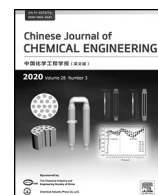




Contents lists available at ScienceDirect

Chinese Journal of Chemical Engineering

journal homepage: www.elsevier.com/locate/CJChE

Article

Stochastic optimization based on a novel scenario generation method for midstream and downstream petrochemical supply chain



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ARTICLE INFO

Article history:

Received 12 January 2019

Received in revised form 16 June 2019

Accepted 25 June 2019

Available online 15 July 2019

Keywords:

Petroleum

Two-stage

Optimization

Scenario generation

Parameter estimation

ABSTRACT

A two-stage mixed integer linear programming model (MILP) incorporating a novel method of stochastic scenario generation was proposed in order to optimize the economic performance of the synergistic combination of midstream and downstream petrochemical supply chain. The uncertainty nature of the problem intrigued the parameter estimation, which was conducted through discretizing the assumed probability distribution of the stochastic parameters. The modeling framework was adapted into a real-world scale of petrochemical enterprise and fed into optimization computations. Comparisons between the deterministic model and stochastic model were discussed, and the influences of the cost components on the overall profit were analyzed. The computational results demonstrated the rationality of using reasonable numbers of scenarios to approximate the stochastic optimization problem.

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1. Introduction

It is through supply chains that raw materials are acquired, stored, and transformed into products, which are then delivered to customers. Information, materials and financial flows occur among different echelons over the time horizon of the supply chain [1]. The petrochemical industry is often considered as three major segments: upstream, midstream, and downstream [2]. The midstream and downstream segments cover the crude oil transformation, production of petrochemical products, inventory and distribution of end products to consumers. As a complex and dynamic system, the petrochemical supply chain is subjected to uncertainties involved in the entire procedures. Most often, the uncertain factors involved in the petrochemical supply chain are fluctuations of production levels, product prices and unforeseeable demands of the products [3]. For the deterministic models, those early works on planning and scheduling of petrochemical supply chains [4–6] cannot capture the uncertain feature of most real-world applications. The perturbations of uncertain factors may cause potentially significant impacts on the overall financial outcomes, characterizing the dynamic behaviors of the large-scale petrochemical industry, especially when one considers it as a capital intense infrastructure. In order to maintain the operation profitability, the aforementioned uncertainty factors must be taken into consideration.

To deal with uncertainty factors in the optimization problem, different approaches employing robust optimization [7,8], chance constraint

optimization [9,10], fuzzy programming [11,12], and stochastic programming [13–15] have been proposed. The stochastic programming methods were shown to exhibit good performance when the collected data have a particular distribution [16]. In addition, Lima *et al.* [17], Al-Othman *et al.* [18], and Leiras *et al.* [19] showed that discretizing the normal distribution of the values of the uncertain parameters into different scenarios would be computationally more tractable and industrially more applicable than handling the continuous random parameters involved in the stochastic programming methods.

In spite of a considerable amount of research focusing on scenario-based stochastic programming methods to deal with the uncertainty of the petrochemical supply chain [18–20], most articles refer to the segmentation of the scenarios only with limited number of scenarios. One of the first works addressing the scenario discretization was by Al-Othman *et al.* [18], whose work dealt with the uncertainty of market demand and price based on the two-stage problem with finite numbers of scenarios. Leiras *et al.* [19] proposed a simplified scenario tree with 9 scenarios based on data collected from industrial experts and from secondary research like historical economic data. Zhao *et al.* [20] followed the similar approach and the independent uncertain parameters (product price and demand) were measured with three levels of realizations (high, medium and low, and the 3 realizations were assigned with probabilities of 25%, 50% and 25%, respectively), so 9 scenarios were generated.

However, limited numbers of scenarios proposed in his work did not capture the uncertainty of the problem and calculation inaccuracy cannot be ignored. If this method were adopted to discretize the stochastic parameters into more refined grids of scenarios to embed more possible

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incidents, the computational burden would be a significant issue. To the best of our knowledge, few previous works have done any explorations on the midpoint between the calculation accuracy and computational burden.

Based on the shortcomings and gaps identified from the literature review, the contributions of this paper can be summarized as follows: the first novelty of this work is that it highlights the relationship between scenario generation and the probability distribution of the uncertain parameters, which can make the scenario generation more rational and can avoid the arbitrary assigning of probability to each scenario. The second novelty is that this work analyzed the trade-off between calculation accuracy and computational time and proposed a criterion for choosing the midpoint. The third novelty is that this work analyzed the influence of each cost component on the overall profit of the supply chain model.

The remainder of the paper is organized as follows. In Section 2 the problem is stated, and assumptions are offered for simplification of the subsequent model. Section 3 is dedicated to the formulation of a scenario-based two stage stochastic optimization model. In Section 4, a case study in the context of large-scale petrochemical supply chain industry is conducted, more scenarios are generated in this section, and influences of the cost components on the overall profit were analyzed. Conclusions are elaborated in Section 5, and some final remarks close the paper.

2. Problem Statement

A superstructure of the petrochemical supply chain with four levels of participants: suppliers, production centers, distribution centers and consumers [19], is illustrated in Fig. 1.

The participants in the supply chain denoted by the nodes in the superstructure in Fig. 1 can be described as:

- 1) Both the oil field (OF) and the terminal (TE) are suppliers of raw materials. Meanwhile, the terminal functions as a receiver of final products that are to be exported.
- 2) The refineries (R: r1, r2, r3) function as warehouses for the raw materials and production centers transforming the raw materials to the products, which are then transported to distribution bases (B: b1, b2, b3) and/or the terminal.
- 3) Both the distribution bases and the terminal act as warehouses for the products.

- 4) Products stocked in distribution bases are targeted at domestic customers (C: c1, c2, c3, c4, c5), while products stocked in terminal are targeted at overseas customers (OC: oc1, oc2).

The number of nodes in the four levels can be adjusted according to different scales of the real cases.

When product demand of customers goes beyond the upper limit of refinery production, extra products need to be procured from overseas with possibly a higher price at the terminal to compensate for the existing demand. Extra products can be sold on site to the overseas customers or can be transported to the distribution bases to be sold to the domestic customers.

For the sake of simplification, the following assumptions are adopted in the present work:

- 1) The physical structure of the supply chain has been predefined and will have no alterations during the whole-time horizon.
- 2) The stochastic parameters are defined as the uncertain prices and demands of the products and can be represented as stochastic parameters with normal distribution of probabilities, the means and standard deviations of which are able to be forecasted via market data mining and analyses.
- 3) Parameters with respect to each node in the supply chain structure in Fig. 1, such as the prices and properties of each material, the yield ratio, properties and kinds of product produced by each refinery, the upper and lower bounds of each kind of capacity constraint, and the unit price of each kind of cost component, are given and will remain constant for each time period discussed.
- 4) Each node (including the refineries) in the supply chain is regarded as black box, with inner and outer flow of products and materials being monitored.

