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Optimal Distribution-Inventory Planning of Industrial Gases. II. MINLP Models and Algorithms for Stochastic Cases

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ABSTRACT: In this article, we consider inventory-distribution planning under uncertainty for industrial gas supply chains by extending the continuous approximation solution strategy proposed in part I of this work. A stochastic inventory approach is proposed and incorporated into a multiperiod two-stage stochastic mixed-integer nonlinear programming (MINLP) model to handle uncertainty in demand and loss or addition of customers. This nonconvex MINLP formulation takes into account customer synergies and simultaneously predicts the optimal sizes of customers' storage tanks, the safety stock levels, and the estimated delivery cost for replenishments. To globally optimize this stochastic MINLP problem with modest computational time, we develop a tailored branch-and-refine algorithm based on successive piecewise-linear approximation. The solution from the stochastic MINLP is fed into a detailed routing model with a shorter planning horizon to determine the optimal deliveries, replenishments, and inventories. A clustering-based heuristic is proposed for solving the routing model with reasonable computational effort. Three case studies including instances with up to 200 customers are presented to demonstrate the effectiveness of the proposed stochastic models and solution algorithms.

1. INTRODUCTION

The design and operation of industrial gas inventory-distribution systems involve uncertainties at the strategic and operational levels. In the short term, the most common uncertainty is concerned with the product consumption and demands of the customers. In addition to demand fluctuations, it is common to have losses or additions of customers due to contract termination or new contracts that are signed. A deterministic planning model[1] is a useful tool to help reduce costs by taking into account customer synergies in inventory-distribution planning and integrating strategic tank sizing-decisions with operational vehicle routing decisions. However, uncertain demand fluctuations and uncertain additions and losses of customers can significantly affect the decision-making across the industrial gas supply chain. Thus, it is necessary to extend deterministic planning models to address these uncertainties and develop effective optimization algorithms for these problems.

A key component of decision-making under uncertainty is the representation of the stochastic parameters. There are two distinct ways of representing uncertainties. The scenario-based approach[2−6] attempts to capture the uncertainties by representing them in terms of a number of discrete realizations of the stochastic parameters, where each complete realization of all uncertain parameters gives rise to a scenario. In this way, all possible future outcomes are taken into account through the use of scenarios, in which recourse actions are anticipated for each scenario realization. The objective is to find a solution that, on average, performs well under all scenarios. This approach provides a straightforward way of formulating the problem, but its major drawback is that it typically relies on either a priori forecasting of all possible outcomes or the explicit/implicit discretizations of continuous probability distributions. Thus, the problem size increases exponentially as the number of uncertain parameters and scenarios increases. This is particularly true when using continuous multivariate probability distributions with Gaussian quadrature integration schemes. Alternatively, Monte Carlo sampling could be used, but it also requires a rather large number of samples to achieve a desired level of accuracy.

The uncertainty can also be addressed through a chance constraint approach, which considers the uncertainty by treating one or more parameters as random variables with known probability distributions. Through multivariate integration over the continuous probability distribution functions, this approach can lead to a reasonable-size deterministic equivalent representation of the probabilistic model. It circumvents the exponentially growing number of scenarios from explicit/implicit discretization or sampling, at the expense of introducing a certain number of nonlinear terms into the model.[7−9] Although this approach has the limitation of not explicitly integrating recourse actions, it can effectively handle demand uncertainty at the operational level, where the probabilistic description renders some operational planning variables stochastic. Based on the chance constraint method and some features of demand uncertainty, You and Grossmann[10−12] recently proposed stochastic inventory models to deal with demand uncertainty in the design and operation of process systems. In their works, the uncertain demand is hedged by holding a certain amount of safety stocks before demand

Received: August 21, 2010
Accepted: December 20, 2010
Revised: November 29, 2010
Published: January 28, 2011

dx.doi.org/10.1021/ie101758u | Ind. Eng. Chem. Res. 2011, 50, 2928–2945

realization. The safety stock level is estimated by using a chance constraint that links service level with a demand probability distribution. The need to allow recourse actions as in stochastic programming,[13] which can significantly increase problem size, is obviated by taking proactive action with the safety stocks. The stochastic attributes of the problem are translated into a deterministic optimization problem at the expense of adding nonlinear safety stock terms into the model.

As argued by Zimmermann,[14] the choice of the appropriate method for modeling the stochastic parameters is context-dependent, with no single theory being sufficient to model all kinds of uncertainty. The problem addressed in this article includes two types of uncertainty: customer demand fluctuation at the operational level and uncertain changes in the distribution network due to loss or addition of customers at the strategic level. Based on the nature of these nonlinearities, we employ the stochastic inventory approach to deal with demand uncertainty and use the scenario-based stochastic programming approach to handle the uncertain loss or addition of customers in the distribution network. We extend the continuous approximation approach, which is an efficient computational strategy for large-scale inventory-distribution planning of industrial gases, to address the two aforementioned types of uncertainty. The stochastic version of the continuous approximation solution strategy includes a two-stage stochastic mixed-integer nonlinear programming (MINLP) problem in the upper level and a decomposable mixed-integer linear programming (MILP) problem in the lower level. A global optimization method based on successive piecewise-linear approximation is proposed to effectively solve the stochastic MINLP at the upper level, and a clustering-based heuristic is proposed for solving the routing model at the lower level with reasonable computational effort. We present the model formulations and computational strategies in this article. Three case studies with up to 200 customers are solved to illustrate the application of the proposed models and the performance of the solution algorithms.

The rest of this article is organized as follows: The general problem statement is provided in section 2, which is followed by the proposed stochastic continuous approximation method in section 3. The model formulation of the stochastic continuous approximation model and the global optimization algorithm for solving it effectively are given in sections 4 and 5, respectively. In section 6, we present computational results for three case studies. The last section concludes this article, and the clustering-based heuristic method for solving the routing problem is given in the Appendix.

2. PROBLEM STATEMENT

We are given an industrial gas distribution network consisting of a production plant and a set of customers $n \in N$. The locations of the plant and customers, as well as the distances between them, are given as well. We are also given a set of tanks with different sizes $i \in I$. The lower and upper bounds for tanks with size i are given as T_i^{L} and T_i^{U}, respectively. We set the parameter $\mathrm{ot}_{i,n} = 1$ if customer n has an existing tank with size i and set it to zero otherwise. Similarly, the parameter $\mathrm{new}_n = 1$ if customer n is a new customer without any existing tank; otherwise, it is set to be zero. Each newly installed tank is full of merchant liquid product at the beginning. That is, the initial inventory, $\mathrm{Vzero}_{n,y}$, is assumed to be the same as the tank capacity for the new customers. For customers with existing tanks, their initial inventory levels are given. There is a set of trucks $j \in J$ with maximum capacities Vtruck_j. The delivery cost per distance traveled is given as ck_j. All trucks are assumed to have an average traveling speed (speed) and a maximum number of working hours per day, hpd. For each delivery by truck, there is a fixed percent of product loss, denoted as loss, and a minimum unloaded fraction given as frac. The capital cost of tank with size $i \in I$ is given as Ccap_i, and the service cost of installing, upgrading, or downgrading a tank with size $i \in I$ is Cser_i. Both capital cost and service costs are discounted with a working capital discount factor wacc and a depreciation period in years given as dep.

