about $\left(x^{n+1,m}, z^{n+1,m}\right), m \in M$ and add to the current relaxation master problem MILP.

(4) Solve the current MILP, getting a set of new integer assignment. Set $n = n+1$.

UNTIL (Termination conditions)

5.2. Numerical experiments

In this section, 12 different numerical examples are considered with different number of feedstocks and furnace based on the presented formulation in Section 4. The detailed data are from the real production processes and the references (Jain&Grossmann[13], Liu, Xu&Li[14], Han &Wang[25], Wang[27]). The production time horizon is 70~110 days. The final products considered are only ethylene and propylene. The number of feedstocks ranges from 2 to 7, and the number of furnaces from 2 to 5. The preset number of production runs is from 5 to 8. We limit the maximum number of feedstocks in one production run to 2 in order to control the problem size, which also satisfies the operational demand. Other data are listed in Table 1. It should be noted that for the parameters γ_{ij}, which determinates the convexity of the proposed MINLP, are all greater than 1. Therefore, the computational cases are all convex MLNLPs.

Table 1. Ranges of parameters for the production run scheduling formulation[13,14,25,27]

Parameters	c_{ijl}	F_{ij} (ton/d)	Is_{ik} (ton)	Q_l (10^3ton)	R_{ij}	Sf_i (ton/d)	$\lambda_{ii'}$	γ_{ij}
Range	0.06~0.63	40~220	500~1000	2.8~176	0.06~0.12	70~130	-0.2~0.2	2~3

The production run scheduling formulation was implemented in GAMS 24.2 (Brooke et al.[29]). The computer operating system is Windows 7, and Intel Core 2 Duo, CPU 2.6 GHz and 4 GB of RAM. The solutions of the NLP problems are obtained using the CONOPT3 solver, and the solutions of the MILP problems are obtained using CPLEX12.6. The stopping criterion of the DICOPT solver is set to the option one in which the objective of the last MIP master problem is worse than the best NLP solution found, namely a "crossover" occurred, and the other is maximum major iterations. The major iteration limit is 50. The same convergence rules are set for MC-OA.

Illustration case

The illustration case is one with 3 types of feedstocks, 2 furnaces and a time horizon of 110 days. Based on the same data, we present two optimal scheduling results with one and two event points (|S|), which are shown in Fig. 6 and Fig. 7.