3. Mathematical Model

A two-stage stochastic linear programming method with resource was first proposed by Beale [21] and Danzig [22]. In their approach, some decisions, termed as resource actions, are made after uncertainty is disclosed, and the decision variables can thus be categorized according to stages [23]. Based on the two-stage model, Zhao *et al.* [20] developed a two-stage scenario-based mixed-integer linear programming (MILP) method for the optimization of petrochemical supply chain. In the following subsections, the model by Zhao is employed as a basis. The

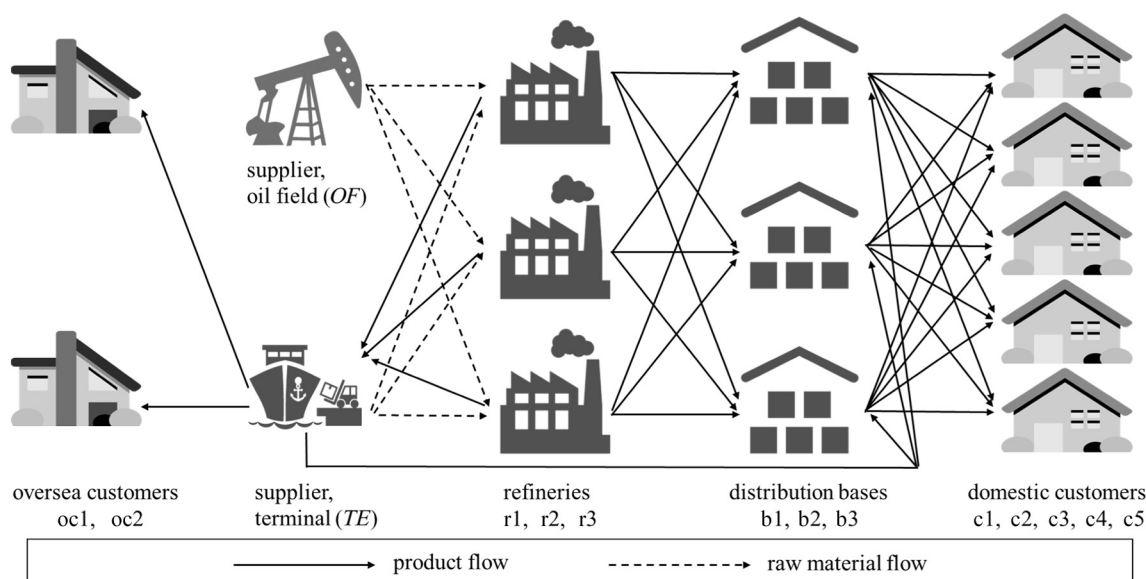


Fig. 1. Petroleum supply chain network.

terms in the objective function are categorized into two stages. The cost of materials purchased at each supplier and the cost of materials transported between nodes that are involved in the supply chain are defined as the first stage terms and therefore scenario-independent, while the other terms are sorted as the second stage ones, which are scenario-dependent.

3.1. Objective function

The objective of the supply chain optimization is to maximize the expected profit, which follows the basic rule of sales subtract costs, as given by Eq. (1). The costs include those for material purchase (Cmp), material transportation ($Cmtr$), carbon emission tax ($Cctax$), refinery operation (Cro), inventory (Cin), product transportation ($Cptr$), extra product purchase ($Ccpp$), production surplus penalty ($Csur$), and production backlog penalty ($Cbck$).

$$\begin{aligned} \text{Max } E[\text{profit}] = & -Cmp - Cmtr - Cctax \\ & - \sum_{sc^n \in SC} \text{PROB}^{sc^n} \cdot (Sales^{sc^n} - Cro^{sc^n} - Cin^{sc^n} - Cptr^{sc^n} - Ccpp^{sc^n} - Csur^{sc^n} - Cbck^{sc^n}) \end{aligned} \quad (1)$$

In the function given by Eq. (1), sc^n refers to 'scenario n ', PROB^{sc^n} refers to the probability of scenario n .

The sale is given by

$$\begin{aligned} Sales^{sc^n} = & \sum_{p \in P} \sum_{oc \in OC} \sum_{te \in TE} \sum_{tp \in TP} PUP_{p,te}^{sc^n,tp} \cdot qps_{p,oc,te}^{sc^n,tp} \\ & + \sum_{p \in P} \sum_{c \in C} \sum_{b \in B} \sum_{tp \in TP} PUP_{p,b}^{sc^n,tp} \cdot qps_{p,c,b}^{sc^n,tp} \end{aligned} \quad (2)$$

where $PUP_{p,te}^{sc^n,tp}$ and $PUP_{p,b}^{sc^n,tp}$ refer to the unit price for product p purchased at time period tp of scenario sc^n at respectively, terminal te and distribution b ; $qps_{p,oc,te}^{sc^n,tp}$ and $qps_{p,c,b}^{sc^n,tp}$ refer to the quantity of product p sold at time period tp of scenario sc^n at respectively, terminal te to overseas customer oc and distribution b to domestic customer c .

The costs in Eq. (1) are as follows:

The material purchase:

$$\begin{aligned} Cmp = & \sum_{m \in M} \sum_{te \in TE} \sum_{r \in R} \sum_{tp \in TP} MUP_{m,te}^{tp} \cdot qmp_{m,te,r}^{tp} \\ & + \sum_{m \in M} \sum_{of \in OF} \sum_{r \in R} \sum_{tp \in TP} MUP_{m,of}^{tp} \cdot qmp_{m,of,r}^{tp} \end{aligned} \quad (3)$$

where $MUP_{m,te}^{tp}$ and $MUP_{m,of}^{tp}$ refer to the unit prices of material m purchased during time period tp at respectively terminal te and oil field of ; $qmp_{m,te,r}^{tp}$ and $qmp_{m,of,r}^{tp}$ refer to quantity of material m purchased by refinery r during time period tp at respectively terminal te and oil field of .

The material transportation:

$$Cmtr = \sum_{m \in M} \sum_{n \in N} \sum_{n' \in N} \sum_{tr \in TR} \sum_{tp \in TP} MTUP_{m,n,n',tr}^{tp} \cdot DIS_{n,n'} \cdot qmtr_{m,n,n',tr}^{tp} \quad (4)$$

where $MTUP_{m,n,n',tr}^{tp}$ refers to the unit price of material transportation for material m by transportation tool tr at time period tp from node n to node n' ; $DIS_{n,n'}$ refers to the distance between nodes n and n' ; and $qmtr_{m,n,n',tr}^{tp}$ refers to quantity of material m transported from node n to n' by transportation tool tr at time period tp .