The uncertainties arise from demand fluctuations and the losses or gains of customers in the distribution network. We assume that customer demands follow normal distributions, and the uncertain losses/additions of customers are represented through a set of scenarios $s \in S$. We assume that all contracts are terminated or signed at the beginning of each year. Thus, the losses or additions of customers happen at the beginning of each year, which then defines a network structure for that year in the given scenario (see Figure 1 for an example). The probability of each scenario is given or can be derived from the probabilities of gaining or losing customers.

The problem is then to simultaneously determine the tank sizes and modification decisions at each customer location, as well as the schedule and quantity of each delivery for all possible realizations of uncertainty. The objective is to minimize the total expected cost.

Based on the aforementioned discussion, the major assumptions of this problem are listed as follows:

- Only one type of industrial gas is considered.
- Scenarios with different network structures and the associated probabilities can be obtained.
- Customers are added/lost at the beginning of the time period (year).
- Customer demand fluctuations follow a normal distribution.

For the continuous approximation approach, the major assumptions are as follows:

- Inventory routing is cyclic.
- All customers have the same replenishment lead time.
- The replenishment lead times are all the same in a year of a scenario.
- Only one type of truck is used in a given year of a scenario.

3. SOLUTION STRATEGY

We use the continuous approximation approach of part I[1] to deal with industrial gas inventory-distribution planning under uncertainty for two major reasons. The first one is its computational efficiency. As shown through the case studies in our previous work,[1] this approach is much more efficient than the integrated MILP approach and the route selection-tank-sizing approach for solving large-scale problems, with little sacrifice of the solution quality. By decoupling the decision-making at the strategic and operational levels and using a continuous approximation to estimate the routing cost, the proposed model can establish the optimal tradeoff between the strategic tank-sizing cost and the approximate routing cost to predict optimal tank-sizing decisions in the upper level. The lower level problem is then decomposed and solved as a vehicle routing problem with

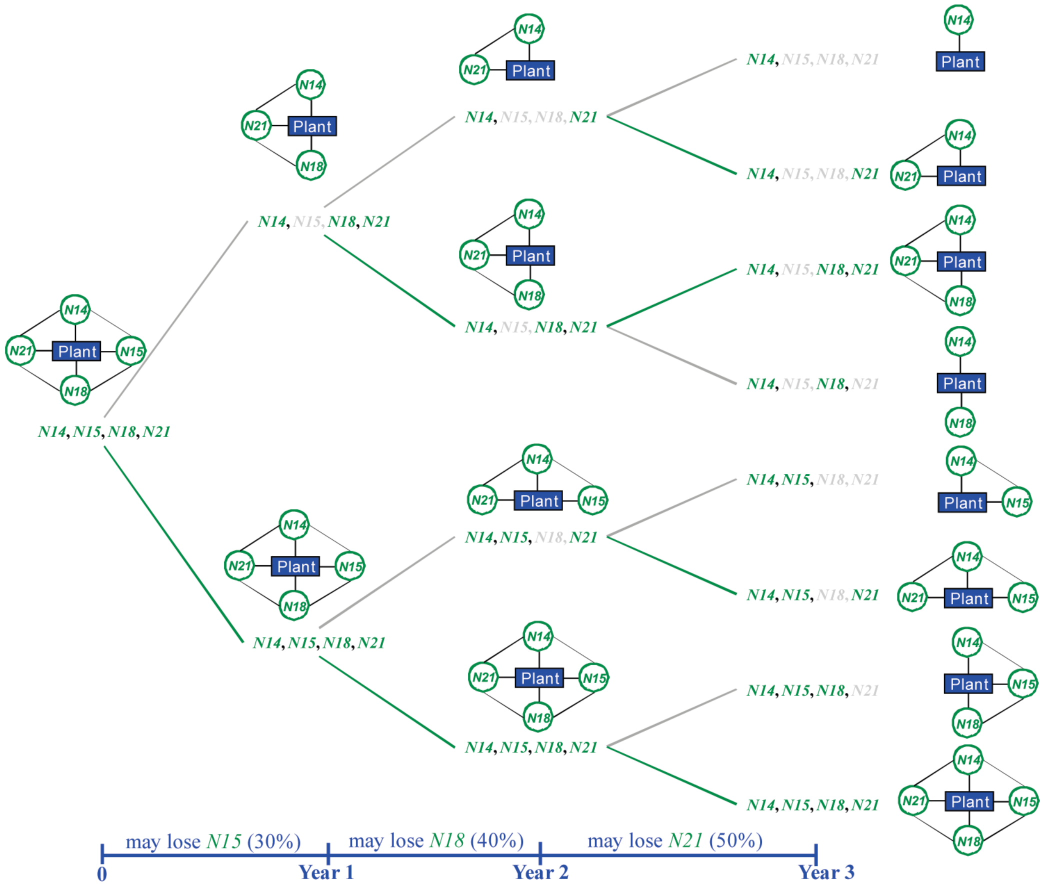


Figure 1. Industrial gas distribution network under uncertain loss of customers over time.

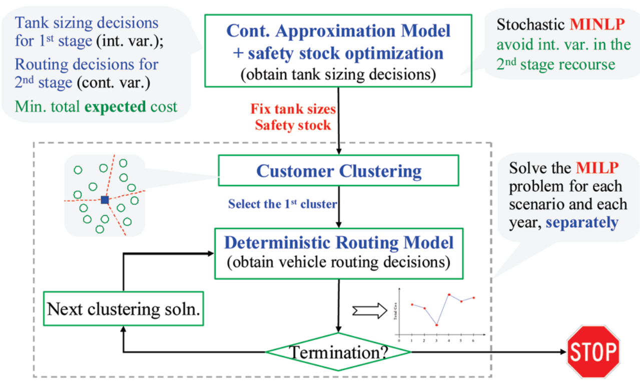


Figure 2. Inventory profile of a customer under cyclic inventory routing.

fixed tank sizes and shorter time horizon. The second major reason for using the continuous approximation approach is that the first stage decisions (here-and-now) of this problem are the tank-sizing decisions and the second stage decisions (wait-and-see) are the routing decisions. These decisions are usually modeled with binary variables, and their presence in the second stage of the stochastic programming problem gives rise to a significant computational challenge. However, the continuous approximation model can handle this challenge because it relies on very few binary variables and most discrete decisions are approximated using "continuous" functions. Therefore, the continuous approximation model is expected to have higher computational efficiency than other approaches that also incorporate stochastic programming.