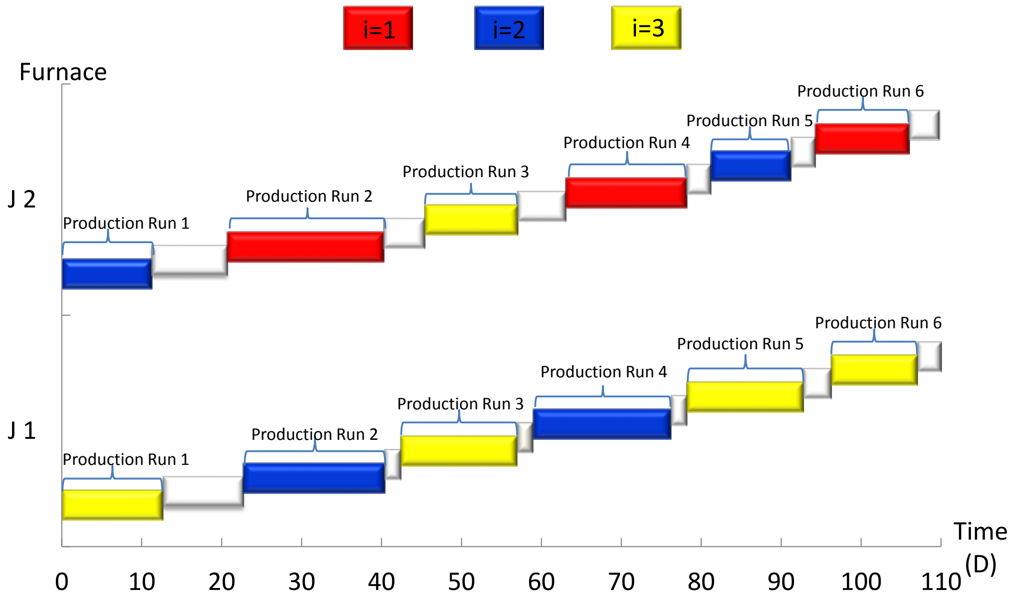

Fig. 6. Optimal scheduling for the illustrated case with limitation of $|S| = 1$

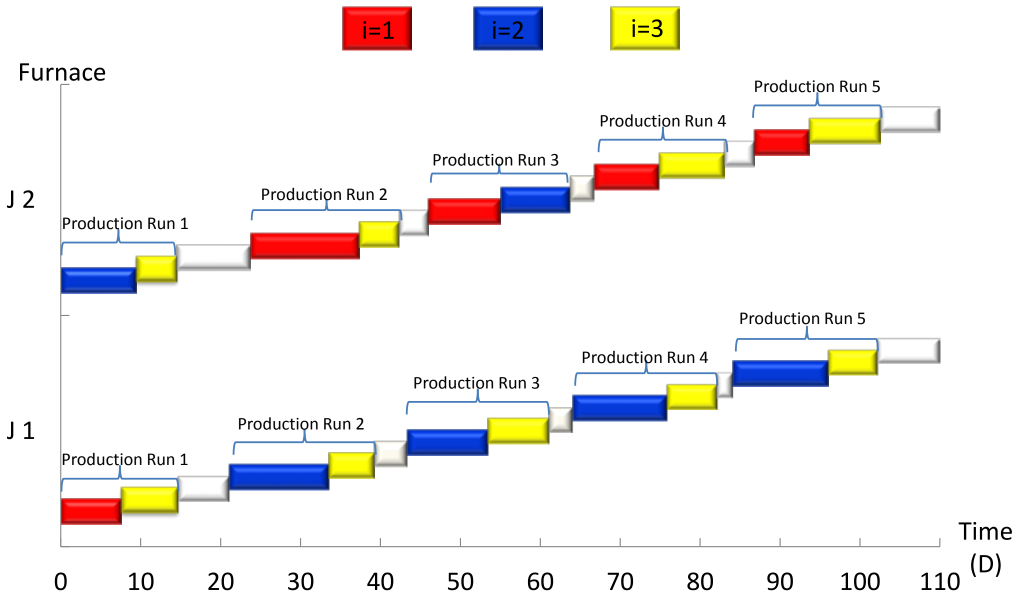

Fig. 7. Optimal scheduling for the illustrated case with limitation of $|S| = 2$

For the case with $|S| = 1$, the active number of production run is 6, more than the case with $|S| = 2$. The operation mode in Fig. 6 involves shorter production runs and more cleanups than the operation mode in Fig. 7. And the total product quantity of ethylene and propylene in Fig. 6 is 16541.7ton, compared with 17415.7ton in Fig. 7. The optimal net profit of the scheduling in Fig. 6 is 103 million USD compared with the optimal net profit of the scheduling in Fig. 7 is 118 million USD, which is increased 15.2%. In addition, we solve the case with the event point $|S| = 3$, which result is equal to the case of $|S| = 2$. That means it is not beneficial for the objective value with more event points, considering the changeover cost.

The active number of production runs in Fig. 7 is 5, which are all composed of two types of cracked feedstocks. When the initial inventory of feedstocks is small, the supplying rates of feedstocks determine the lengths of production runs and compositions of the scheduling. The cracking sequence in one production run is determined by the dependent coking factor between the two types of feedstocks. The idle time of the furnaces occur at the beginning and end of the time horizon, which can be explained by the fact that the accumulated inventory of feedstocks at the beginning and the left time of H is not enough. The workload on two units is almost balanced as it is expected.

The ratio of energy consumption cost to the total cost here is 9.12%. If we ignore the energy cost in the proposed model for the case $|S| = 2$, we get a new scheduling illustrated in Fig. 8. The result is similar to the Fig. 7 which is also 5 production runs with multiple feedstocks in one run. The duration and composition of scheduling in Fig. 8 is more cyclic than Fig. 7, which are only dependent on the limitation of coke thickness. In Fig.8, the coke thicknesses reach to the limitation for every production run of each furnace. Without consideration of energy cost, the optimal scheduling is only determined by the material balance of feedstocks and the limitation of coke thickness.