The carbon emission tax:

The environmental influence in the form of carbon emission tax ($Cctax$) was incorporated into the objective function in the following three forms: material transportation carbon emission tax ($Cmtrctax$), refinery operation carbon emission tax ($Croctax$), and product transportation carbon emission tax ($Cptrctax$).

$$Cctax^{sc^n} = Cmtrctax + \sum_{sc^n \in SC} \text{PROB}^{sc^n} (Croctax^{sc^n} + Cptrctax^{sc^n}) \quad (5)$$

$$Cmtrctax = \text{TAXC} \cdot \sum_{m \in M} \sum_{n \in N} \sum_{n' \in N} \sum_{tr \in TR} \sum_{tp \in TP} \text{CCOEF}_{tr} \cdot DIS_{n,n'} \cdot qmtr_{m,n,n',tr}^{tp} \quad (6)$$

$$Croctax^{sc^n} = \text{TAXC} \cdot \sum_{m \in M} \sum_{r \in R} \sum_{tp \in TP} \text{ECr} \cdot qmo_{r,m}^{sc^n,tp} \quad (7)$$

$$Cptrctax^{sc^n} = \text{TAXC} \cdot \sum_{p \in P} \sum_{n \in N} \sum_{n' \in N} \sum_{tr \in TR} \sum_{tp \in TP} \text{CCOEF}_{tr} \cdot DIS_{n,n'} \cdot qptr_{p,n,n',tr}^{sc^n,tp} \quad (8)$$

TAXC is the tax per ton of CO_2 emitted, and can take the value of 10 Chinese Yuan per ton in the Chinese market [20]. CCOEF refers to carbon emission coefficient of different transportation modes. According to The Greenhouse Gas Protocol and the European Chemical Industry Association [24], the carbon emission coefficients of road, railway, water for freight are $3.27 \times 10^{-5} \text{ t CO}_2 \cdot (\text{t} \cdot \text{km})^{-1}$, $2.8 \times 10^{-5} \text{ t CO}_2 \cdot (\text{t} \cdot \text{km})^{-1}$, $5.3 \times 10^{-5} \text{ t CO}_2 \cdot (\text{t} \cdot \text{km})^{-1}$, respectively. The pipeline transportation is approximated as non-carbon emission. ECr is the quantity of CO_2 emitted per ton of material operated at refinery R , readers interested in the calculation process can refer to the work of Jiang [25].

The refinery operation of scenario n :

$$Cro^{sc^n} = \sum_{r \in R} \sum_{m \in M} \sum_{tp \in TP} \text{ROUP}_{r,m}^{tp} \cdot qmo_{r,m}^{sc^n,tp} \quad (9)$$

where $\text{ROUP}_{r,m}^{tp}$ refers to the operation unit price [20] of refinery r to process material m at time period tp and $qmo_{r,m}^{sc^n,tp}$ refers to the quantity of material m operated by refinery r at time period tp of scenario sc^n .

The inventory of scenario n :

$$\begin{aligned} Cin^{sc^n} = & \sum_m \sum_r \sum_{tp} \text{IVUP}_{m,r}^{tp} \cdot qmsto_{m,r}^{sc^n,tp} + \sum_p \sum_{te} \sum_{tp} \text{IVUP}_{p,te}^{tp} \\ & \cdot qpsto_{p,te}^{sc^n,tp} + \sum_p \sum_b \sum_{tp} \text{IVUP}_{p,b}^{tp} \cdot qpsto_{p,b}^{sc^n,tp} \end{aligned} \quad (10)$$

where $\text{IVUP}_{m,r}^{tp}$, $\text{IVUP}_{p,te}^{tp}$, and $\text{IVUP}_{p,b}^{tp}$ refer to the inventory unit price at time period TP for material M in refinery r , for product p in terminal te , and for product p in distribution base b , respectively. $qmsto_{m,r}^{sc^n,tp}$, $qpsto_{p,te}^{sc^n,tp}$, and $qpsto_{p,b}^{sc^n,tp}$ refer to the quantity of material m stocked at refinery r , quantity of product p stocked at terminal te , and quantity of product p stocked at distribution b , respectively, at time period tp of scenario sc^n .

The product transportation of scenario n :

$$Cptr^{sc^n} = \sum_{p \in P} \sum_{n \in N} \sum_{n' \in N} \sum_{tr \in TR} \sum_{tp \in TP} \text{PTUP}_{p,n,n',tr}^{tp} \cdot DIS_{n,n'} \cdot qptr_{p,n,n',tr}^{sc^n,tp} \quad (11)$$

where $\text{PTUP}_{p,n,n',tr}^{tp}$ refers to the transportation unit price for product p from node n to n' by transportation tool tr at time period tp ; $DIS_{n,n'}$ refers to the distance between nodes n and n' , as mentioned above; and $qptr_{p,n,n',tr}^{sc^n,tp}$ refers to the quantity of product p transported by transportation tool tr from node n to n' at tp of scenario sc^n .

The extra product purchase of scenario n :

$$Cepp^{sc^n} = \sum_{p \in P} \sum_{te \in TE} \sum_{tp \in TP} EPUP_{p,te}^{tp} \cdot qepp_{p,te}^{sc^n, tp} \quad (12)$$

where $EPUP_{p,te}^{tp}$ refers to the unit price of extra product p purchased at terminal te at time period tp and $qepp_{p,te}^{sc^n, tp}$ refers to quantity of extra product purchased at terminal te at time period tp of scenario sc^n .

The production surplus penalty of scenario n :

$$Csur^{sc^n} = \sum_{c \in C} \sum_{p \in P} \sum_{tp \in TP} SUR_p^{tp} \cdot qsp_{p,c}^{sc^n, tp} + \sum_{oc \in OC} \sum_{p \in P} \sum_{tp \in TP} SUR_p^{tp} \cdot qsp_{p,oc}^{sc^n, tp} \quad (13)$$

where SUR_p^{tp} refers to the penalty for production surplus per ton of product p produced and $qsp_{p,c}^{sc^n, tp}$ and $qsp_{p,oc}^{sc^n, tp}$ refer to the quantity of surplus product p to be purchased at time period tp of sc^n by domestic customer c , and overseas customer oc , respectively. The surplus penalty accounts for all the cost of coupons and discounts in order to sell the products to domestic and overseas customers.

The production backlog penalty of scenario n :

$$Cbck^{sc^n} = \sum_{c \in C} \sum_{p \in P} \sum_{tp \in TP} BCK_p^{tp} \cdot qbp_{p,c}^{sc^n, tp} + \sum_{oc \in OC} \sum_{p \in P} \sum_{tp \in TP} BCK_p^{tp} \cdot qbp_{p,oc}^{sc^n, tp} \quad (14)$$

where BCK_p^{tp} refers to the penalty for production backlog per ton of product p not being able to be produced and $qbp_{p,c}^{sc^n, tp}$ and $qbp_{p,oc}^{sc^n, tp}$ refer to the quantity of backlog product p needed at time period tp of scenario n by domestic customer c , and by overseas customer oc , respectively. The backlog penalty accounts for all the penalty for not being able to satisfy the amounts of products as signed in the contracts.

3.2. Constraints equations

The variations of the variables are subjected to the following constraints.

Material balance:

$$\sum_{te \in TE} qmp_{m,te,r}^{tp} + \sum_{of \in OF} qmp_{m,of,r}^{tp} + qmsto_{m,r}^{sc^n, tp-1} = qmo_{m,r}^{sc^n, tp} + qmsto_{m,r}^{sc^n, tp} \quad (15)$$

$$\forall m \in M, \forall r \in R, \forall tp \in TP, \forall sc^n \in SC$$

where $qmsto_{m,r}^{sc^n, tp}$ refers to the quantity of material m stocked at refinery r at time period tp of scenario sc^n .