The detailed algorithmic framework of the stochastic continuous approximation approach is given in Figure 2. At the upper level, we solve a stochastic version of the continuous approximation model by incorporating a stochastic inventory model for safety stock optimization. Although the deterministic continuous approximation model can be reformulated as an MILP, the inclusion of stochastic inventory approach introduces additional nonlinear terms (square-root terms) and renders the model as an MINLP. The stochastic continuous approximation model also includes a two-stage stochastic programming element by treating all the tank-sizing decisions as the first stage decisions and the remaining ones as the second stage. In this way, we avoid a large number of integer variables from detailed routing in the second stage of the stochastic programming model. Note that in principle, the problem could be formulated as a multistage stochastic programming model, but we only consider a two-stage approach in order to reduce the computational effort. Section 4 presents the detailed model formulation of the stochastic continuous approximation model and section 5 introduces an efficient global optimization algorithm to solve this upper level problem.

After solving the upper level stochastic continuous approximation model to obtain the optimal tank sizes and safety stocks, these decisions are passed to the lower level for detailed routing. Since both kinds of uncertainty are taken into account in the stochastic continuous approximation model, we only need to solve a deterministic version of the detailed routing problem for each year and each scenario, which includes a specific network structure. The detailed routing model is the same as the integrated MILP model presented in part I,[1] except that all the decisions for tank sizing and safety stocks are fixed using the values from the optimal solution of the stochastic continuous approximation model. Thus, the model formulation of the detailed routing problem is omitted in this paper. Vehicle routing problems have been well studied in the past decades and there are many heuristic methods that can be used to improve the computational efficiency.[15] In this work we use a clustering-based heuristic that is described in the Appendix.

4. STOCHASTIC CONTINUOUS APPROXIMATION MODEL

The stochastic continuous approximation model is a stochastic MINLP that simultaneously considers tank sizing, safety stock optimization and approximated vehicle routing. The detailed model formulation is given below, and a list of indices, sets, parameters and variables are given in the Appendix.

4.1. Objective Function. The objective function of this model is to minimize the total expected cost, including capital cost, service cost and distribution cost as given in eq 1.

$$\min : E[\text{cost}] = \sum_s \text{prob}_s(\text{capcost}_s + \text{servcost}_s + \text{distcost}_s) \quad (1)$$

where prob_s is the probability of scenario s and the detailed cost components are listed in constraints 2 − 5.

$$\text{capcost}_s = \frac{1}{\text{dep}}\left(\sum_i \text{Ccap}_i \times \sum_y \left[\sum_{\substack{n|\text{new}_n=0\wedge\text{tsize}_n=0\\ \wedge n\in N_{y,s}}} \frac{\text{ot}_{i,n}}{(1+\text{wacc})^{y-1}} + \sum_{\substack{n|\text{new}_n=0\wedge\text{tsize}_n=1\\ \wedge\text{espace}_n=0\wedge n\in N_{y,s}}} \frac{\text{yt}_{i,n}}{(1+\text{wacc})^{y-1}} + \sum_{\substack{n|\text{new}_n=0\wedge\text{tsize}_n=1\\ \wedge\text{espace}_n=1\wedge n\in N_{y,s}}} \frac{\text{ot}_{i,n}+\text{et}_{i,n}}{(1+\text{wacc})^{y-1}} + \sum_{\substack{n|\text{new}_n=1\\ \wedge n\in N_{y,s}}} \frac{\text{yt}_{i,n}}{(1+\text{wacc})^{y-1}}\right]\right) \quad (2)$$

Equation 2 is for the capital cost of scenario s. The four terms correspond to rating (no tank sizing), replacing an existing tank, adding a tank to the extra space an existing customer and sizing the tank at a new customer location, respectively. $N_{y,s}$ is a subset of customers included in the distribution network of scenario s in year y.

Any tank change or addition leads to a service cost, as shown in eqs 3 and 4. The total distribution cost equals to the sum of discounted annual routing cost as in eq 5, where $crot_{y,s}$ is the estimated routing cost of scenario s in year y coming from the continuous approximation. Note that the capital, service and distribution costs are all discounted with the working capital discount factor *wacc*.

$$\text{servcost}_s = \frac{1}{\text{dep}}\left(\sum_i \sum_{n\in N_{y,s}} \text{Cser}_i \sum_y \frac{\text{tins}_{i,n}+\text{et}_{i,n}}{(1+\text{wacc})^{y-1}}\right) \quad (3)$$

where

$$\text{tins}_{i,n} \geq \text{yt}_{i,n} + \text{ot}_{i,n} \quad (4)$$

$$\text{distcost}_s = \sum_y \frac{\text{crot}_{y,s}}{(1+\text{wacc})^y} \quad (5)$$

We note that the distribution cost given in objective function 5 is the estimation cost of vehicle routing from the "continuous approximation method", and it is not the exact routing cost that can be derived from solving the detailed routing problem.

4.2. Tank-Sizing Constraints. Tank-sizing decisions are the first-stage decisions in the stochastic programming model, and they are independent of the scenarios. Although a potentially better approach for capital investment planning would be to allow the tank size to change every year using a multiperiod formulation for tank selection, we assume in this work that the tank sizes will not change in the planning horizon after installation in the first year as in part I.[1] Given that the market is dynamic in nature and that uncertainty in customer demand and in its set of neighbors grows in the future, capital investment decisions are made in the present, and the model is optimized on a periodic basis to assess potential changes in the capacity of the network

First, the two parameters tsize_n and espace_n are introduced to define the conditions for tank sizing. We set $\text{espace}_n = 1$ if there is extra space for installing another tank at customer n; otherwise, it is set it to be zero. Similarly, $\text{tsize}_n = 1$ if the tanks at customer n need to be sized or changed; otherwise, $\text{tsize}_n = 0$.

If the tank of customer n needs to be sized or changed, either a new tank will be installed in the extra space, or the current tank will be changed. If no tank is sized, no modification will be made. This relationship can be modeled by the constraint

$$\sum_i (\text{yt}_{i,n} + \text{et}_{i,n}) \leq \text{tsize}_n, \quad \forall n\in N_{y,s} \quad (6)$$

where $\text{yt}_{i,n}$ is also a binary variable that equals 1 if customer n will have a tank of size i installed and $\text{et}_{i,n}$ is a binary variable that equals 1 if customer n has a tank of size i installed in the extra space.

