



## Modeling and Optimization of Chemical Fertilizers Supply Chain Using Hybrid Whale Optimization and Simulated Annealing

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**Revise Date:** 01 December 2022 **Abstract**

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Phosphorus is a basic constituent of chemical fertilizers and plays a pivotal role in crop yield enhancement in agriculture systems. Considering the growing demands for phosphorus and the limited resources of this vital substance, sustainable supply chain management (SCM) of chemical fertilizers is of great importance. In the present study, a mathematical model for sustainable chemical fertilizer SCM is presented. Taking into account the adverse environmental effects of the production and consumption of chemical fertilizers, the present study attempts to design a sustainable SCM concerning economic, environmental, and social factors. To solve the problem, a hybrid metaheuristic algorithm incorporating whale optimization and simulated annealing is used considering a multi-objective function. The simulation results obtained from a real case study of the chemical fertilizers supply chain network in Iran proved the effectiveness and applicability of the proposed model and solution method. Obtained results show the effectiveness of the proposed method compared with other algorithms with respect to economic, social, and environmental factors.

### Keywords:

Chemical fertilizers

Phosphorus

Sustainable supply chain management

Whale optimization algorithm

Simulated annealing

## INTRODUCTION

Phosphorus-based chemical fertilizers play a significant role in increasing productivity and product quality in the agriculture industry. Phosphorus (P) is regarded as the most widely used element in the chemical fertilizer industry. Phosphate rock (PR), as a limited and non-renewable material, is considered the main source of phosphorus (Scholz et al., 2013). Modern agriculture consumes a large quantity of phosphate in order to make crops grow, and as a result, with growing of the population in the world and the increased demand for agricultural products, phosphorus consumption is increasing (Roos et al., 2013). Given this increase in demand, some underground phosphorus mines are close to being run out. Also, the world's known PRs are located in limited countries, which has become a matter of concern (Gong et al., 2022a). In this regard, some countries have to import PR or ready-made chemical fertilizers from other countries.

Current strategies for the management of P production and consumption suffer from the depletion of PRs, low PUE (P-use efficiency), and high P-induced environmental factors (Luo et al., 2017). One of the important concerns in this regard is to provide a strategy in order to conserve the environment (Simons et al., 2014). Considering the limited PR mines and environmental issues of the chemical fertilizers, especially on the ecosystem, as well as the adverse effects of excessive use of P, sustainable management of P-use should give particular attention to understanding the prerequisites for adequate P supply. In this regard, societies can prevent water pollution and ensure long-term food security as well as the potential negative effects of P crops on terrestrial biodiversity (Garske & Ekardt, 2021). Technically, in order to ensure the system's survival, sustainability and flexibility should be taken into account simultaneously by exploiting synergies of these two issues. Furthermore, the supply chain must be flexible so that it can maintain its sustainable performance, especially considering the environmental dimension (Mehrjerdi & Shafiee, 2021). Despite the great importance of P supply

chain network optimization, it has been a long time since this issue has not received enough attention from researchers, especially by mathematical modeling from the operations research point of view.

In recent years, researchers have paid special attention to phosphorus as a rare and critical resource. Generally, P-based chemical fertilizers including medium-low PR processing fertilizers such as single super P (SSP), triple super P (TSP) and calcium magnesium P (CMP), and high PR processing such as mono-ammonium P (MAP), di-ammonium P (DAP) and nitrogen P potassium (NPK) (Gong et al., 2022a). Most of the wastes caused by the application of fertilizers on the soil to the branch point are observed in the wastewater of agricultural lands (Scholz & Welmer, 2015). Research on phosphorus production and its use show that 80% of wastes originate from mine to the branch point, while 10% of the processed phosphorus fertilizer is consumed by humans (Cordell et al., 2009). According to UNWA (United Nations Wastewater Assessment) reports, insufficient wastewater imposes adverse effects on human health, the environment, and the economy (Zhongming et al., 2021). Phosphorus wastewater and untreated phosphorus sewage are considered the main causes of the development or expansion of "dead zones" (Nedelciu et al., 2020). This phenomenon imposes tangible adverse effects on the environment and the livelihood of people who live in these areas. P-rich wastewater is also considered as a threat to marine biodiversity (Martinez-Escobar & Mallela, 2019). The PR extraction and refinement for the production of phosphorus fertilizers can be regarded as the main cause of almost all impacts of the phosphorus supply chain on climate and air quality (Oberle et al., 2019).

### **Phosphorus fertilizer supply chain management**

Modeling and optimization of the phosphorus supply chain network play an effective role in management's decision-making on the reliable P stock flow among the different levels of the P supply chain, from the suppliers to the consumers. In particular, studies in the literature that consider important concerns of the P SCMs, e.g., flexibility

and sustainability challenges, are worthy of attention. In addition, regional discordances of fertilizer requirements and environmental issues on P-SCM have not so far received enough attention. The literature in the field of phosphorus supply chain typically uses quantitative models to evaluate phosphorus deficiency. In these researches, it is assumed that the recycling of the phosphorus-containing waste in their model involved the reabsorption of phosphorus materials in food industry wastes. To address concerns about phosphorus depletion, Van Vuuren et al. (2010) developed a production and exchange model, concluding that phosphorus will not be depleted in the short or medium term. Mohr & Evans (2013) presented a model of demand-production interaction, which considers low, high, and best estimation modes of maximum phosphate production.

Some studies focus on the analysis and improvement of the yield of phosphorus products and the management of environmental activities of the phosphorus supply chain (Gong et al., 2022a; Rabbani et al., 2022; Shokouhifar et al., 2023). Researchers have applied a series of integrated and single-factor methods in order to improve the efficiency of phosphorus fertilizer use in agricultural systems (Bai et al., 2013; Withers et al., 2014; Gong et al., 2022b). They have a yield response to phosphorus fertilizer to evaluate the optimized usage of phosphorus fertilizers for soil with phosphorus deficiencies (Bai et al., 2013). Also, Li et al. (2011) proposed a maintenance and compensation technique for management of phosphorus with P abundance. In another research, a practical approach has been examined to reduce environmental effects of phosphorus fertilizer (Gong et al., 2022b). In addition, the replacement strategy indicates that feeding the roots of crops instead of the soil can result in high efficiency of phosphorus fertilizer application (Withers et al., 2014).

In terms of sustainable approaches in agriculture, phosphorus supply chain management faces problems related to PR extraction, phosphorus fertilizer production, and crop production. The impact of different phosphorus fertilizers on PUE should be quantitatively calculated and analyzed

from the supply chain perspective (Nedelciu et al., 2020). The nature and magnitude of the flow of phosphorus materials in the supply chain should be determined as well (Chowdhury et al., 2016). Recent studies have used these two approaches in order to identify general trends in P flow.