Product balance:

$$qmo_{m,r}^{sc^n, tp} \cdot YDR_{r,m,p} = \sum_{te \in TE} qpte_{p,r,te}^{sc^n, tp} + \sum_{b \in B} qpb_{p,r,b}^{sc^n, tp} \quad (16)$$

$$\forall m \in M, \forall p \in P, \forall r \in R, \forall tp \in TP, \forall sc^n \in SC$$

where $YDR_{r,m,p}$ refers to the yield ratio of material m to product p at refinery r and $qpte_{p,r,te}^{sc^n, tp}$ and $qpb_{p,r,b}^{sc^n, tp}$ refer to the quantity of product p produced by refinery r sold at tp of scenario sc^n at terminal te , and at distribution b , respectively.

The product balance constraint at terminal is given by

$$\sum_{r \in R} qpte_{p,r,te}^{sc^n, tp} + qepp_{p,te}^{sc^n, tp} - \sum_{b \in B} qeph_{p,b,te}^{sc^n, tp} + qpsto_{p,te}^{sc^n, tp-1} = \sum_{oc \in OC} qps_{p,oc,te}^{sc^n, tp} + qpsto_{p,te}^{sc^n, tp} \quad \forall p \in P, \forall te \in TE, \forall tp \in TP, \forall sc^n \in SC \quad (17)$$

where $qeph_{p,b,te}^{sc^n, tp}$ refers to the quantity of extra product p purchased at te to be sold at distribution b at time period tp of scenario sc^n .

Function (18) gives the product balance constraint at distribution base.

$$\sum_{r \in R} qpb_{p,r,b}^{sc^n, tp} + \sum_{te \in TE} qeph_{p,b,te}^{sc^n, tp} + qpsto_{p,b}^{sc^n, tp-1} = \sum_{c \in C} qps_{p,c,b}^{sc^n, tp} + qpsto_{p,b}^{sc^n, tp} \quad \forall p \in P, \forall b \in B, \forall tp \in TP, \forall sc^n \in SC \quad (18)$$

Sulfur content restriction

This constraint gives the logical relations of the sulfur content between the processed materials and the corresponding products, and would control the procurement for materials with different qualities.

$$\sum_{m \in M} qmo_{r,m}^{sc^n, tp} \cdot SC_m^{tp} \cdot YDR_{r,m,p} \cdot (1 - DSR_{r,m}) \leq \left(\sum_{m \in M} qmo_{r,m}^{sc^n, tp} \cdot YDR_{r,m,tp} \right) \cdot SC_p^{tp} \quad \forall p \in P, \forall r \in R, \forall tp \in TP, \forall sc^n \in SC \quad (19)$$

where SC_m^{tp} and SC_p^{tp} refer to the sulfur content at time period tp of material m and of product p , respectively and $DSR_{r,m}$ refers to the desulfurization ratio of material m at refinery r .

Procurement capacity limits

$$\sum_{r \in R} qmp_{m,te,r}^{tp} + \sum_{r \in R} qmp_{m,of,r}^{tp} \leq MPU_m^{tp} \quad (20)$$

$$\forall m \in M, \forall te \in TE, \forall of \in OF, \forall tp \in TP$$

where MPU_m^{tp} refers to the purchase upper limit of material m at time period tp .

For the extra product procurement capacity, we have

$$\sum_{te \in TE} qepp_{p,te}^{sc^n, tp} \leq EPPU_p^{tp} \quad \forall p \in P, \forall tp \in TP, \forall sc^n \in SC \quad (21)$$

where $EPPU_p^{tp}$ refers to the purchase upper limit of extra product p at time period tp .

Refinery operation

$$CAPL_{r,m}^{tp} \leq qmo_{r,m}^{sc^n, tp} \leq CAPU_{r,m}^{tp} \quad \forall r \in R, \forall m \in M, \forall tp \in TP, \forall sc^n \in SC \quad (22)$$

where $CAPL_{r,m}^{tp}$ and $CAPU_{r,m}^{tp}$ refer to the lower and upper limits of operation capacity of refinery r to process material m at time period tp , respectively.

Inventory capacity upper limits

$$qmsto_{m,r}^{sc^n, tp} \leq IVU_{m,r}^{tp} \quad (23a)$$

$$qpsto_{p,te}^{sc^n, tp} \leq IVU_{p,te}^{tp} \quad (23b)$$

$$qpsto_{p,b}^{sc^n, tp} \leq IVU_{p,b}^{tp} \quad (23c)$$

$$\forall m \in M, \forall p \in P, \forall r \in R, \forall te \in TE, \forall b \in B, \forall tp \in TP, \forall sc^n \in SC$$

where $IVU_{m,r}^{tp}$ refers to the inventory upper limit of refinery r for material m at time period tp ; $IVU_{p,te}^{tp}$ and $IVU_{p,b}^{tp}$ refer to inventory upper limit for product p at time period tp in terminal te , and in distribution base b , respectively.

Capacity for mixed flows

This constraint limits the maximum amount of flows transported by transportation tool tr between nodes involved at time period tp .

$$\sum_{m \in M} mf_{m,n,n',tr}^{tp} + \sum_{p \in P} pf_{p,n,n',tr}^{tp} \leq TCAU_{n,n',tr}^{tp} \quad (24)$$

$$\forall n \in N, \forall n' \in N, \forall tr \in TR, \forall tp \in TP$$

where $mf_{m,n,n',tr}^{tp}$ and $pf_{p,n,n',tr}^{tp}$ refer to the flow of material m , and of product p , respectively, from node n to n' by transportation tool tr at time period tp and $TCAU_{n,n',tr}^{tp}$ refers to the transportation upper limit from node n to n' by transportation tool tr at time period tp .

A set of constraints as follows gives the logical relations of mixed flows at each node.

$$qmp_{m,te,r}^{tp} = \sum_{tr \in TR} mf_{m,te,r,tr}^{tp} \quad (25a)$$

$$qmp_{m,of,r}^{tp} = \sum_{tr \in TR} mf_{m,of,r,tr}^{tp} \quad (25b)$$

$$qpb_{p,r,b}^{sc^n, tp} = \sum_{tr \in TR} pf_{p,r,b,tr}^{sc^n, tp} \quad (25c)$$

$$qpte_{p,r,te}^{sc^n, tp} = \sum_{tr \in TR} pf_{p,r,te,tr}^{sc^n, tp} \quad (25d)$$

$$qps_{p,b,c}^{sc^n, tp} = \sum_{tr \in TR} pf_{p,b,c,tr}^{sc^n, tp} \quad (25e)$$

$$qps_{p,te,oc}^{sc^n, tp} = \sum_{tr \in TR} pf_{p,te,oc,tr}^{sc^n, tp} \quad (25f)$$

$$qepb_{p,te,b}^{sc^n, tp} = \sum_{tr \in TR} pf_{p,te,b,tr}^{sc^n, tp} \quad (25g)$$

$$\forall m \in M, \forall p \in P, \forall r \in R, \forall of \in OF, \forall te \in TE,$$

$$\forall b \in B, \forall oc \in OC, \forall c \in C, \forall tp \in TP, \forall sc^n \in SC$$

Product demands

This set of constraints denotes the demand constraint of overseas and domestic customers respectively.