If there is no extra space ($\text{espace}_n = 0$), then no tank should be installed in the extra space, and at least one type of tank should be selected to replace the existing tank. On the other hand, if the storage tanks at customer n should be upgraded ($\text{tsize}_n = 1$) and there is extra space, then at most one type of tank should be selected to be installed at the extra space (i.e., one binary variable $\text{et}_{i,n}$ must be selected), and at the same time, there is no change to the existing tank (i.e., all $\text{yt}_{i,n}$ variables are zero). These logic relationships can be modeled by

$$\sum_i \mathrm{yt}_{i,n} = 1 - \mathrm{espace}_n, \quad \forall n \in N_{y,s} \text{ such that } \mathrm{tsize}_n = 1 \tag{7}$$

$$\sum_i \mathrm{et}_{i,n} \le \mathrm{espace}_n, \quad \forall n \in N_{y,s} \tag{8}$$

The minimum and maximum inventory levels of customer n depend on the storage tank(s) installed for this customer. Thus, they are modeled through the two equations

$$\mathrm{Vl}_n = \sum_i T_i^{\mathrm{L}}(\mathrm{ot}_{i,n} + \mathrm{yt}_{i,n} + \mathrm{et}_{i,n}), \quad \forall n \in N_{y,s} \tag{9}$$

$$\mathrm{Vu}_n = \sum_i T_i^{\mathrm{U}}(\mathrm{ot}_{i,n} + \mathrm{yt}_{i,n} + \mathrm{et}_{i,n}), \quad \forall n \in N_{y,s} \tag{10}$$

If a new customer n joins the distribution network, at least one new tank is selected to be installed, and the tank is assumed to be at full level; otherwise, the initial inventory level parameters are given

$$\mathrm{Vzero}_n = \mathrm{Vu}_n, \quad \forall n \in N_{y,s} | \mathrm{new}_n = 1 \tag{11}$$

4.3. Truck Constraints. Similarly to the deterministic version of this model, we assume that only one type of truck is selected for delivery in each year and each scenario. This assumption implies that all trucks have the same capacity and unit cost in each year and each scenario, although we do not explicitly account for truck availability in the continuous approximation. However, it should be noted that the "one-type-of-truck" assumption is associated with the continuous approximation, which is used at the strategic level for tank-sizing decisions. The availability of the trucks is considered in the lower-level detailed routing model (see part I[1] for details).

We note that different scenarios in different years might have different network structures and thus different selection of trucks. The following constraints are used to define the truck selection

$$\sum_j \mathrm{tru}_{j,y,s} = 1, \quad \forall y, s \tag{12}$$

$$\mathrm{cunit}_{y,s} = \sum_j \mathrm{ck}_j \mathrm{tru}_{j,y,s}, \quad \forall y, s \tag{13}$$

$$\mathrm{ccapic}_{y,s} = \sum_j \mathrm{tru}_{j,y,s} \mathrm{Vtruck}_j (1 - \mathrm{loss}), \quad \forall y, s \tag{14}$$

Constraint 12 shows that only one type of truck is selected per year, and $\mathrm{tru}_{j,y,s}$ is a binary variable that is equal to 1 if truck j is selected for delivery in year y and scenario s and 0 otherwise-zero. Constraints 13 and 14 are for the unit transportation cost ($\mathrm{cunit}_{y,s}$) in year y of scenario s and the effective delivery capacity ($\mathrm{ccapic}_{y,s}$) after adjustment of loss of the truck for a scenario in a specific year.

The lead time of a replenishment cycle ($\mathrm{LT}_{y,s}$) in year y of scenario s should not be less than the sum of the total travel time, which is given by the minimum routing distance ($\mathrm{mrt}_{y,s}$) divided by the traveling speed and the working hours per day (hpd), and the total loading time, which includes the loading times at the customer locations and at the plant. There will be at least $|N_{y,s}|$ times of loading in the customers as each customer will be visited at least once in a replenishment cycle. The loading time at the plant should be greater than the loading time of deliveries from the plant (FT_del). Thus, the lead-time constraint is given by

$$\mathrm{LT}_{y,s} \ge \frac{\mathrm{mrt}_{y,s}}{\mathrm{speed} \times \mathrm{hpd}} + \mathrm{FT\_load}|N_{y,s}| + \mathrm{FT\_del}, \quad \forall y, s \tag{15}$$

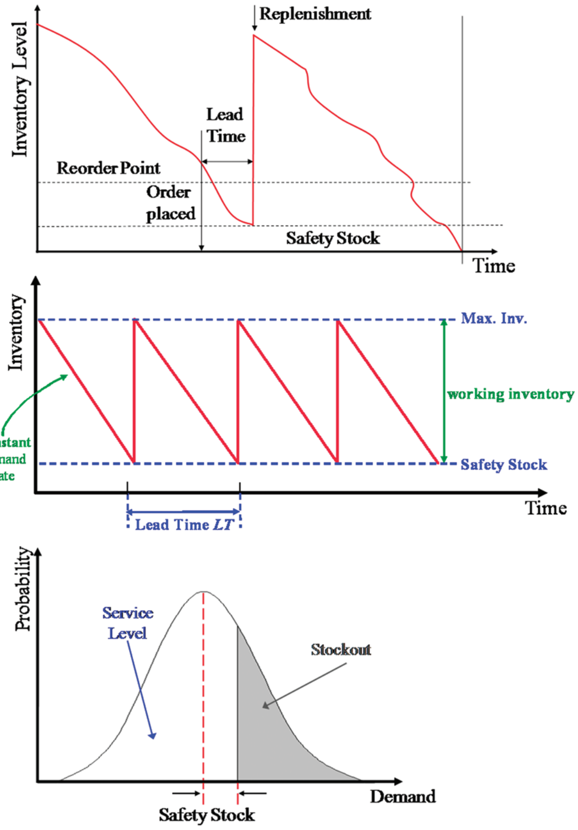


Figure 3. Stochastic inventory system under continuous approximation.

4.4. Cyclic Inventory Routing under Uncertainty Based on Continuous Approximation. Because the focus of this work is on strategic tank-sizing decisions, we employed a continuous approximation method to estimate the optimal routing cost as a result of different tank-sizing decisions. By using the continuous approximation, we simplify the detailed routing problem, while still capturing the tradeoff between capital costs and routing costs at the strategic level.

With the proposed approach, we approximate the discrete variables and parameters associated with vehicle routing using continuous functions, which represent distributions of customer locations and demands. The profile of an inventory system under uncertain demand is given in Figure 3a. Similarly to the deterministic case, we assume cyclic inventory routing for each scenario in each year because of their potentially different network structures and demands. Thus, the inventory profile of a customer for a scenario in a specific year is given in Figure 3b. From this figure, we have the tank size no less than the maximum inventory level, which is the sum of the working inventory and the safety stock.