### **Our contributions to the literature**

Despite extensive research in the field of chemical fertilizer production and consumption management, there are very limited studies with a focus on the issues related to the P-based chemical fertilizer sustainable SCM. To fill these gaps, we introduce a multi-objective model considering the economic, social, and environmental issues of the SCM. In addition to the economic costs (e.g., purchase of raw materials, production, maintenance, and transportation), the presented model evaluates the improvement of PUE (as a social objective) as well as the reduction of adverse environmental effects from the supply chain perspective. Finally, we propose a hybrid metaheuristic algorithm based on whale optimization and the simulation annealing to solve the model. This model allows the decision-maker to make a compromise between conflicting objectives. The most important specific innovations presented by this study versus existing research are summarized as follows:

- Modeling a sustainable supply chain for phosphorus-based chemical fertilizers considering the concerns of raw material supply, production, and chemical fertilizer distribution.
- Providing a multi-objective optimization model with mathematical modeling taking into account the economic, social, and environmental considerations.
- Presenting an ensemble metaheuristic utilizing whale optimization and simulation annealing (WOASA), to simultaneously take advantage of the local and global search capabilities of these two algorithms and as a result, increase the speed of convergence and achieve a better solution.
- Using a real case study on the chemical fertilizer supply chain conducted in Iran, which studies 3 PR mines, 9 ammonia

supply factories, 7 phosphoric acid supply factories, 36 sulfuric acid supply factories, 40 chemical fertilizer production factories, and 32 distribution centers (provincial centers of Iran).

In the remainder of this study, the problem modeling and the proposed solution method are respectively introduced in Sections 2 and 3. The case study and simulation results are reported in Section 4. Finally, concluding remarks are discussed in Section 5.

### PROBLEM MODELING

In this section, we introduce a multi-objective mathematical model for sustainable chemical fertilizer supply chain management taking the economic, social, and environmental issues into account. In this regard, we consider not only the economic costs such as the purchase of raw materials, production, maintenance, and transportation costs, but also the PUE as a social issue and the reduction of adverse environmental effects of the supply chain. In the following, the problem statement is provided in Section “Supply chain model”, and then, the mathematical model is presented in Section “Objective function”.

#### Supply chain model

In this study, we consider a three-stage fertilizer SCM consisting of primary raw material suppliers, fertilizer producers, and distribution centers (provincial centers). The supply chain network model can be seen in Fig. 1. The proposed model is investigated in  $T$  time periods (months). Each distributor  $d$  may face the demand  $D_{dpt}$  for fertilizer type  $p$  in each month  $t$ . The list of notations in this paper is provided in Table 1. The following conditions are assumed in order to determine the obstacles of the model:

- Raw materials include phosphorus (P), ammonia (A), phosphoric acid (PA), and sulfuric acid (SA).
- Chemical fertilizers include TSP, SSP, and DAP.
- SSP consists of SA and P.
- TSP consists of PA and S.
- DAP consists of PA and A.
- Suppliers have limited capacity.
- The number of raw materials for a producer can be provided from different suppliers.
- Each producer may save some of the fertilizers at end of every month.
- Each distributor is able to buy from different producers until their need for different fertilizers is met.
- Each distributor is able to store some of the fertilizers that are surplus to consumption at end of each month.
- The delivery lead time between each supplier and producer as well as between each producer and distributor is ignored (zero). In other words, raw materials/fertilizers ordered at the beginning of month  $t$  are delivered to the producer/distributor in the same month  $t$ .
- Each producer may have one or more producing lines for the production of TSP, SSP, or DAP.
- Producers have limited capacities for the production of each fertilizer.
- Quantity of raw materials supplied by each supplier as well as the quantity demanded by each distributor for each period of time is assumed to be definite and scheduled.

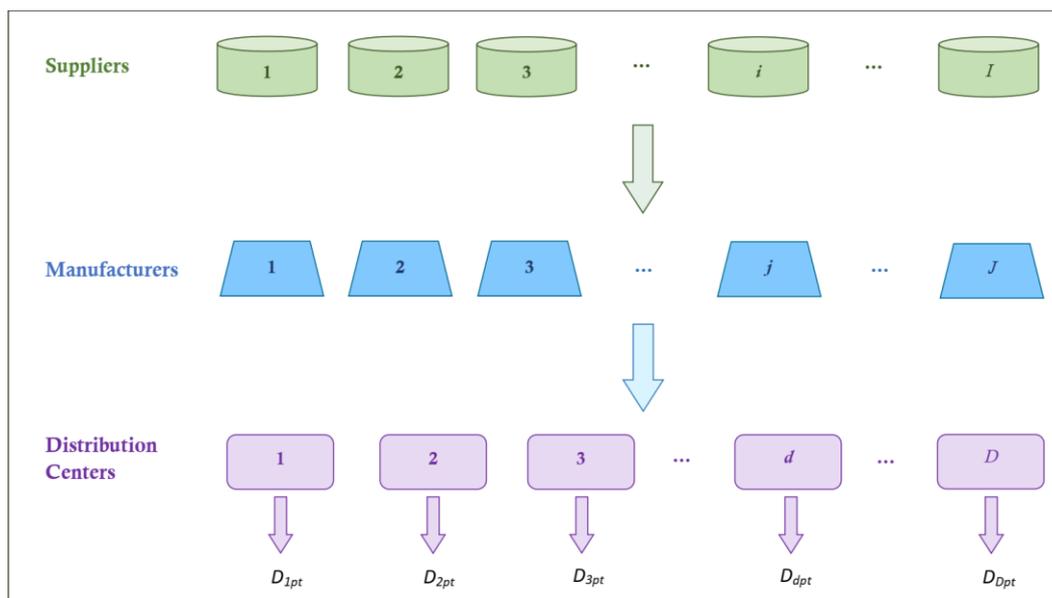


Fig. 1. Three-level model of chemical fertilizer supply chain.

Table 1: Notations.