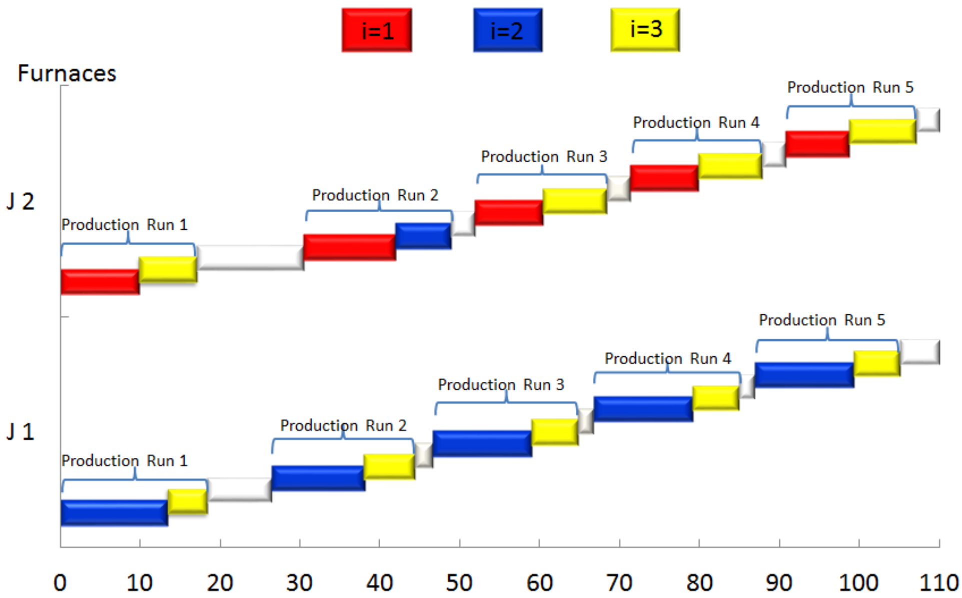

Fig. 8. Optimal scheduling for the illustrated case $|S| = 2$ without energy cost

Computational results

The computational statistics are shown in Table 2 including problem size, relaxed and optimal objective values, number of iterations and CPU times of DICOPT and MC-OA.

Table 2. Statistics computational results for the proposed model with DICOPT and MC-OA[a]

No. J	No. I	No. K	No. Bin./Cont./Cons.	RMINLP Value	DICOPT Iters	DICOPT CPU(s)	DICOPT Opt.	MC-OA Iters.	MC-OA CPU(s)	MC-OA Opt.	Gap %[b]
2	2	8	176/257/767	120.8	3	1.7	118.2	3	3.2	118.2	2.1
2	3	8	288/417/1152	106.4	50	97.3	102.7	6	19.7	102.8	3.5
2	4	8	432/641/1665	125.0	50	231.8	113.6	10	82.2	114.0	9.1
3	3	8	456/617/1852	153.3	50	716.5	146.0	17	241.6	145.3	4.8
3	4	6	504/715/1963	101.6	50	1095.1	95.4	34	262.0	95.2	6.1
3	5	6	702/1039/2684	100.9	50	2123.7	92.2	23	383.2	91.2	8.6
4	3	6	480/613/1974	146.9	50	969.3	141.1	50	232.7	141.3	3.8
4	4	6	696/949/2743	167.7	50	26268.8	158.0	50	1584.2	158.2	5.7
4	5	6	960/1381/3704	154.8	50	33728.1	149.0	50	4074.2	149.0	3.8
4	6	5	1060/1591/4043	111.5	50	12869.3	106.7	50	3923.7	106.8	4.3
4	7	5	1360/2111/5164	94.0	50	10447.5	86.9	50	740.5	86.5	7.6
5	3	5	525/636/2181	104.2	50	1795.8	96.1	50	412.4	96.1	7.8

[a] The parameters of CPLEX solution pool are that SolnPoolIntensity is set 4, SolnPoolPop is set 1, SolnPoolCapacity is set 3, SolnPoolReplace is set 1.

[b] The optimal solutions are the best lower bound objective function when the method terminates, with units of million USD. The gaps mean the relative gaps between the relaxed objective function values and the optimal one.