The working inventory equals the demand rate times the replenishment lead time. The safety stock level can be determined by using the stochastic inventory approach as follows: A storage facility under demand uncertainty might not always have sufficient stock to handle the changing demand. If the inventory level is less than the demand during the replenishment lead time, stockout might happen. Type I service level is defined as the probability that the total inventory on hand is more than the demand (as shown Figure 3b). If the demand is normally distributed with mean μ and standard deviation σ, the optimal safety stock level to guarantee a service level α is $z_\alpha\sigma$, where z_α is a standard normal deviate such that $\Pr(z \le z_\alpha) = \alpha$.[16] If the demand rate is normally distributed with mean μ and standard deviation σ, then the uncertain demand over the replenishment lead time LT also follows a normal distribution with mean μLT and variance $\sigma^2\cdot$LT. Thus, the optimal safety stock level to guarantee a service level α is $z_\alpha\sqrt{\sigma^2\cdot LT} = z_\alpha\cdot\sigma\cdot\sqrt{LT}$.[16] Note that the accepted practice in this field is to assume a normal distribution of the demand, although, of course, other distribution functions can be specified. The stochastic inventory model has been shown to provide very good approximations for inventory systems under demand uncertainty.[17] In this way, the maximum inventory level is modeled as a nonlinear function of the replenishment lead time and demand probability distribution. A tradeoff between the inventory and routing costs is also established. If the replenishment frequency is high, the routing cost could also be high, but the working inventory level might be low, so only a small tank is needed, and vice versa.

If we use $x_{y,s}$ to denote the number of replenishment cycles in year y of scenario s. Then, the corresponding replenishment lead time ($\mathrm{LT}_{y,s}$) should satisfy the equation

$$\mathrm{LT}_{y,s}x_{y,s} = \mathrm{Hz}_y, \quad \forall y, s$$

where Hz_y is the time duration of year y. Note that both Hz_y and $\mathrm{LT}_{y,s}$ are in terms of physical days instead of working days, as customers consume demand continuously. The above equation has a bilinear term on the left-hand side. To linearize this term, similarly to part I,[1] the integer variable $x_{y,s}$ can be reformulated with binary variables $\mathrm{Ix}_{k,y,s} \in \{0,1\}$ as follows

$$x_{y,s} = \sum_k 2^{|k|-1}\mathrm{Ix}_{k,y,s}, \quad \forall y, s \tag{16}$$

where $\mathrm{Ix}_{k,y,s}$ determines the value of the kth digit, $k \in K$, of the binary representation of $x_{y,s}$. Note that the elements in set K depend on the upper bound of $x_{y,s}$. For example, if $x^{\mathrm{U}}_{y,s} = 63$, we can set K = 1, 2, 3, 4, 5, or 6.

With eqs 16, we can linearize the nonlinear constraint $\mathrm{LT}_{y,s}$-$x_{y,s} = \mathrm{Hz}_y$ as $\mathrm{LT}_{y,s}x_{y,s} = \sum_k 2^{|k|-1}\mathrm{LT}_{y,s}\mathrm{Ix}_{k,y,s}$. By introducing a nonnegative continuous variable $\mathrm{LTIx}_{k,y,s} = \mathrm{LT}_{y,s}\mathrm{Ix}_{k,y,s}$, we have the following reformulated constraint

$$\sum_k 2^{|k|-1}\mathrm{LTIx}_{k,y,s} = \mathrm{Hz}_y, \quad \forall y, s \tag{17}$$

We also need the following linearization constraints to define the new variable $\mathrm{LTIx}_{k,y,s}$[18,19]

$$\mathrm{LTIx}_{k,y,s} + \mathrm{LTIx1}_{k,y,s} = \mathrm{LT}_{y,s}, \quad \forall k, y, s \tag{18.1}$$

$$\mathrm{LTIx}_{k,y,s} \le \mathrm{LT}^{\mathrm{U}}_{y,s}\mathrm{Ix}_{k,y,s}, \quad \forall k, y, s \tag{18.2}$$

$$\mathrm{LTIx1}_{k,y,s} \le \mathrm{LT}^{\mathrm{U}}_{y,s}(1 - \mathrm{Ix}_{k,y,s}), \quad \forall k, y, s \tag{18.3}$$

$$\mathrm{Ix}_{k,y,s} \in \{0,1\}, \quad \mathrm{LTIx}_{k,y,s} \ge 0, \quad \mathrm{LTIx1}_{k,y,s} \ge 0, \quad \forall k, y, s \tag{18.4}$$

where $\mathrm{LTIx1}_{k,y,s}$ is an auxiliary variable and the upper bound of $\mathrm{LT}_{y,s}$ ($\mathrm{LT}^{\mathrm{U}}_{y,s}$) is given by the time duration of year y (Hz_y).

Let $\mathrm{Vm}_{n,y,s}$ be the maximum inventory level of customer n in scenario s and year y. From Figure 3, we know that the maximum inventory level should be no less than the sum of the working inventory ($\mathrm{winv}_{n,y,s}$), the safety stock ($\mathrm{safety}_{n,y,s}$), and the minimum volume of the tank in customer n in year y (Vl_n) defined in constraint 9. Thus, we have the constraint

$$\mathrm{Vm}_{n,y,s} \ge \mathrm{winv}_{n,y,s} + \mathrm{safety}_{n,y,s} + \mathrm{Vl}_n, \quad \forall n, y, s \tag{19}$$

The maximum inventory level should not exceed the maximum volume of the tank defined by the tank size of customer n in constraint 10

$$\mathrm{Vm}_{n,y,s} \le \mathrm{Vu}_n, \quad \forall n, y, s \tag{20}$$

As discussed above, the safety stock level should be equal to the product of the service level parameter z_α, the standard deviation of daily demand $\sigma_{n,y}$, and the square root of replenishment lead time $\mathrm{LT}_{y,s}$, which is measured in days

$$\mathrm{safety}_{n,y,s} = z_\alpha\sigma_{n,y}\sqrt{\mathrm{LT}_{y,s}}, \quad \forall n, y, s \tag{21}$$

For customer n, the working inventory ($\mathrm{winv}_{n,y,s}$) is the replenishment that it receives in a replenishment cycle. Thus, the working inventory times the number of replenishment cycles should be equal to the annual amount of product delivered from the plant to customer n in scenario s and year y ($\mathrm{Trp}_{n,y,s}$)

$$\mathrm{winv}_{n,y,s}x_{y,s} = \mathrm{Trp}_{n,y,s}, \quad \forall n, y, s$$

Based on eqs 16, we can reformulate the bilinear term on the left-hand side of the above equatioin as $\mathrm{winv}_{n,y,s}x_{y,s} = \sum_k 2^{|k|-1}\mathrm{winv}_{n,y,s}\mathrm{Ix}_{k,y,s}$. By introducing the nonnegative continuous variable $\mathrm{wIx}_{k,n,y,s} = \mathrm{winv}_{n,y,s}\mathrm{Ix}_{k,y,s}$, we can obtain the following reformulated linear constraint

$$\sum_k 2^{|k|-1}\mathrm{wIx}_{k,n,y,s} = \mathrm{Trp}_{n,y,s}, \quad \forall n, y, s \tag{22}$$