**Indices and sets:**

- $i \in I$  suppliers
- $j \in J$  producers
- $d \in D$  distributors
- $r \in R$  raw materials (A, P, SA, PA)
- $p \in P$  chemical fertilizers (TSP, SSP, DAP)
- $t \in T$  months (time periods)

**Parameters:**

- $A_{ir}$  equal to 1 if material  $r$  is provided by supplier  $i$  and equal to 0 otherwise.
- $U_{rp}$  equal to 1 if material  $r$  is used for production of fertilizer  $p$  and equal to 0 otherwise.
- $CapS_{irt}$  quantity of material  $r$  supplied by supplier  $i$  in month  $t$  (tons)
- $CapP_{jpt}$  capacity of fertilizer  $p$  in production center  $j$  in each month for each month (tons)
- $WS_{jr}$  storage capacity of producer  $j$  in each month for material  $r$  (tons)
- $WP_{jp}$  storage capacity of producer  $j$  in each month for fertilizer  $p$  (tons)
- $WD_{dp}$  capacity of distribution center  $d$  in each month for fertilizer  $p$  (tons)
- $\alpha_{rp}$  quantity of material  $r$  needed for production of fertilizer  $p$  (%)
- $D_{dpt}$  demand of distribution center  $d$  for fertilizer  $p$  in month  $t$  (tons)
- $TS_r$  truck size for transporting material  $r$  (tons)
- $TP_p$  truck size for transporting fertilizer  $p$  (tons)
- $dS_{ij}$  distance between supplier  $i$  and production center  $j$  (kilometers)
- $dP_{jd}$  distance between production center  $j$  and distribution center  $d$  (kilometers)
- $FTCS_{ijr}$  fixed transporting cost of material  $r$  between supplier  $i$  and producer  $j$  (\$ per truck)
- $FTCP_{jdp}$  fixed transporting cost of fertilizer  $p$  between country  $k$  and distribution center  $d$  (\$ per truck)
- $VTCS_{ijr}$  variable transporting cost of material  $r$  between supplier  $i$  and production center  $j$  (\$ per truck per kilometer)
- $VTCP_{jdp}$  variable transporting cost of fertilizer  $p$  between producer  $j$  to distribution center  $d$  (\$ per truck per kilometer)
- $BCS_{ir}$  purchase cost of material  $r$  from supplier  $i$  (\$ per ton)
- $PC_{jp}$  producing cost of fertilizer  $p$  by producer  $j$  (\$ per ton)
- $ICS_{jr}$  cost of holding inventory of material  $r$  in producer  $j$  for each month (\$ per ton)
- $ICP_{jp}$  cost of holding inventory of fertilizer  $p$  in producer  $j$  for each month (\$ per ton)
- $ICD_{dp}$  cost of holding inventory of fertilizer  $p$  in distribution center  $d$  for each month (\$ per ton)
- $PY_p$  increase in the average yield of crops with fertilizer  $p$  (%)
- $G$  fuel consumption of vehicles (liters per kilometer)
- $e_t$  quantity of greenhouse gas emissions (tons) resulting from fuel per liter of gasoline
- $e_p$  greenhouse gas emissions (tons) resulting from production of type  $p$  products

$e_r$  greenhouse gas emissions (tons) resulting from production of type  $r$  material

**Direct decision variables:**

- $O_{jp}$  equal to 1 if producer  $j$  generates fertilizer  $p$ , otherwise equal to 0
- $P_{jpt}$  quantity of fertilizer production in producer  $j$  in month  $t$  (tons)
- $XS_{ijrt}$  equal to 1 if supplier  $i$  supplies material  $r$  to producer  $j$  in month  $t$  and equal to 0 otherwise.
- $XP_{jdpt}$  equal to 1 if producer  $j$  distributes fertilizer  $p$  to distribution center  $d$  in month  $t$  and equals 0 otherwise.
- $YS_{ijrt}$  quantity of material  $r$  transported from supplier  $i$  to production center  $j$  in month  $t$  (tons)
- $YP_{jdpt}$  quantity of fertilizer  $p$  delivered from production center  $j$  to distributor  $d$  in month  $t$  (tons)

**Indirect decision variables:**

- $SD_{dpt}$  delivered demands of distribution center  $d$  for fertilizer  $p$  in month  $t$  (tons)
- $SM_{jrt}$  delivered demands of producer  $j$  for material  $r$  in month  $t$  (tons)
- $US_{jrt}$  equal to 0 if the demand of producer  $j$  for material  $r$  is completely delivered in month  $t$ , and 1 otherwise.
- $UD_{dpt}$  equal to 0 if the demand of distribution center  $d$  for fertilizer  $p$  is completely delivered at month  $t$  and 1 otherwise.
- $IS_{jrt}$  quantity of inventory of material  $r$  kept in producer  $j$  in month  $t$  (tons)
- $IP_{jpt}$  quantity of inventory of fertilizer  $p$  kept in producer  $j$  in month  $t$  (tons)
- $ID_{dpt}$  quantity of inventory of fertilizer  $p$  kept in distribution center  $d$  in month  $t$  (tons)

**Objective function**

**Economic function**

Overall economic costs of the model contain the cost of raw material purchased from suppliers (CB), producers' production cost (CP), raw material and fertilizer inventory holding costs at producers and distributors (CI), and transportation costs (CT). These costs are respectively presented by Eqs. (1) - (4).

$$C_B = \sum_i \sum_r (BCS_{ir} \sum_t \sum_j YS_{ijrt} XS_{ijrt}) \quad (1)$$

$$C_P = \sum_j \sum_p PC_{jp} O_{jp} \sum_t P_{jpt} \quad (2)$$

$$C_I = \sum_t \sum_j \sum_r (ICS_{jr} IS_{jrt}) + \sum_t \sum_j \sum_p (ICP_{jp} IP_{jpt}) + \sum_t \sum_j \sum_p (ICD_{dp} ID_{dpt}) \quad (3)$$

$$C_T = \sum_t \sum_i \sum_j \sum_r \left( (FTCS_{ijr} + VTCS_{ijr} dS_{ij}) \left[ \frac{YS_{ijrt} XS_{ijrt}}{TS_r} \right] \right) + \sum_t \sum_j \sum_d \sum_p \left( (FTCP_{jdp} + VTCP_{jdp} dP_{jd}) \left[ \frac{YP_{jdpt} XP_{jdpt}}{TP_p} \right] \right) \quad (4)$$

Therefore, overall economic objective can be calculated as follows:

$$Z_{EC} = C_B + C_P + C_I + C_T = \left( \sum_i \sum_r (BCS_{ir} \sum_t \sum_j YS_{ijrt} XS_{ijrt}) \right) + \left( \sum_j \sum_p PC_{jp} O_{jp} \sum_t P_{jpt} \right) + \left( \sum_t \sum_j \sum_r (ICS_{jr} IS_{jrt}) + \sum_t \sum_j \sum_p (ICP_{jp} IP_{jpt}) + \sum_t \sum_j \sum_p (ICD_{dp} ID_{dpt}) \right) + \left( \sum_t \sum_i \sum_j \sum_r \left( (FTCS_{ijr} + VTCS_{ijr} dS_{ij}) \left[ \frac{YS_{ijrt} XS_{ijrt}}{TS_r} \right] \right) + \sum_t \sum_j \sum_d \sum_p \left( (FTCP_{jdp} + VTCP_{jdp} dP_{jd}) \left[ \frac{YP_{jdpt} XP_{jdpt}}{TP_p} \right] \right) \right) \quad (5)$$