As there are 4-index discrete variables and continuous variables in the proposed model, the problem-size is somewhat large for even small numbers of units and feedstocks. When we solve the reformulated MINLP model using DICOPT, the convergence of the solution is slow as the problem size increases. The solution of the master problem of OA is especially time consuming at the beginning of the major iterations for even small cases. The upper bounds from the master problem are almost unchanged, and the lower bound changes slowly. Therefore, there is only one case in which DICOPT terminates when crossover occurs. Compared with DICOPT, the improved MC-OA (Su, Tang&Grossmann[24]) obtains almost the same quality of solutions with fewer iterations and smaller CPU times.

The range of relative gaps between the objective function value of RMINLP and optimum are between 2.1% and 9.1%, which means that the formulation is tight. The reasons that the solution methods converge slowly is that there are many alternative solutions that are equivalent, and the approximate master problems are large.

5.3. Sensitivity analysis

The optimal objective function values are not monotonic with the number of furnace for the length of scheduling horizon and the feed rates for different cases are different. For the example of 4 furnaces and 6 types of feedstocks with time horizon of 110 days, we demonstrate the optimal production run scheduling solution in Fig. 9, and the averaged inventory quantity of each feedstock in the end of each production run in Fig. 10.

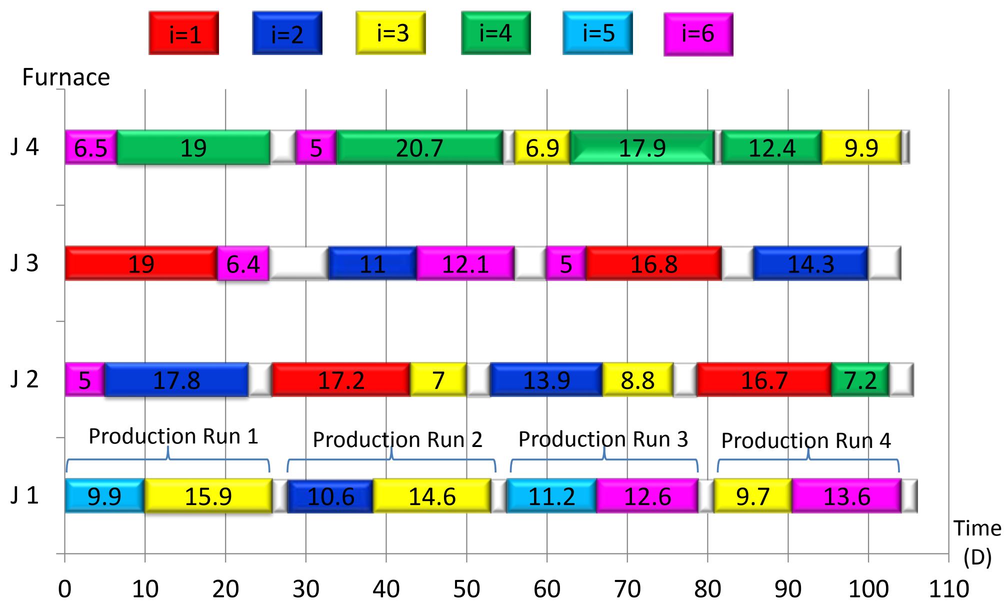

Fig. 9. Optimal scheduling for the case with 6 kind of feedstocks and 4 cracking furnace

According to the scheduling results, the composition of a production run for one furnace changes with the inventory quantity of each feedstock. Multiple feedstocks in one production run for one furnace occurs when feedstocks are insufficient; otherwise, single feedstocks are used when raw materials are sufficient. The production run scheduling solution demonstrates that dominated yield or coking rate of each feedstock determines the allocation between feedstocks and furnaces. The feedstocks with worse product yields or high coking rates are chosen to satisfy the mass balance and the continuity of the cracking process. Moreover, the optimal production run scheduling keeps some regularity, which is easy to operate in real production. We find that the inventory of feedstock 5 is the most abundant among all feedstock at the end of the horizon, which explains that the lowest product yield is of feedstock 5.