We also need the following linearization constraints to define $\mathrm{wIx}_{k,n,y,s}$

$$\mathrm{wIx}_{k,n,y,s} + \mathrm{wIx1}_{k,n,y,s} = \mathrm{winv}_{n,y,s}, \quad \forall k, n, y, s \tag{23.1}$$

$$\mathrm{wIx}_{k,n,y,s} \le \mathrm{winv}^{\mathrm{U}}_{n,y,s}\mathrm{Ix}_{k,y,s}, \quad \forall k, n, y, s \tag{23.2}$$

$$\mathrm{wIx1}_{k,n,y,s} \le \mathrm{winv}^{\mathrm{U}}_{n,y,s}(1 - \mathrm{Ix}_{k,y,s}), \quad \forall k, n, y, s \tag{23.3}$$

$$\mathrm{Ix}_{k,y,s} \in \{0,1\}, \quad \mathrm{wIx}_{k,n,y,s} \ge 0, \quad \mathrm{wIx1}_{k,n,y,s} \ge 0, \quad \forall k, n, y, s \tag{23.4}$$

where $\mathrm{wIx1}_{k,n,y,s}$ is an auxiliary variable.

Based on mass balance, the total amount of product delivered from plant to customer n in year y ($\mathrm{Trp}_{n,y,s}$) is given by the constraints

$$\mathrm{Trp}_{n,y,s} = \mathrm{dem}_{n,y} + \mathrm{Vend}_{n,y,s} - \mathrm{Vzero}_n + \mathrm{Vl}_n + \mathrm{safety}_{n,y,s}, \quad \forall n, s, y = 1 \tag{24}$$

$$\mathrm{Trp}_{n,y,s} = \mathrm{dem}_{n,y} + \mathrm{Vend}_{n,y,s} - \mathrm{Vend}_{n,y-1,s}, \quad \forall n,s,y|y \geq 2 \tag{25}$$

$$\mathrm{Vend}_{n,y,s} \leq \mathrm{winv}_{n,y,s}, \quad \forall n,s,y \tag{26}$$

where $\mathrm{dem}_{n,y}$ is the demand rate of customer n in year y and $\mathrm{Vend}_{n,y,s}$ is the inventory level of customer n in scenario s at the end of year y after adjustment for minimum tank volume and safety stocks which should be less than the working inventory level. Note that in the first year we need to account for the initial inventory level and adjust for minimum tank volume and safety stocks.

4.5. Continuous Approximation for Routing Cost. The capacitated vehicle routing cost is estimated by a continuous approximation approach. Let $\mathrm{Trp}_{n,y,s}$ be the total amount of product delivered from the plant to customer n in scenario s and year y, $\mathrm{ccapic}_{y,s}$ be the effective truck capacity (truck capacity after accounting for product loss), rr_n be the distance between the plant and customer n, and $\mathrm{TSP}_{y,s}$ be the length of the optimal traveling salesman tour by which all customers included in scenario s and year y are visited once. Based on a continuous approximation, the minimum routing distance for each replenishment cycle in scenario s and year y ($\mathrm{mrt}_{y,s}$) can be approximated as[1]

$$\mathrm{mrt}_{y,s} \approx 2\left(\frac{\sum_{n \in N_{y,s}} \mathrm{Trp}_{n,y,s}\mathrm{rr}_n}{x_{y,s}\mathrm{ccapic}_{y,s}}\right) + \left(1 - \frac{1}{\mathrm{ccapic}_{y,s}}\right)\mathrm{TSP}_{y,s}, \quad \forall y,s$$

To reduce the nonlinearities, we introduce the new positive variable $\mathrm{seg}_{y,s}$ such that

$$\mathrm{seg}_{y,s} = \frac{\sum_{n \in N_{y,s}} \mathrm{Trp}_{n,y,s}\mathrm{rr}_n}{x_{y,s}\mathrm{ccapic}_{y,s}}, \quad \forall y,s$$

which is equivalent to the constraint

$$\mathrm{seg}_{y,s}x_{y,s}\mathrm{ccapic}_{y,s} = \sum_{n \in N_{y,s}} \mathrm{Trp}_{n,y,s}\mathrm{rr}_n = \sum_{n \in N_{y,s}} \mathrm{winv}_{n,y,s}x_{y,s}\mathrm{rr}_n$$
$$= x_{y,s}\sum_{n \in N_{y,s}} \mathrm{winv}_{n,y,s}\mathrm{rr}_n, \quad \forall y,s$$

Because $x_{y,s}$ is a positive integer variable, the above equation is equivalent to

$$\mathrm{seg}_{y,s}\mathrm{ccapic}_{y,s} = \sum_{n \in N_{y,s}} (\mathrm{winv}_{n,y,s}\mathrm{rr}_n), \quad \forall y,s$$

Based on eq 14, we can reformulate the bilinear term on the left-hand side of the above equation as $\mathrm{seg}_{y,s}\mathrm{ccapic}_{y,s} = \sum_j \mathrm{seg}_{y,s}\mathrm{tru}_{j,y,s}\mathrm{Vtruck}_j(1 - \mathrm{loss})$. By introducing the nonnegative continuous variable $\mathrm{TruSeg}_{j,y,s} = \mathrm{seg}_{y,s}\mathrm{tru}_{j,y,s}$, we have the following reformulated linear constraint

$$\sum_j \mathrm{TruSeg}_{j,y,s}\mathrm{Vtruck}_j(1 - \mathrm{loss}) = \sum_{n \in N_{y,s}} (\mathrm{winv}_{n,y,s}\mathrm{rr}_n), \quad \forall y,s \tag{27}$$

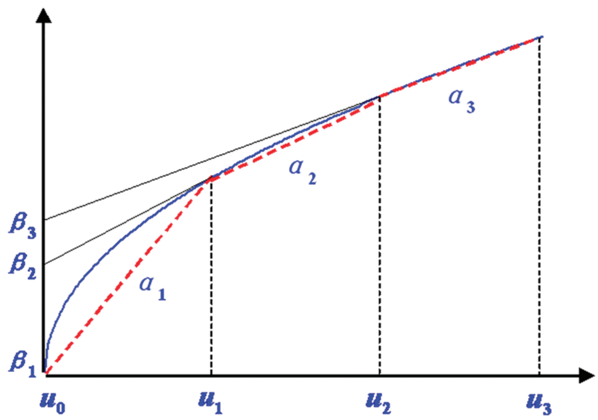


Figure 4. Piecewise-linear underestimator of a concave term.