**Social function**

Social objective can be defined to increase the average crop yields, which is calculated as:

$$Z_{SC} = \sum_p PY_p \left( \sum_t \sum_d SD_{dpt} \right) / \sum_p \sum_t \sum_d SD_{dpt} \quad (6)$$

**Environmental function**

Environmental objective is defined to reduce the total emission of greenhouse gases caused by the

raw material production, chemical fertilizer production, and transportation. This function can be calculated as follows:

$$\begin{aligned}
 Z_{EN} &= \left\{ \sum_t \left( \sum_p \sum_j P_{jpt} \cdot e_p + \sum_j \sum_r \sum_i YS_{ijrt} \cdot e_r \right) \right. \\
 &+ \left( \sum_i \sum_j \sum_r \left[ \frac{YS_{ijrt}XS_{ijrt}}{TS_r} \right] \cdot dS_{ij} \right. \\
 &\left. \left. + \sum_j \sum_d \sum_p \left[ \frac{YP_{jdpt}XP_{jdpt}}{TP_p} \right] \cdot dP_{jd} \right) \cdot G.et \right\} \quad (7)
 \end{aligned}$$

**Overall objective function**

The weighted average method is used to solve the multi-objective model. In this method, first, each objective function is normalized in the interval [0,1] with the aim of minimization using the Min-Max method. Then the overall objective function is expressed as a weighted average of three normalized objective functions according to the following equation:

$$OBJ = (w_{EC}Z_{EC} + w_{SC}Z_{SC} + w_{EN}Z_{EN}) \times PF \quad (8)$$

where w<sub>EC</sub>, w<sub>SC</sub> and w<sub>EN</sub> denote constant weighting coefficients in the interval [0,1] (w<sub>EC</sub>+w<sub>SC</sub>+w<sub>EN</sub>=1), which determine the relative significance of the three partial objective functions in the overall objective function; and PF represents a penalty function that is calculated as in the following relation:

$$PF = NUC + N_{US} \times (1 + AP_{US}) + N_{UD} \times (1 + AP_{UD}) \quad (9)$$

where NUC denotes the number of constraints which have not been satisfied. Moreover, NUS and NUD correspond to the unsatisfied demands of raw materials and chemical fertilizers, respectively. Finally, APUS and APUD represent the percentage of unsatisfied demands of producers and distributors, respectively.

**Constraints**

In the following, the problem constraints are expressed in three levels for distributors, producers, and suppliers, respectively.

$$\sum_t \sum_d SD_{dpt} \geq D_{dpt} \quad \forall p, \forall d, \forall t \quad (10)$$

$$ID_{dp0} = 0 \quad \forall d, \forall p \quad (11)$$

$$ID_{dpt-1} + \sum_j YP_{jdpt}XP_{jdpt} \geq SD_{dpt} \quad \forall d, \forall p, \forall t \quad (12)$$

$$\begin{aligned}
 ID_{dpt} &= ID_{dpt-1} + \sum_j YP_{jdpt}XP_{jdpt} \\
 &\quad - SD_{dpt} \quad \forall d, \forall p, \forall t \quad (13)
 \end{aligned}$$

$$ID_{dpt} \leq WD_{dp} \quad \forall p, \forall d, \forall t \quad (14)$$

$$XS_{ijrt} \leq \max_p(U_{rp}O_{jp}) \quad \forall i, \forall j, \forall r, \forall t \quad (15)$$

$$XP_{jdpt} \leq O_{jp} \quad \forall j, \forall d, \forall p, \forall t \quad (16)$$

$$P_{jpt}O_{jp} \leq CapP_{jp} \quad \forall j, \forall p, \forall t \quad (17)$$

$$IS_{jr0} = 0 \quad \forall j, \forall r \quad (18)$$

$$\begin{aligned}
 IS_{jrt-1} + \sum_t YS_{ijrt}XS_{ijrt} \\
 \geq \sum_p \alpha_{rp}P_{jpt}O_{jp} \quad \forall j, \forall r, \forall t \quad (19)
 \end{aligned}$$

$$\begin{aligned}
 IS_{jrt} = IS_{jrt-1} + \sum_t YS_{ijrt}XS_{ijrt} \\
 - \sum_p \alpha_{rp}P_{jpt}O_{jp} \quad \forall j, \forall r, \forall t \quad (20)
 \end{aligned}$$

$$IP_{jp0} = 0 \quad \forall j, \forall p \quad (21)$$

$$IP_{jpt-1} + P_{jpt}O_{jp} \geq \sum_d YP_{jdpt}XP_{jdpt} \quad \forall j, \forall p, \forall t \quad (22)$$

$$\begin{aligned}
 IP_{jpt} = IP_{jpt-1} + P_{jpt}O_{jp} \\
 - \sum_d YP_{jdpt}XP_{jdpt} \quad \forall j, \forall p, \forall t \quad (23)
 \end{aligned}$$

$$IS_{jrt} \leq WS_{jr} \quad \forall r, \forall j, \forall t \quad (24)$$

$$IP_{jpt} \leq WP_{jp} \quad \forall p, \forall j, \forall t \quad (25)$$

$$XS_{ijrt} \leq A_{ir} \quad \forall i, \forall j, \forall r, \forall t \quad (26)$$

$$\sum_j YS_{ijrt}XS_{ijrt} \leq CapS_{irt} \quad \forall i, \forall r, \forall t \quad (27)$$

Constraints (10)-(14) are associated with the distributors. Constraint (10) indicates that the total delivered fertilizer p to all distribution centers in month t should be equal to or more than their demand. Constraint (11) shows that the initial inventory in distributor d is zero. Constraint (12) expresses that the summation of inventory of fertilizer p in distributor d in month t and the purchased fertilizers should satisfy its demand. Constraint (13) shows the inventory of distribution center d for fertilizer p after delivery of demands at the end of month t. Constraint (14) expresses that inventory of fertilizer p in distribution center d in month t must not exceed the storage capacity.