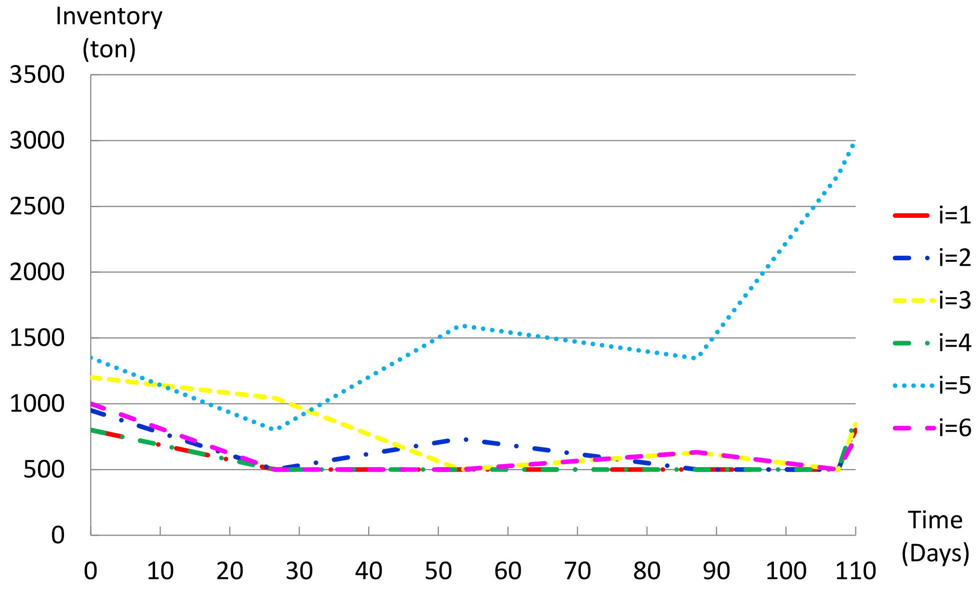

Fig. 10. Inventory curves of the feedstocks for the case with 6 kind of feedstocks and 4 cracking furnace

In this scheduling problem, the key factors influencing the scheduling result include limitation of coke thickness and production run length, which are partly set artificially.

In the case with 6 feedstocks and 4 furnaces, we change the four types of related data to investigate the sensitivity of the proposed model. Four scenarios are set in Table 3 with changes in the range of production run lengths, limitation of coke thickness and energy cost. The evaluated targets are shown including the net profit, total products quantity and number of active production runs.

Table 3. Summary of the three scenarios for the case with 6 feedstocks and 4 furnaces

Scenarios	Basic Scenario	Scenario1	Scenario2	Scenario3	Scenario4
maximal production run length (days)	28	30	28	28	28
minimal production run length (days)	5	5	8	5	5
limitation of coke thickness (cm)	[2.0, 2.5]	[2.0, 2.5]	[2.0, 2.5]	[2.5, 3.0]	[2.0, 2.5]
cost of energy consumption	Y	Y	Y	Y	N
total products quantity (ton)	34,933	34,859	34,855	34,818	36,450
no. of active production run	4	4	4	4	4
optimal net profit (million USD)	106.7	106.8	105.5	106.5	126.8

For the former 4 cases, the basic scenario obtains the maximum products amount, and scenario 1 yields the maximum net profit. The net profit of the scenario 2 and the total products quantity of the scenario 3 are the lowest. In general, the variations for the former 3 scenarios are not very large. The scenario 4 without the consideration of energy cost obtains more products amount and the net profit than the former 4 cases. Based on the result of the scenario 4, energy cost influences the duration of production run. In addition, the computation iterations and CPU time of the scenario 4 is 2 iterations and 52.7 sec. using DICOPT solver, compared with 50 iterations and 12869.3 sec. of other iterations. Therefore, it becomes more complicated with the consideration of energy cost.

6. Conclusion

In this paper, we have considered the new operating mode of ethylene production process, where the target is to ensure constant final product yields with higher producing cost under limitation of raw materials and energy consumption. The short-term scheduling problem for the cracking process was introduced with the definition of production run to describe the cracking process. The mass balance of feedstocks on each production run, coking factor and non-simultaneous decoking operations for each equipment were considered.