We also need the following linearization constraints

$$\mathrm{TruSeg}_{j,y,s} + \mathrm{TruSeg1}_{j,y,s} = \mathrm{seg}_{y,s}, \quad \forall j,y,s \tag{28.1}$$

$$\mathrm{TruSeg}_{j,y,s} \leq \mathrm{seg}^{\mathrm{U}}_{y,s}\mathrm{tru}_{j,y,s}, \quad \forall j,y,s \tag{28.2}$$

$$\mathrm{TruSeg1}_{j,y,s} \leq \mathrm{seg}^{\mathrm{U}}_{y,s}(1 - \mathrm{tru}_{j,y,s}), \quad \forall j,y,s \tag{28.3}$$

$$\mathrm{tru}_{j,y,s} \in \{0,1\}, \quad \mathrm{TruSeg}_{j,y,s} \geq 0, \quad \mathrm{TruSeg1}_{j,y,s} \geq 0, \quad \forall j,y,s \tag{28.4}$$

where $\mathrm{TruSeg1}_{j,y,s}$ is an auxiliary variable and the upper bound of $\mathrm{seg}^{\mathrm{U}}_{y,s}$ is given by a sufficient large number (e.g., $|N_r|\max\{\mathrm{rr}_n\}$).

Thus, the continuous approximation of the minimum routing distance for each replenishment cycle is given by

$$\mathrm{mrt}_{y,s} = 2\mathrm{seg}_{y,s} + \left(1 - \frac{1}{\mathrm{ccapic}_{y,s}}\right)\mathrm{TSP}_{y,s}, \quad \forall y,s$$

Further, the reciprocal of $\mathrm{ccapic}_{y,s}$ ($\mathrm{Tccapic}_{y,s}$) can be modeled through the linear equation

$$\mathrm{Tccapic}_{y,s} = \sum_j \frac{\mathrm{tru}_{j,y,s}}{\mathrm{Vtruck}_j(1 - \mathrm{loss})}, \quad \forall y,s \tag{29}$$

which comes directly from eq 14.

Based on eq 29, we can easily reformulate the minimum routing distance constraint as

$$\mathrm{mrt}_{y,s} = 2\mathrm{seg}_{y,s} + (1 - \mathrm{Tccapic}_{y,s})\mathrm{TSP}_{y,s}, \quad \forall y,s \tag{30}$$

If the unit distance transportation cost of scenario s in year y ($\mathrm{cunit}_{y,s}$) is known, then the total delivery cost of this scenario in this year ($\mathrm{crot}_{y,s}$) is the product of the unit transportation cost, the number of replenishment cycles, and the minimum routing distance of each replenishment cycle

$$\mathrm{crot}_{y,s} = \mathrm{cunit}_{y,s}\mathrm{mrt}_{y,s}x_{y,s}, \quad \forall y,s$$

Based on eqs 13 and 16, similarly to part I,[1] we have $\mathrm{cunit}_{y,s}\mathrm{mrt}_{y,s}x_{y,s} = \sum_j\sum_k(2^{|k|-1}\mathrm{ck}_j\mathrm{tru}_{j,y,s}\mathrm{Ix}_{k,y,s}\mathrm{mrt}_{y,s})$. If we set $\mathrm{mrIx}_{k,y,s} = \mathrm{Ix}_{k,y,s}\mathrm{mrt}_{y,s}$ and $\mathrm{mrItru}_{j,k,y,s} = \mathrm{tru}_{j,y,s}\mathrm{mrIx}_{k,y,s}$, then the above nonlinear constraint can be linearized as

$$\mathrm{crot}_{y,s} = \sum_j\sum_k 2^{|k|-1}\mathrm{ck}_j\mathrm{mrItru}_{j,k,y,s}, \quad \forall y,s \tag{31}$$

We also need the following linear constraints

$$\mathrm{mrIx}_{k,y,s} + \mathrm{mrIx1}_{k,y,s} = \mathrm{mrt}_{y,s}, \quad \forall y, s \tag{32.1}$$

$$\mathrm{mrIx}_{k,y,s} \le \mathrm{mrt}^{\mathrm{U}}_{y,s}\mathrm{Ix}_{k,y,s}, \quad \forall y, s \tag{32.2}$$

$$\mathrm{mrIx1}_{k,y,s} \le \mathrm{mrt}^{\mathrm{U}}_{y,s}(1 - \mathrm{Ix}_{k,y,s}), \quad \forall k, y, s \tag{32.3}$$

$$\mathrm{Ix}_{k,y,s} \in \{0, 1\}, \quad \mathrm{mrIx}_{k,y,s} \ge 0, \quad \mathrm{mrIx1}_{k,y,s} \ge 0 \tag{32.4}$$

$$\mathrm{mrItru}_{j,k,y,s} + \mathrm{mrItru1}_{j,k,y,s} = \mathrm{mrIx}_{k,y,s}, \quad \forall j, k, y, s \tag{33.1}$$

$$\mathrm{mrItru}_{j,k,y,s} \le \mathrm{mrt}^{\mathrm{U}}_{y,s}\mathrm{tru}_{j,y,s}, \quad \forall j, k, y, s \tag{33.2}$$

$$\mathrm{mrItru1}_{j,k,y,s} \le \mathrm{mrt}^{\mathrm{U}}_{y,s}(1 - \mathrm{tru}_{j,y,s}), \quad \forall j, k, y, s \tag{33.3}$$

$$\mathrm{tru}_{j,y,s} \in \{0, 1\}, \quad \mathrm{mrItru}_{j,k,y,s} \ge 0, \quad \mathrm{mrItru1}_{j,k,y,s} \ge 0, \quad \forall j, k, y, s \tag{33.4}$$

where $\mathrm{mrIx1}_{k,y,s}$ and $\mathrm{mrItru1}_{j,k,y,s}$ are auxiliary variables.

4.6. Stochastic MINLP Reformulation. After reformulation and linearization, the stochastic continuous approximation model is a nonconvex MINLP with the objective function given in eq 1 and constraints 2−33.4. The remaining nonlinear nonconvex term in this model is the square-root term in safety stock constraint 21.