Constraints (15) - (25) are related to producers. Constraint (15) stipulates that if producer j needs material r for the production of fertilizers, it can get raw material r from different suppliers in any month. Constraint (16) ensures that if there are no lines for producing fertilizer p in producer j, the producer cannot send any fertilizer of type p to a distributor. Constraint (17) ensures that the

quantity of fertilizer  $p$  in producer  $j$  in month  $t$  must not exceed its capacity. Constraint (18) indicates that the initial inventory of material  $r$  in producer  $j$  is zero. Constraint (19) shows that there is enough material for the production of fertilizer  $p$  in producer  $j$  in month  $t$ . Constraint (20) measures inventory of material  $r$  in producer  $j$  in month  $t$ . Constraint (21) indicates that the initial quantity of fertilizer  $p$  in producer  $j$  is zero. Constraints (22)-(23) ensure that the inventory of fertilizer  $p$  and the quantity of this fertilizer produced by producer  $j$  can meet the demand of period  $t$ . Constraints (24)-(25) ensure that the inventory of material or fertilizer stored in the warehouse of producer  $j$  does not exceed its capacity.

Constraints (26) and (27) are related to suppliers. Constraint (26) indicates that if material  $r$  is supplied by supplier  $i$ , the raw material required by producer  $j$  can be delivered from supplier  $i$ . Constraint (27) shows that the quantity of material  $r$  delivered and supplied by supplier  $i$  to all the producers in month  $t$  does not exceed the production capacity of supplier  $i$ .

### SOLUTION METHOD

Given that the supply chain management problem suffers from NP-hardness (Shokouhifar et al., 2021; Sohrabi et al., 2023), the best option to solve the proposed problem is to apply metaheuristic algorithms. Metaheuristics are either population-based having a suitable global search strategy (exploration), or single population-based (solution-based) using a local search strategy (exploitation) (Shokouhifar, 2021). In this paper, we apply a population-based metaheuristic based on WOA, a solution-based metaheuristic based on SA, and a hybrid metaheuristic based on WOA and SA (called WOASA algorithm) to optimize the proposed supply chain model. These algorithms are presented in the following.

#### Whale optimization algorithm

Whale optimization algorithm (WOA) is a swarm intelligence algorithm that was first introduced by Mirjalili & Lewis (2016). In each WOA iteration, the existing population is updated by the use of three search mechanisms, i.e., search for prey,

encircling prey, and bubble-net attacking (Ghasemi Darehnaei et al., 2021).

#### 3.2.1. Encircling prey

Assuming that the global best whale is optimal or close to the optimal solution ( $S^*$ ), each whale tries to move its position closer to  $S^*$ . This operator satisfies the following relation:

$$\vec{S}(t+1) = \vec{S}^*(t) - \vec{A} \cdot |2\vec{r} \cdot \vec{S}^*(t) - \vec{S}(t)| \quad (28)$$

$$\vec{A} = 2\vec{a} \cdot \vec{r} - \vec{a} \quad (29)$$

where  $\vec{r}$  denotes a random vector with elements in interval  $[0,1]$ ,  $t$  is the algorithm iteration number, and the elements of vector  $\vec{a}$  decrease linearly from the initial value 2 to the final value 0 in the process of running the WOA algorithm.

#### 3.2.2. Bubble-net attacking

A whale can be updated by modeling the process of whales attacking the bubble net as:

$$\vec{S}(t+1) = |\vec{S}^*(t) - \vec{S}(t)| \cdot e^{bl \cos(2\pi l)} + \vec{S}^*(t) \quad (30)$$

where  $l$  is a uniform random parameter in interval  $[-1,1]$ , and  $b$  is a fixed parameter that models the helix-shape motion of whales.

#### 3.2.3. Search for prey

If  $|A| > 1$ , the whale may move towards a completely random solution. This operator allows WOA to more explore in the entire search space. Using this operator, a whale is updated to a random whale ( $S_{rnd}$ ) as follows:

$$\vec{S}(t+1) = \vec{S}_{rand}(t) - \vec{A} \cdot |C \cdot \vec{S}_{rand}(t) - \vec{S}(t)| \quad (31)$$

#### Simulated annealing

Simulated annealing (SA) was first presented in 1983 inspired by the metal refrigeration process (Kirkpatrick et al., 1983). In SA, every possible solution is equivalent to the state of the system, and the objective is to minimize the internal energy of the system. The goal is to transfer the system from a random initial state to a state where the system contains the lowest energy (Behmanesh-Fard et al., 2023). In SA, first, an initial solution is randomly generated, and then, a new solution iteratively is constructed in the vicinity of the old solution. If the quality of the generated solution is higher than that of the old solution, SA considers it; otherwise, the new solution is accepted with probability  $P_{acp}$ , which is calculated as:

$$P_{acp} = \exp\left(-\frac{OF^{new} - OF^{current}}{T}\right) \quad (32)$$

where  $T$  is the temperature of the algorithm in the current iteration.

### Hybrid WOASA algorithm

As mentioned above, population-based metaheuristics have a better global search strategy (exploration). On the other hand, solution-based metaheuristics have suitable exploitation. To simultaneously take advantage of the two mentioned methods, we present a hybrid metaheuristic algorithm using WOA and SA (called WOASA algorithm) with the aim of efficiently optimizing the supply chain model. The proposed WOASA algorithm starts its search

by generating a random initial population of feasible solutions (whales), and then, in an iterative process, the quality of this population is improved with the help of the WOA operators. After running the WOA algorithm, the best global solution is provided to the SA algorithm as its initial solution. Then, SA tries to improve the quality of the existing solution by the use of local search operators. Algorithm 1 presents the pseudo-code of WOASA for optimization of the proposed supply chain model.

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**Algorithm 1.** Proposed WOASA algorithm.

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#### WOA:

1. Generation of a random population of whales:  $S_w$  ( $w=1,2,\dots,PopSize$ )
2. Calculation of  $OBJ$  for each solution using Eq. (8)
3.  $i = 0$
4. **while** ( $i \leq MaxIter_{WOA}$ )
5.     **for** each whale  $w$
6.         Update  $a$ ,  $p$ , and  $l$
7.         **if** ( $p > 0.5$ )
8.             Update solution  $w$  by *bubble-net attacking*
9.         **else**
10.             **if**  $|A| > 1$ , update solution  $w$  by the *search for prey*, otherwise, using *encircling prey*
11.         **end**
12.         Amend whale  $w$  if goes beyond the search space
13.     **end**
14. Calculation of  $OBJ$  for each solution using Eq. (8)
15. Updating GBS (global best solution)
16.  $i = i + 1$
17. **end**

#### SA:

1. Considering GBS as initial solution of SA:  $S^*$
2.  $j = 0$
3. **while** ( $j \leq MaxIter_{SA}$ )
4.     Generation of a neighbor  $S^*_{new}$
5.     Replace  $S^*$  by  $S^*_{new}$ , if  $OBJ^*_{new} < OBJ^*$  or  $rand < P_{acp}$
6.     Updating GBS
7.     Update  $T$
8.      $j = j + 1$
9. **end**

**Return GBS as the optimized supply chain model**

---

### Representation of a solution

As seen in Fig. 2, a possible solution to the problem is encoded as a hybrid structure consisting of 3 binary and 3 integer matrices. The

decision variables comprise S.O to specify the lines of fertilizer productions in producers, S.P to determine the quantity of producing fertilizers by different production centers for each month, two

binary matrices to determine the connections in the supply chain, and two integer matrices to specify the quantity of material/fertilizer

transportation between different levels of the supply chain.