$$qps_{p,oc,te}^{sc^n, tp} = DEM_{p,oc}^{sc^n, tp} + qsp_{p,oc}^{sc^n, tp} - qbp_{p,oc}^{sc^n, tp} \quad \forall p \in P, \forall oc \in OC, \forall tp \in TP, \forall sc^n \in SC \quad (26a)$$

$$qps_{p,c,b}^{sc^n, tp} = DEM_{p,c}^{sc^n, tp} + qsp_{p,c}^{sc^n, tp} - qbp_{p,c}^{sc^n, tp} \quad \forall p \in P, \forall c \in C, \forall tp \in TP, \forall sc^n \in SC \quad (26b)$$

where $DEM_{p,oc}^{sc^n, tp}$ and $DEM_{p,c}^{sc^n, tp}$ refer to the demand for product p at time period tp of scenario sc^n of overseas customer oc and of domestic customer c , respectively; $qsp_{p,oc}^{sc^n, tp}$ and $qsp_{p,c}^{sc^n, tp}$ refer to the quantity of surplus product p to be purchased at tp of sc^n 'by overseas customer oc ' and 'by domestic customer c ', respectively; and $qbp_{p,oc}^{sc^n, tp}$ and $qbp_{p,c}^{sc^n, tp}$ refer to the quantity of backlog product p needed 'by overseas customer oc ',

and 'by domestic customer c ', respectively, at time period tp of scenario sc^n .

The upper bounds of each kind of product surplus or backlog are given as follows.

$$qsp_{p,oc}^{sc^n, tp} \leq iqsp_{p,oc}^{sc^n, tp} \cdot QSU_{p,oc}^{tp} \quad (27a)$$

$$qsp_{p,c}^{sc^n, tp} \leq iqsp_{p,c}^{sc^n, tp} \cdot QSU_{p,c}^{tp} \quad (27b)$$

$$qbp_{p,oc}^{sc^n, tp} \leq iqbp_{p,oc}^{sc^n, tp} \cdot QBU_{p,oc}^{tp} \quad (27c)$$

$$qbp_{p,c}^{sc^n, tp} \leq iqbp_{p,c}^{sc^n, tp} \cdot QBU_{p,c}^{tp} \quad (27d)$$

$$\forall p \in P, \forall oc \in OC, \forall c \in C, \forall tp \in TP, \forall sc^n \in SC$$

where $iqsp_{p,oc}^{sc^n, tp}$, $iqbp_{p,oc}^{sc^n, tp}$, $iqsp_{p,c}^{sc^n, tp}$, $iqbp_{p,c}^{sc^n, tp}$ are 0–1 variables, with values of 1 and 0 denoting the situation of happening and not happening of the corresponding incident as above, respectively; $QSU_{p,oc}^{tp}$ and $QSU_{p,c}^{tp}$ refer to the upper limit of surplus product p to be purchased at time period tp 'by overseas customer oc ', and 'by domestic customer c ', respectively; and $QBU_{p,oc}^{tp}$ and $QBU_{p,c}^{tp}$ refer to the upper limit of backlog product p needed at time period tp 'by overseas customer oc ', and 'by domestic customer c ', respectively.

Since the surplus and backlog of one kind of product cannot happen at the same time period, the constraints as follows give the logical relationship.

$$iqsp_{p,oc}^{sc^n, tp} + iqbp_{p,oc}^{sc^n, tp} \leq 1 \quad (28a)$$

$$iqsp_{p,c}^{sc^n, tp} + iqbp_{p,c}^{sc^n, tp} \leq 1 \quad (28b)$$

4. Case Study

The numerical data in the case study were collected both from real petrochemical market and secondary research like historical data, and the scale of this numerical example can be regarded as the same magnitude of a real world problem.

The time horizon in this study is one season and is divided into 3 time periods (tp1, tp2, tp3), each period accounts for one month. Materials include 2 kinds of crude oil (cof1, cof2) provided by the oil field, 6 kinds of crude oil (cote1, cote2, cote3, cote4, cote5, cote6) and 3 other materials (l-naphtha, h-naphtha, mix-xylene) provided by the terminal, the 11 kinds of materials mentioned above differ in their sulfur content and prices. There are 15 kinds of different products being produced by the three refineries, with 9 kinds of the products targeted at both overseas and domestic customers while other 6 products targeted only at domestic customers. The transportation network involves 4 kinds of transportation modes: ocean, pipeline, railway, and road transportation.

4.1. Scenario generation for deterministic model

The first step before diving into the task of scenario generation was to calculate the deterministic model as the contrast group. The deterministic model was defined as an exceptional case where the prices and demands of products remain constant, as μ_p and μ_d . Table 1 presents the results for the deterministic model.

Table 1 shows that the profit for the deterministic model is 6.42×10^7 USD (noted as profit⁰), and this would be the benchmark for the following groups with more scenarios. The deterministic model required a much lower computational effort (with an execution time of 0.078 s), but it cannot capture the truly dynamic and uncertain behavior of the stochastic problem.

Table 1
Deterministic model: Optimal profit and costs

Item	Value $\times 10^7$ /USD
Profit	6.4204611
Sales	15.573179
Materials purchase cost	6.1126469
Transportation cost	0.8806403
Operations cost	1.3364521
Inventory cost	0.0209382
Extra products purchase cost	0.5196594
CO ₂ tax cost	0.0585877
Surplus cost	0.0529190
Backorder cost	0.1708746

4.2. Generation of more scenarios

As was mentioned in Section 2, the stochastic parameters in this case study were defined as the prices and demands of the products, and their probability distributions all follow the pattern of normal distribution, with the means (μ) and standard deviation (σ) being able to be forecasted. For the better illustration of the problem, we take one of the products as an example and denote the mean of this product as μ_p and the standard deviation as σ_p , and the same for the product demand: μ_d and σ_d .

Considering the symmetry of the normal distribution, using $1\sigma_p$ as the discretization unit can divide the whole probability space of the product price into N parts, and for a case of $N = 5$, probabilities of each part are specified in Table 2. As predefined in Section 1, the random variables involved in this study are independent, so the demand component of the stochastic vector can be treated in a likely manner with the probability space of the product demand being divided into 5 parts as well. When the two components of the parameter vector were combined, 25 scenarios were generated. Other products are processed in the same manner.

A series of scenario generation with discretization index of $1/2\sigma$, $2/5\sigma$, $1/4\sigma$, and $1/5\sigma$ can be proceeded in a similar fashion, and the sketched map of the 5 kinds of discretization for respectively $N = 5$, 11, 15, 23, and 29 is shown in Fig. 2.

The five sets of the aforementioned parameter discretization were fed into the original model to substitute the deterministic pattern, and statistics on the GAMS model with different numbers of scenarios are presented in Table 3.

Fig. 3 suggests that the discretization of the values of the uncertain parameters tends to overestimate the expected profit. When the discretization is increasingly refined (value of N getting higher), the expected profit approaches the real value (the one with the continuous distributions). On the other hand, as the number of scenarios increased, the execution of the program required more computational efforts, denoted by the increase of elapsing time of the computation.

Facing the contradiction shown in Fig. 3, a proper value of N needs to be determined to balance the calculation inaccuracy and the computational effort. Fig. 4 gives the trend of cumulative probability (probability of scenarios with profit greater than profit⁰ are counted into the cumulative probability) with respect to N , it can be seen that the overall trend goes flat when it passes $N = 15$ (225 scenarios), which indicates that scenarios more than 225 would achieve almost no more benefit.