Based on continuous-time description, the hybrid MINLP/GDP formulation was presented, which includes nonlinear objective function, disjunctive and linear constraints. Through the convex hull reformulation, the model was transformed into an MINLP. In order to solve the MINLP model efficiently, we applied the improved multi-generation cuts for OA (Su, Tang&Grossmann[24]) with problem-specific integer cuts to solve the formulated production run scheduling problem. As shown in the three scenarios analysis, the proposed model is relatively robust to input data.

The cracking process of ethylene production is a continuous parallel-process, which is popular in chemical process. Therefore, the model presented in this paper can be extended to the short-term scheduling for other similar production processes. The hybrid MINLP/GDP modelling method can be used to develop more complex optimization models in process system engineering. Also the MC-OA with problem-specific improved cuts is also a general method for the large scale MINLP problems.

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Appendix

We transform the disjunctive constraints (14, 17, 19, 22 and 24) in the proposed model into the mixed integer constraints(14r, 17r, 19r, 22r and 24r) according to the convex hull relaxation method (Lee&Grossmann[18]). Considering some linear constraints in disjunctions, the disjunctive eq. 14 and eq. 22 can be simplified. The reformulated eq.14 is as follows.

$$T_j^L \cdot \tilde{x}_{ijk} \le ps_{ijk} \le T_j^U \cdot \tilde{x}_{ijk} \quad \forall i, j, k \tag{14r}$$

By introducing the disaggregated variables $ts_{jk}^{x1}, ts_{jk}^{x2}$, the disjunctive eq. 17 is reformulated as

$$\left.\begin{aligned}
& ts_{jk} = ts_{jk}^{x1} + ts_{jk}^{x2} \\
& p_{jk} \le T_j^U \cdot \hat{x}_{jk} \\
& \tau_{jk} = \tau_j \cdot \hat{x}_{jk} \\
& ts_{jk}^{x1} \le H \cdot \hat{x}_{jk} \\
& ts_{jk}^{x2} \le H \cdot \left(1 - \hat{x}_{jk}\right) \\
& ts_{jk}^{x1} + p_{jk} + \tau_{jk} \le ts_{jk+1}^{x1} \\
& ts_{jk}^{x2} \le ts_{jk+1}^{x2}
\end{aligned}\right\} \quad \forall j, k < K \tag{17r}$$

As the special case of eq. 17, the disjunctive eq. 19 is reformulated as eq. 19r.

$$\left.\begin{aligned}
& ts_{jk} = ts_{jk}^{x1} + ts_{jk}^{x2} \\
& p_{jk} \le T_j^U \cdot \hat{x}_{jk} \\
& \tau_{jk} = \tau_j \cdot \hat{x}_{jk} \\
& ts_{jk}^{x1} \le H \cdot \hat{x}_{jk} \\
& ts_{jk}^{x2} \le H \cdot \left(1 - \hat{x}_{jk}\right) \\
& ts_{jk}^{x1} + p_{jk} + \tau_{jk} \le H
\end{aligned}\right\} \quad \forall j, k = K \tag{19r}$$

The disjunctive eq. 22 is reformulated as follows.

$$\left.\begin{array}{l}\lambda_{ii'jk} = \lambda_{ii'} \cdot y_{ii'jk} \\ Cg_{ii'jk} = Cg_{ii'} \cdot y_{ii'jk}\end{array}\right\} \quad \forall i \neq i', j, k \tag{22r}$$

By introducing the disaggregated variables $ts_{jk}^{z1}, ts_{jk}^{z2}$, the disjunctive eq. 24 is reformulated as

$$\left.\begin{array}{l}ts_{jk} = ts_{jk}^{z1} + ts_{jk}^{z2} \\ ts_{jk}^{z1} \leq H \cdot z_{jj'k} \\ ts_{jk}^{z2} \leq H \cdot \left(1 - z_{jj'k}\right) \\ ts_{jk+1}^{z1} + \tau_{j'k} \cdot z_{jj'k} \leq ts_{j'k+1}^{z1} \\ ts_{j'k+1}^{z2} + \tau_{jk} \cdot \left(1 - z_{jj'k}\right) \leq ts_{jk+1}^{z2}\end{array}\right\} \quad \forall j \neq j', k < K \tag{24r}$$

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