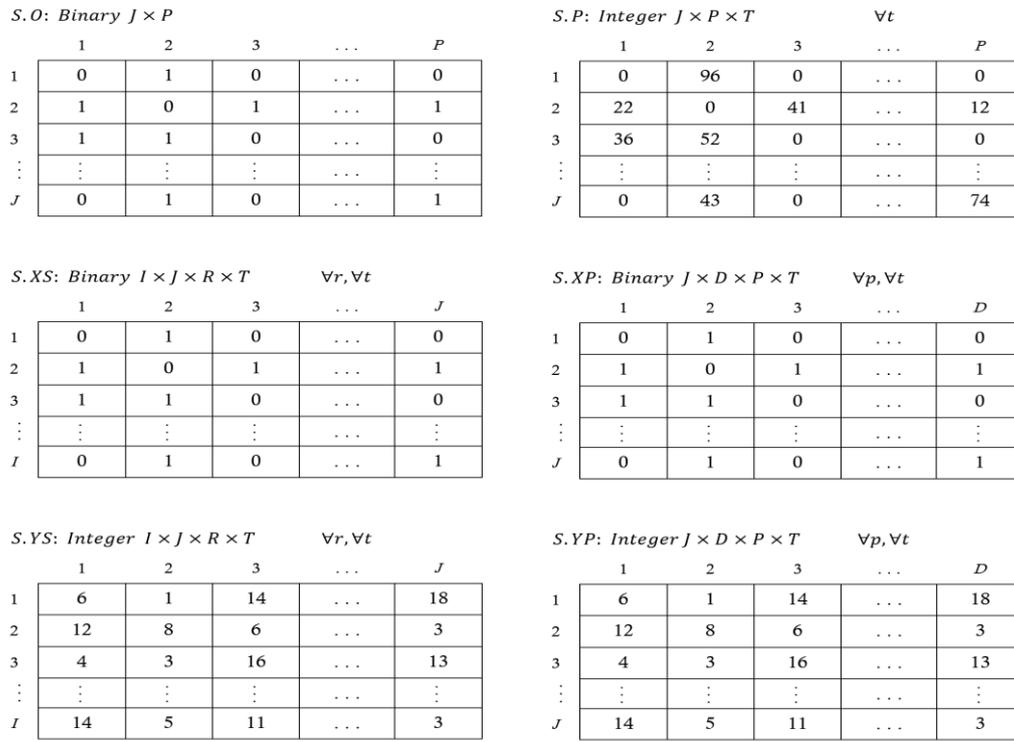


Fig. 2. Probabilistic solution coding.

**Global search using WOA**

At the beginning of the WOA algorithm, a population of whales is randomly generated. In each WOA iteration, the current population is updated using the search for prey, encircling prey, and bubble-net attacking operators. In order to update a whale, a uniform random parameter  $p$  in the interval of  $[0,1]$  is generated. If  $p \geq 0.5$ , the solution would be updated through the bubble-net attack operator, and when  $p < 0.5$ , a vector  $A$  is randomly constructed. Then, if  $|A| < 1$ , encircling prey is run, and otherwise, the solution would be updated by using search for prey.

**Local search using SA**

As stated above, in the proposed hybrid WOASA algorithm, the final global solution of the WOA is provided to the SA as the initial solution. In each iteration, a solution is constructed in the vicinity of the old solution. Then, SA may consider the new solution or not by checking the acceptance

rule. At the beginning of SA, a large value is assumed for the temperature  $T$  so that worse solutions can be accepted with a higher probability. As the temperature gradually decreases during the algorithm running, the probability of accepting worse solutions decreases. In this study, the temperature value decreases linearly from  $T_{initial}$  to  $T_{final}$  during the algorithm running. In order to develop a neighbor solution in the vicinity of the old one, the first one of the 6 structures in the solution is randomly selected. Then, depending on the selected structure, a local binary or integer operator is performed. Examples of binary and integer local search operators are shown in Figs. 3 and 4, respectively.

$S^*$	0	1	0	1	0	...	0
	1	1	1	0	1	...	0
	1	0	0	1	1	...	0
	0	1	0	0	1	...	1
$S^*_{new}$	0	1	0	1	0	...	0
	1	1	1	0	0	...	0
	1	0	0	1	1	...	0
	0	1	0	0	1	...	1

Fig. 3. Binary local search operator.

$S^*$	4	23	46	15	32	...	26
	20	41	16	25	36	...	51
	61	36	44	54	22	...	17
	28	45	33	16	51	...	73
$S^*_{new}$	4	23	46	15	32	...	26
	20	41	16	25	15	...	51
	61	36	44	54	22	...	17
	28	45	33	16	51	...	73

Fig. 4. Integer local search operator.

### SIMULATION

The data required for the case study of this research was collected from the statistical reports of the Soil and Water Research Institute (SWRI) of Iran and the experts' opinions. SSP, TSP, and DAP are the three types of phosphorus-based chemical fertilizers having the most application in Iran's agriculture. The raw materials for the production of these fertilizer types include A, P, SA, and PA. The details of the case study dataset are provided in Appendix 1.

#### Settings

The presented model was coded in the MATLAB R2020b environment and was solved with the help of the WOASA algorithm. All the simulations were performed on a PC with an i7,

2.56 GHz processor, 16 GB of memory, and Windows 10. Different values were evaluated in order to set each controllable parameter in the proposed algorithm, and finally, the best value in terms of convergence speed and accuracy was considered for the final simulations. Table 2 lists the controllable parameters of the proposed algorithm.

Table 2: Parameters of WOASA.