Table 2
Parameter discretization of price ($\Delta = 1\sigma_p$)

Scenario	Product price	Probability/%
1	$\mu_p - 2\sigma_p$	2.28
2	$\mu_p - 1\sigma_p$	13.59
3	μ_p	68.26
4	$\mu_p + 1\sigma_p$	13.59
5	$\mu_p + 2\sigma_p$	2.28

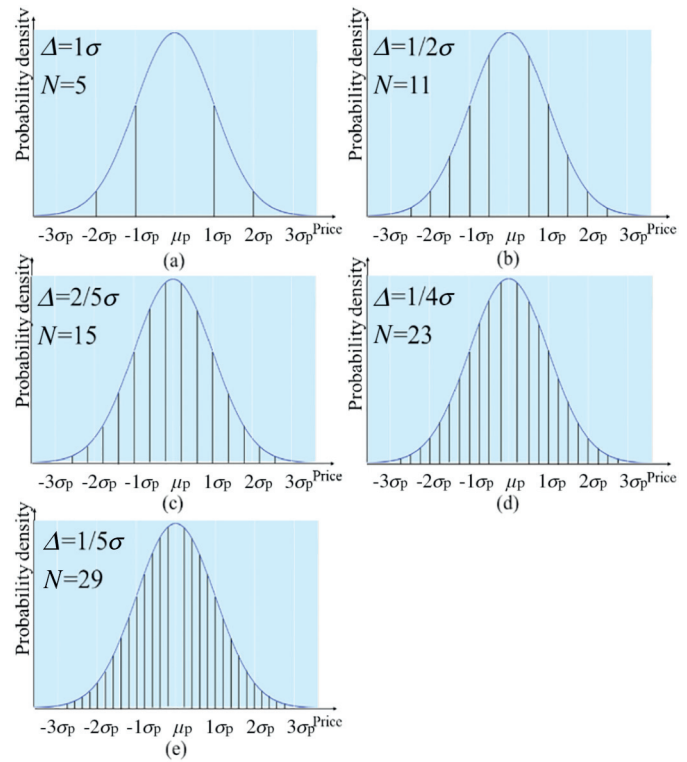


Fig. 2. Sketch map for stochastic parameter discretization.

As a result, the trends presented in Figs. 3 and 4 jointly pinpointed $N = 15$ as the compromise of computational burden and accuracy of measurement. For a general problem, the ratio of the slope around an N value can be calculated and used as a criterion to determine the desirable N value. For an N value in the i th trial, namely N_i , the criterion ε can be defined as

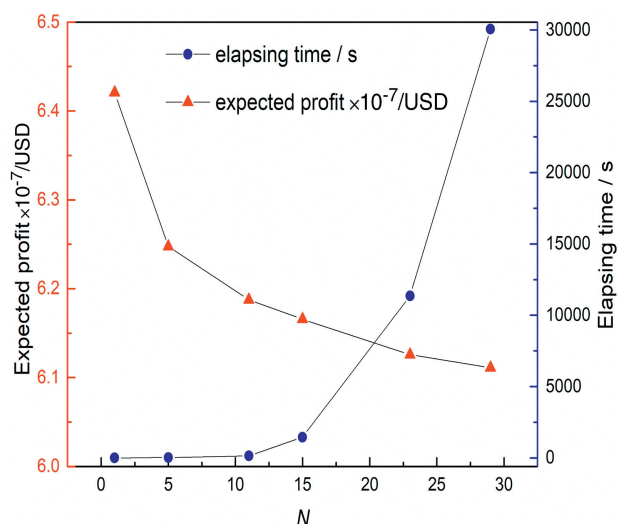
$$\varepsilon = \frac{[(\sum P)_{i+1} - (\sum P)_i](N_i - N_{i-1})}{[(\sum P)_i - (\sum P)_{i-1}](N_{i+1} - N_i)} \quad (29)$$

In the particular example shown above when $N_i = 15$ (while $i = 4$), $\varepsilon = 0.02975$, which can be known as sufficiently small and can also be suggested for general applications. For more general cases, $\varepsilon < 0.05$ can be regarded as the criterion for determining N .

After pinpointing the optimal value of N as 15 for the case study, the distribution of the profits of the 225 scenarios should be explored. Fig. 5 gives the distribution of profits with respect to different product price and demand. The red curved surface is constituted by 225 dots, obviously the number of N determines the smoothness of the surface. If the value of N is too small, the surface would appear jagged, while when the value of N approaches infinite, the surface would be close to the situation when the stochastic variables (product price and demand) in the problem are continuous. The blue plane with profit of 6.42×10^7 USD (profit⁰) divides the whole space into 2 parts, and the dots above the blue plane represent scenarios with profit larger than profit⁰.

Table 3
Statistics of the GAMS model with uncertainty

Number of scenarios	25	121	225	529	841
Blocks of equations	91	91	91	91	91
Single equations	123,565	596,461	1,108,765	2,606,269	4,143,181
Blocks of variables	52	52	52	52	52
Single variables	158,626	764,290	1,420,426	3,338,362	5,306,770
Nonzero elements	1,306,732	6,314,764	11,740,132	27,598,900	43,875,004
Discrete variables	13,950	67,518	125,550	295,182	469,278

Fig. 3. Expected profits and elapsing time with respect to N .

4.3. Global sensitivity analysis

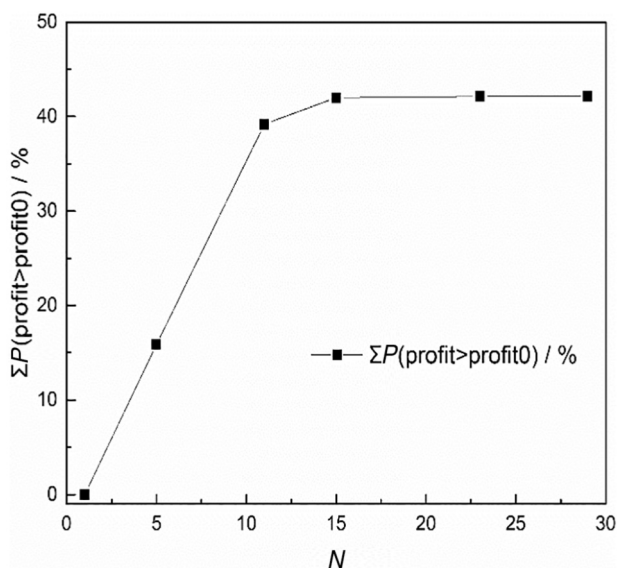
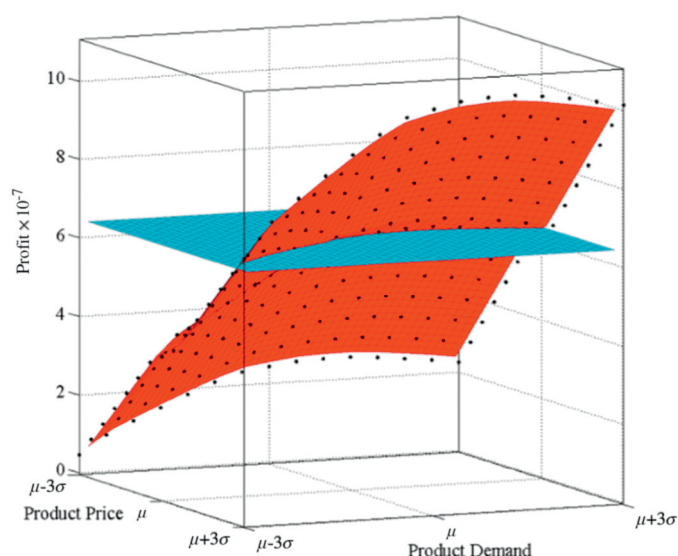
In order to investigate the contributions of the uncertainty of each cost component on the output of the model, sensitivity analysis needs to be conducted. Local sensitivity analysis (LSA) method was frequently carried out to pinpoint the influential factors in different echelons of the petrochemical supply chain model [26–28], but it can only assess one single factor at a time by keeping all the other input parameters at their nominal values [29,30]. While the global sensitivity analysis (GSA) takes the full rank of uncertainties of the input variables, and all the uncertainty factors can be simultaneously evaluated. In this paper, the GSA method of Sobol'–Jansen (variance-based method) [31,32] is applied to identify the influential cost components. The following steps are conducted in the GSA method:

Step1: determine the objective function.

The objective function of this problem can be rewritten as:

$$\text{profit} = \text{Sales} - \text{Cmp} - \text{Ctr} - \text{Cro} - \text{Cin} - \text{Cepp} - \text{Cctax} - \text{Csur} - \text{Cbck} \quad (30)$$

where Ctr is the sum of Cmtr and Cptr .

Fig. 4. Cumulative probability of scenarios with respect to N .Fig. 5. Distribution of optimal profits ($N = 15$).

Step2: determine the input variables of the model.

Since the target of the sensitivity analysis is to determine the influence of the 8 cost components on the overall profit, each cost component is regarded as an input variable and is assigned a coefficient x_i ($i = 1, 2, \dots, 8$).

$$\text{profit} = \text{Sales} - x_1 \text{Cmp} - x_2 \text{Ctr} - x_3 \text{Cro} - x_4 \text{Cin} - x_5 \text{Cepp} - x_6 \text{Cctax} - x_7 \text{Csur} - x_8 \text{Cbck} \quad (31)$$

Step3: generate samples from the distribution of input variables

Considering the nature of the cost component in the economic context, the x_i takes the value from 0.5 to 2.0 (denoting that the corresponding cost component takes the value from twice to half of its original value), and is assumed to follow the uniform distribution. The Monte Carlo method is applied, and 200 samples of the input variables are generated.

Step4: perform the sensitivity analysis

When the goal is to determine the most important input variable, the first order sensitivity index is calculated, that is,

$$S_i = \frac{\text{Var}[E(\text{profit}|x_i)]}{\text{Var}(\text{profit})} \quad (32)$$

The total sensitivity index indicates the magnitude of the interactions between the i^{th} cost component and other components,

$$ST_i = \frac{E[\text{Var}(\text{profit}|x_i)]}{\text{Var}(\text{profit})} \quad (33)$$

For details of this calculation process please refer to the work of Lilburne and Tarantola [33]. The interpretation of the index is straightforward, the higher the first order sensitivity index (S_i) of an input variable, the greater their influence on the model output. While the lower the total sensitivity index (ST_i), the less the interactions between i^{th} cost component and other components. Fig. 6 gives the results of the GSA method.

The black dots in Fig. 6 show that the material purchase cost (Cmp), material and product transportation cost (Ctr), and refinery operation cost (Cro) rank as the top three influential cost components for the

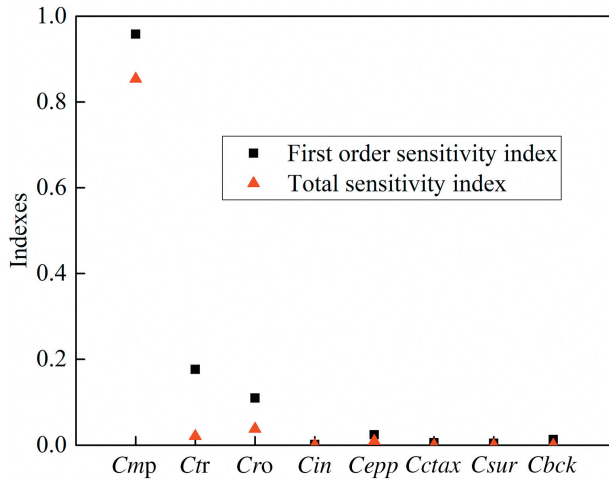


Fig. 6. Results of the global sensitivity analysis.

overall profit. While from the red dots in Fig. 6, one can notice that *Cro* exhibits greater interactions with other components when compared with the *Ctr*, regardless of the higher influence of *Ctr* on the overall profit.

5. Conclusions

This work introduced a novel stochastic scenario generation method based on the probability distribution pattern of the stochastic parameters, and these scenarios were incorporated into the MILP model in order to capture the random factors in the stochastic optimization of the large-scale petrochemical supply chain. The scenario generation method showed good performance in portraying the stochastic characteristics of the petrochemical supply chain optimization problem, and the 225 discretized scenarios can be adequate enough in dealing with the continuous random parameters in the case study.

The best kick-point where computational cost and accuracy of approximations can be compromised was pinpointed, so that conclusions can be drawn as that for the scenario-based stochastic programming, reasonable numbers of discretized scenarios can be good approximations of the continuous random parameters. A criterion ε was established to determine the desirable N value for general cases. In addition, the global sensitivity analyses gave the sequence of cost components' influence on the overall profit and the interactions of each cost component with other components.

For future study, in order to further reduce number of variables, reliable correlations between the random parameters may be incorporated into the model.

Nomenclature

B	set of distribution bases indexed by b1, b2, b3
BCK_p^{tp}	penalty for production backlog per ton of product not being able to be produced at time period tp
C	set of domestic customers indexed by c1, c2, c3, c4, c5
$CAPL_{r,m}^{tp}$	lower limit of operation capacity of refinery r to process material m at time period tp
$CAPU_{r,m}^{tp}$	upper limit of operation capacity of refinery r to process material m at time period tp
$Cbck^{sc^n}$	cost of production backlog penalty of scenario sc^n
$Cctax^{sc^n}$	cost of carbon emission tax of scenario sc^n
$Cepp^{sc^n}$	cost of extra product purchased of scenario sc^n
Cin^{sc^n}	cost of inventory of scenario sc^n
Cmp	cost of material purchase
$Cmtr$	cost of material transportation
$Cptr^{sc^n}$	cost of product transportation of scenario sc^n
Cro^{sc^n}	cost of refinery operation of scenario sc^n