Parameter	value
Iterations of WOA	100
Population of WOA	50
$b$ in WOA	1
Iterations of SA	5000
$T_{initial}$ in SA	2
$T_{final}$ in SA	0
Economic weight ( $w_{EC}$ )	0.5
Social weight ( $w_{SC}$ )	0.25
Environmental weight ( $w_{EN}$ )	0.25

### RESULTS

#### Comparison with exact search

In this section, we compare the WOASA algorithm with the results derived using the exact search for different test examples presented in Table 3 with different problem sizes. Table 4 presents the comparison of the results derived using the exact method and the WOASA algorithm (in 10 consecutive runs). According to this table, the average deviation of the solution of WOASA from the optimal solution ranges between 0 and 0.343% from small to medium problem sizes. Although the running time of the exact search for test problems 1 and 2 is lower than that of the WOASA algorithm, the running time of the exact search exponentially increases as the dimension of the problem increases. As can be seen, the exact method cannot find the optimal solution for large problems in an acceptable running time. However, the computational time to reach the near-optimal solution increases almost linearly as the problem size in the proposed method increases.

Table 3: Dimensions of the problems.

Problem	No. materials	No. products	No. suppliers	No. producers	No. distributors	No. months
1	2	1	1	1	1	3
2	2	1	2	2	2	3
3	2	2	2	3	2	6
4	2	2	3	5	3	6
5	3	2	5	10	3	12
Case study	4	3	45	40	32	12

Table 4: Comparison of WOASA with exact search method for different problems.

Data set	Exact Method (optimal solution)		WOASA (near-optimal solution)		
	OF	CPU Time (s)	OF	CPU Time (s)	Error (%)
1	0.6125	0.9	0.6125	7.3	0.00
2	0.582	4.7	0.582	12.1	0.00
3	0.5451	198	0.5456	38.4	0.092
4	0.6123	27350	0.6144	70.2	0.343
5	N/A	N/A	0.5246	182	N/A
Case study	N/A	N/A	0.5935	712	N/A

## Model analysis

Table 5 presents the results of WOASA to justify its performance for the case study dataset. Given the stochastic nature of metaheuristic algorithms, the results of running WOASA for 10 consecutive runs are reported in this table along with the mean and standard deviation of the results for all the runs. The small value of the standard deviation of the results in 10 consecutive runs indicates the suitable reliability of the proposed algorithm.

Figures 5 and 6 depict the convergence diagrams of WOASA in the running phases of the WOA and SA in 10 consecutive runs, respectively. As shown in Fig. 5, the WOA has a very high

convergence speed at the beginning, so the value of *OBJ* decreases from 0.7029 in the initial iteration to about 0.647 in the 40<sup>th</sup> iteration. However, after about 40 iterations of the WOA running, the convergence speed gradually decreases and no significant improvement is observed in the objective function value. Ultimately, the WOA phase ends with an objective function value of 0.6452 in the last iteration. In addition, as shown in Fig. 6, the local search operators in the SA algorithm once again make a significant improvement in the value of the objective function, resulting in the decrease of the value of the objective function to 0.5935.

**Table 5: Optimal value of objectives for case study dataset, obtained by WOASA.**

Run #	$Z_{EC}$ ( $10^6$ \$)	$Z_{SC}$	$Z_{EN}$ ( $10^6$ )	PF	OF
1	573.6	0.39	8.91	0	0.5932
2	571.3	0.412	8.66	0	0.5999
3	565.7	0.395	8.41	0	0.5855
4	571	0.423	9.1	0	0.6108
5	570.5	0.388	9.18	0	0.594
6	573.8	0.396	9.03	0	0.5978
7	567.1	0.385	8.47	0	0.5819
8	566.4	0.387	8.49	0	0.5828
9	569.7	0.391	8.7	0	0.5891
10	572	0.413	8.58	0	0.5997
Average	570.1	0.398	8.75	0	0.5935
STD %	0.5	3.3	3.2	0	1.52

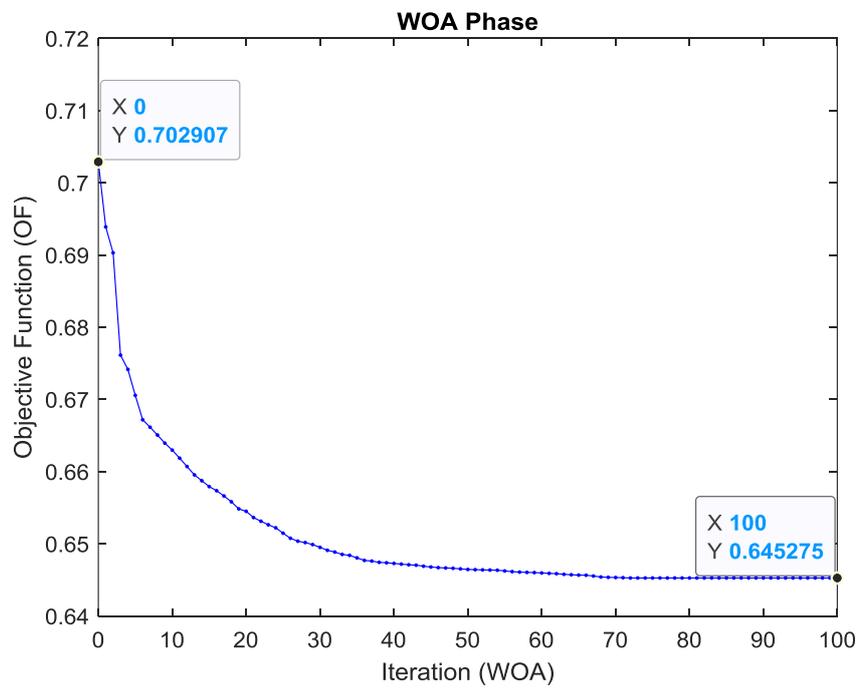


Fig. 5. Convergence diagram of the WOA phase.