$Csur^{sc^n}$	cost of production surplus penalty of scenario sc^n
$DEM_{p,oc}^{sc^n, tp}$	demand for product p of overseas customer oc at time period tp of scenario sc^n
$DEM_{p,c}^{sc^n, tp}$	demand for product p of domestic customer c at time period tp of scenario sc^n
$DIS_{n,n'}$	distance between node n and n'
$DSR_{r,m}$	desulfurization ratio of material m at refinery r
Ecr	quantity of CO ₂ emitted per ton of material operated at refinery r
$EPPU_p^{tp}$	purchase upper limit of extra product p at time period tp
$E[profit]$	expected profit
$EPUP_{p,te}^{tp}$	unit price of extra product p purchased at terminal te at time period tp
$IVU_{m,r}^{tp}$	inventory upper limit of refinery r for material m at time period tp
$IVU_{p,te}^{tp}$	inventory upper limit of terminal te for product p at time period tp
$IVU_{p,b}^{tp}$	inventory upper limit of distribution base b for product p at time period tp
$IVUP_{m,r}^{tp}$	inventory unit price for material m at refinery r at time period tp
$IVUP_{p,te}^{tp}$	inventory unit price for product p at terminal te at time period tp
$IVUP_{p,b}^{tp}$	inventory unit price for product p at distribution base b at time period tp
$iqsp_{p,oc}^{sc^n, tp}, iqbp_{p,oc}^{sc^n, tp}, iqsp_{p,c}^{sc^n, tp}, iqbp_{p,c}^{sc^n, tp}$	are 0–1 variables
M	set of materials indexed by m1, m2, ..., m11
$MUP_{m,of}^{tp}$	unit price of material m purchased at oil field of at time period tp
$MUP_{m,te}^{tp}$	unit price of material m purchased at terminal te at time period tp
$MTUP_{m,n,n',tr}^{tp}$	unit price of transportation for material m by transportation tool tr at time period tp
MPU_m^{tp}	purchase upper limit of material m at time period tp
$m_{m,n,n',tr}^{tp}$	flow of material m from node n to n' by transportation tool tr at time period tp
N	set of nodes in the supply chain model indexed by n and n' ($n \neq n'$)
OC	set of overseas customers indexed by oc1, oc2
OF	set of oil field indexed by of
P	set of products indexed by p1, p2, ..., p15
$PROB^{sc^n}$	probability of scenario sc^n
$PTUP_{p,n,n',tr}^{tp}$	transportation unit price for product p from node n to n' by transportation tool tr at time period tp
$PUP_{p,te}^{sc^n, tp}$	unit price for product p purchased at terminal te at time period tp of scenario sc^n
$PUP_{p,b}^{sc^n, tp}$	unit price for product p purchased at distribution base b at time period tp of scenario sc^n
$p_{p,r,b,tr}^{sc^n, tp}$	flow of product p from refinery r to distribution base b by transportation tool tr at time period tp of scenario sc^n
$p_{p,r,te,tr}^{sc^n, tp}$	flow of product p from refinery r to terminal te by transportation tool tr at time period tp of scenario sc^n
$p_{p,b,c,tr}^{sc^n, tp}$	flow of product p from distribution base b to domestic customer c by transportation tool tr at time period tp of scenario sc^n
$p_{p,te,oc,tr}^{sc^n, tp}$	flow of product p from terminal te to overseas customer oc by transportation tool tr at time period tp of scenario sc^n
$p_{p,te,b,tr}^{sc^n, tp}$	flow of product p from terminal te to distribution base b by transportation tool tr at time period tp of scenario sc^n
$p_{p,n,n',tr}^{tp}$	flow of product p from node n to n' by transportation tool tr at time period tp
$QBU_{p,oc}^{tp}$	upper limit of backlog product p needed by overseas customer oc at time period tp
$QBU_{p,c}^{tp}$	upper limit of backlog product p needed by domestic customer c at time period tp
$QSU_{p,c}^{tp}$	upper limit of surplus product p to be purchased by domestic customer c at time period tp

$QSU_{p, oc}^{tp}$ upper limit of surplus product p to be purchased by oversea customer oc at time period tp

$qbp_{p, c}^{sc^n, tp}$ quantity of backlog product p needed by customer c at time period tp of scenario sc^n

$qbp_{p, oc}^{sc^n, tp}$ quantity of backlog product p needed by oversea customer oc at time period tp of scenario sc^n

$qebp_{p, b, te}^{sc^n, tp}$ quantity of extra product p purchased at terminal te to be sold at distribution b at time period tp of scenario sc^n

$qep_{p, te}^{sc^n, tp}$ quantity of extra product p purchased at terminal te to be sold onsite at time period tp of scenario sc^n

$qmo_{r, m}^{sc^n, tp}$ quantity of material m operated by refinery r at time period tp of scenario sc^n

$qmp_{m, te, r}^{tp}$ quantity of material m purchased at terminal te by refinery r at time period tp

$qmp_{m, of, r}^{tp}$ quantity of material m purchased at oil field of by refinery r at time period tp

$qmsto_{m, r}^{sc^n, tp}$ quantity of material m stocked at refinery r at time period tp of scenario sc^n

$qmr_{m, n, n', r}^{tp}$ quantity of material m transported from node n to n' by transportation tool tr at time period tp

$qpb_{p, r, b}^{sc^n, tp}$ quantity of product p produced by refinery r sold at distribution b at time period tp of scenario sc^n

$qps_{p, oc, te}^{sc^n, tp}$ quantity of product p sold at terminal te to overseas customer oc at time period tp of scenario sc^n

$qps_{p, c, b}^{sc^n, tp}$ quantity of product p sold at distribution b to domestic customer c at time period tp of scenario sc^n

$qpsto_{p, b}^{sc^n, tp}$ quantity of product p stocked at distribution b at time period tp of scenario sc^n

$qpsto_{p, te}^{sc^n, tp}$ quantity of product p stocked at terminal te at time period tp of scenario sc^n

$qpte_{p, r, te}^{sc^n, tp}$ quantity of product p produced by refinery r sold at terminal te at time period tp of scenario sc^n

$qptr_{p, n, n', tr}^{sc^n, tp}$ quantity of product p transported by transportation tool tr from node n to n' at time period tp of scenario sc^n

$qsp_{p, c}^{sc^n, tp}$ quantity of surplus product p to be purchased by customer c at time period tp of scenario sc^n

$qsp_{p, oc}^{sc^n, tp}$ quantity of surplus product p to be purchased by customer oc at time period tp of scenario sc^n

R set of refineries indexed by r_1, r_2, r_3

$ROUP_{r, m}^{tp}$ operation unit price for refinery r to process material m at time period tp

$Sales^{sc^n}$ sales of scenario sc^n

SC set of scenarios indexed by sc^n

SC_m^{tp} sulfur content of material m at time period tp

SC_p^{tp} sulfur content of product p at time period tp

SUP_p^{tp} penalty for production surplus per ton of product p produced at time period tp

$TAXC$ tax per ton of CO_2 emitted

$TCAU_{n, n', tr}^{tp}$ transportation upper limit from node n to n' by transportation tool tr at time period tp

TE set of terminals indexed by te

TP set of time periods indexed by tp_1, tp_2, tp_3

TR set of transportation tools indexed by tr_1, tr_2, tr_3, tr_4

$YDR_{r, m, p}$ yield ratio of material m to product p at refinery r

Acknowledgements

We gratefully acknowledge the support from the National Natural Science Foundation of China (No. 21676183), and State Key Laboratory of Chemical Engineering, Collaborative Innovation of Chemical Science and Engineering (Tianjin).

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