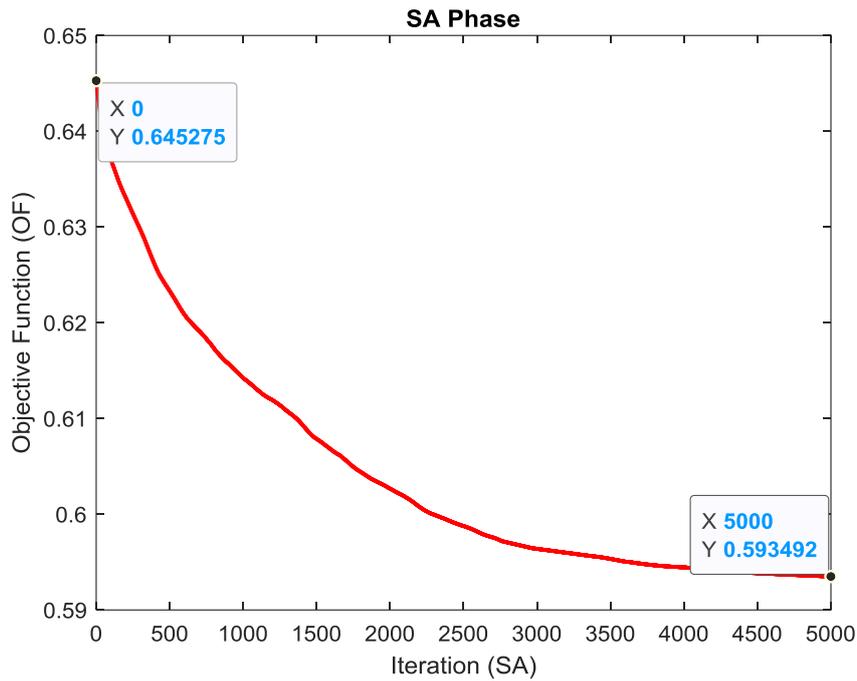


Fig. 6. Convergence diagram of the SA phase.

**Sensitivity Analysis**

The resources that are available in different situations can lead the decision-maker to make different decisions. As a result, sustainability goals (economic, environmental, and social issues) may have different effects (weights). Table 6 reports the results of WOASA according to the variations of these weights, which are used to investigate the effect of different weights on the objective function. The first row of this table shows the default value of these weights. The first three lines are related to the algorithm running

with three objective functions. The second three lines correspond to the algorithm running with two objective functions. Finally, the last three lines correspond to the single-objective running. According to this table, there are correlations between different goals. The social objective function tries to use more DAP fertilizers in order to increase the PUE, which, on the other hand, increases the economic costs. Moreover, the environmental objective seeks to reduce transportation and production quantities to decrease environmental pollution, which in turn demolishes the social objective.

Table 6: Sensitivity analysis of the proposed method by changing the objective function weights.

$w_{EC}, w_{SC}, w_{EN}$	$Z_{EC} (10^6 \$)$	$Z_{SC}$	$Z_{EN} (10^6)$
0.5,0.25,0.25	570.1	0.398	8.75
0.25,0.5,0.25	623.8	0.475	9.23
0.25,0.25,0.5	601.7	0.422	8.11
0,0.5,0.5	745.5	0.483	8.2
0.5,0,0.5	561.3	0.314	7.97
0.5,0.5,0	586	0.455	9.53
1,0,0	512.6	0.321	9.44
0,1,0	769.2	0.51	9.83
0,0,1	611.9	0.355	7.81

## CONCLUSION

In the present study, a mathematical model for the management of a chemical fertilizer sustainable supply chain network is presented and a hybrid metaheuristic algorithm encompassing whale optimization and simulated annealing is introduced to maximize model-solving accuracy. Finally, the designed model and the ensemble metaheuristic algorithm have been evaluated using a real case study dataset. The simulation results are indicative of higher accuracy of the proposed solution method compared to population-based and solution-based algorithms. The presented model helps managers to consider social and environmental issues in addition to economic costs, and try to enhance performance as one of their permanent responsibilities. Since sustainable phosphorus supply chain management has not received adequate attention in the literature, further studies can focus on the optimization of the supply chain of phosphorus

fertilizers using modeling approaches and solution-based methods. The need to establish new factories to solve the issues related to the shortage of fertilizers could also make a perfect and interesting area of study. Similarly, phosphorus recycling could make a research idea to reduce phosphorus dissipation rates and enhance network efficiency. Other metaheuristic algorithms such as Ant Colony Optimization, Aquila Optimizer, Grey Wolf Optimizer, Pareto-based techniques, and hyper-heuristic algorithms can also be recommended to solve the proposed model.

### Appendix 1: Case Study

Table 7 presents the required composition of these materials to produce different chemical fertilizers. Table 8 lists the average monthly demands of distribution centers. Tables 9 and 10 present the supply capacities of the raw materials and production capacities of the chemical fertilizers, respectively.

**Table 7: Characteristics of chemical fertilizers based on the composition of the materials (%).**

Fertilizer	P	A	PA	SA
TSP	40%	0	34%	0
SSP	64%	0	0	37%
DAP	0	23%	47%	0

**Table 8: Average monthly demand of distribution centers (provinces) by fertilizer type (tons).**

Distribution center	SSP	TSP	DAP
1	1679	1633	838
2	1518	1513	910
3	1518	1627	915
4	1257	1338	643
5	563	639	313
6	623	666	385
7	200	215	113
8	496	589	297
9	326	397	197
10	328	387	189
11	2745	2930	1584
12	671	767	389
13	3624	3761	2038
14	769	1018	485
15	263	343	153
16	667	753	397
17	2434	2977	1543
18	956	1153	487
19	270	337	132
20	1181	1363	732
21	1137	1152	623
22	1663	1706	1018
23	289	318	165
24	1775	1913	940

Distribution center	SSP	TSP	DAP
25	1026	1130	661
26	1156	1458	689
27	782	799	438
28	674	618	353
29	493	494	277
30	1440	1320	763
31	232	257	133
32	815	1003	487
Total	33,570	36,574	19,287

Table 9: Monthly capacity of suppliers (tons).

Material	Number of suppliers	Capacity	Total capacity
A	9	(1,350-125,00)	500,000
P	3	(5,000-35,000)	65,000
PA	7	(1,000-21,650)	75,000
SA	26	(1,250-54,150)	300,000

Table 10: Monthly capacity of producers (tons).

Producer No.	SSP	TSP	DAP
1	4650	1530	3090
2	630	510	990
3	2460	3750	3150
4	780	180	0
5	750	390	120
6	990	690	330
7	1740	780	630
8	600	345	300
9	960	330	0
10	1140	1230	0
11	870	450	240
12	1650	0	0
13	720	540	480
14	1350	420	360
15	1440	0	1020
16	990	240	195
17	720	435	0
18	3090	1710	0
19	750	600	330
20	0	4650	0
21	1560	0	720
22	6300	0	4650
23	0	4500	2850
24	2700	3450	1350
25	5550	3720	360
26	1050	900	690
27	630	180	0
28	3240	3690	1650
29	720	300	0
30	1350	195	540
31	1260	0	990
32	2850	600	0
33	510	360	300
34	2850	1440	0
35	540	330	150
36	1050	1200	1080
37	420	195	0
38	660	0	270
39	570	360	0
40	1050	360	300

Producer No.	SSP	TSP	DAP
Total	61,140	40,560	27,135

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