5. GLOBAL OPTIMIZATION ALGORITHM

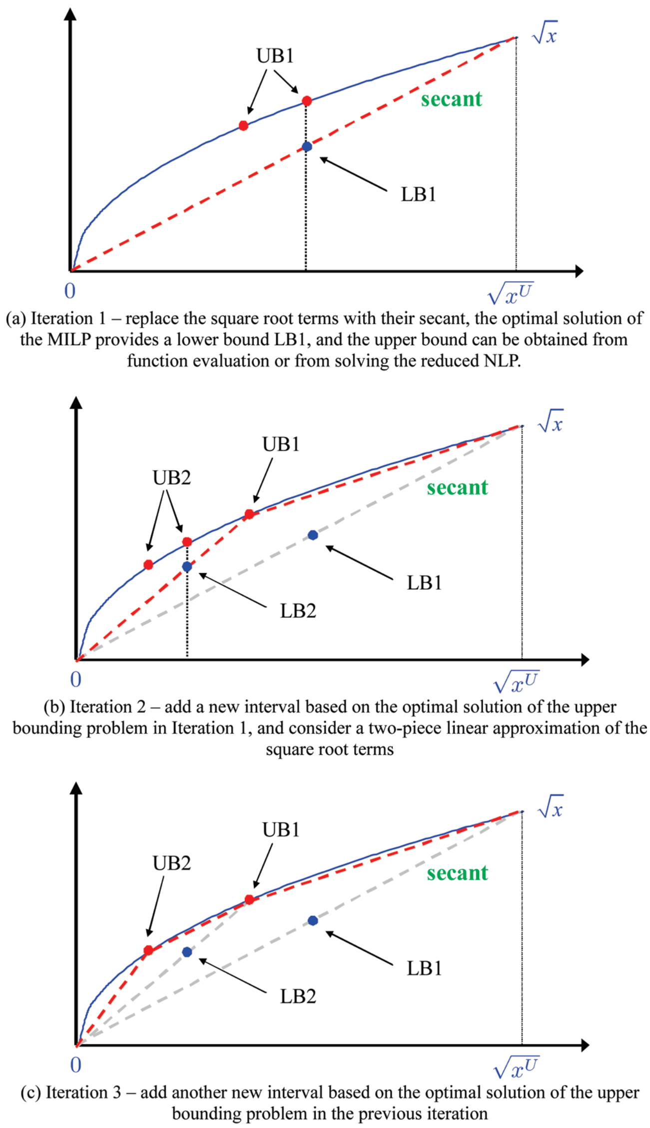
Although small-scale instances of the stochastic continuous approximation model can be solved to global optimality by using a global optimizer, medium- and large-scale problems are often computationally intractable with a direct solution approach because of the combinatorial nature and nonlinear nonconvex terms. In this section, we introduce an efficient global optimization algorithm based on a special property of the model and on successive piecewise-linear approximations to tackle this nonconvex MINLP problem.

An important property of this model is given as follows.

Property 1: If we replace the square-root terms in the safety stock constraint 21 with piecewise-linear underestimators, the solution of the resulting MILP model provides a global lower bound of the global minimum solution of the original MINLP.

We omit the proof because property 1 is straightforward and easy to prove. Based on property 1, we can first construct a lower-bounding MILP problem based on piecewise-linear approximations and then employ a branch-and-refine method to globally optimize the nonconvex stochastic continuous approximation problem.

5.1. Piecewise-Linear Approximation. The only nonlinear terms of the stochastic continuous approximation model are the univariate square-root terms, $(\mathrm{LT}_{y,s})^{1/2}$, in the safety stock constraint 21. To improve computational efficiency, we consider piecewise-linear approximations for the concave square-root terms. There are several different approaches to model piecewise-linear functions for a concave term. In this work, we use the "multiple-choice" formulation[20,21] to approximate the square-root term $(\mathrm{LT}_{y,s})^{1/2}$. Let $P_{y,s} = \{1, 2, 3, ..., p\}$ denote the set of intervals in the piecewise-linear function $\varphi(\mathrm{LT}_{y,s})$ and $u_{y,s,0}$, $u_{y,s,1}$,



(a) Iteration 1 – replace the square root terms with their secant, the optimal solution of the MILP provides a lower bound LB1, and the upper bound can be obtained from function evaluation or from solving the reduced NLP.

(b) Iteration 2 – add a new interval based on the optimal solution of the upper bounding problem in Iteration 1, and consider a two-piece linear approximation of the square root terms

(c) Iteration 3 – add another new interval based on the optimal solution of the upper bounding problem in the previous iteration

Figure 5. Branch-and-refine algorithm based on successive piecewise-linear approximations.

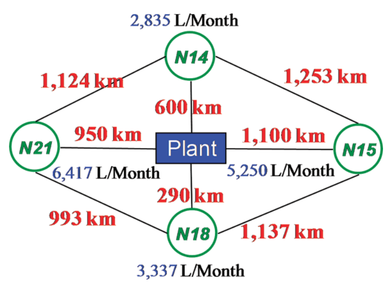


Figure 6. Case study 1: Four-customer industrial gas supply chain.

$u_{y,s,2}$, ..., $u_{y,s,p}$, be the lower and upper bounds of $\mathrm{LT}_{y,s}$ for each interval. The multiple-choice formulation of $\varphi(\mathrm{LT}_{y,s}) = (\mathrm{LT}_{y,s})^{1/2}$ for a given year and scenario is given by

$$\varphi(\mathrm{LT}_{y,s}) = \min \sum_{p} (\beta_{y,s,p}E_{y,s,p} + \alpha_{y,s,p}F_{y,s,p}) \tag{34}$$

subject to

$$\sum_p E_{y,s,p} = 1 \quad (35)$$

$$\sum_p F_{y,s,p} = \mathrm{LT}_{y,s} \quad (36)$$

$$u_{y,s,p-1}E_{y,s,p} \leq F_{y,s,p} \leq u_{y,s,p}E_{y,s,p}, \quad \forall p \quad (37)$$

$$E_{y,s,p} \in \{0,1\}, \quad F_{y,s,p} \geq 0, \quad \forall p \quad (38)$$

with

$$\alpha_{y,s,p} = \frac{\sqrt{u_{y,s,p}} - \sqrt{u_{y,s,p-1}}}{u_{y,s,p} - u_{y,s,p-1}}, \quad \beta_{y,s,p} = \sqrt{u_{y,s,p}} - \alpha_{y,s,p}u_{y,s,p}, \quad p \in P$$

Substituting expressions 34−38 into safety stock constraint 21 yields a mixed-integer linear programming (MILP) model that is a piecewise-linear underestimator of the stochastic MINLP problem. The MILP lower-bounding model formulation is given by

$$\min: E[\mathrm{cost}] = \sum_s \mathrm{prob}_s(\mathrm{capcost}_s + \mathrm{servcost}_s + \mathrm{distcost}_s) \quad (1)$$

subject to constraints 2−20, 22−33.4, and

$$\mathrm{safety}_{n,y,s} = z_\alpha \sigma_{n,y} \sum_p (\beta_{y,s,p}E_{y,s,p} + \alpha_{y,s,p}F_{y,s,p}), \quad \forall n \in N_{y,s}, y, s \quad (39)$$

$$\sum_p E_{y,s,p} = 1, \quad \forall y, s \quad (40)$$

$$\sum_p F_{y,s,p} = \mathrm{LT}_{y,s}, \quad \forall y, s \quad (41)$$

$$u_{y,s,p-1}E_{y,s,p} \leq F_{y,s,p} \leq u_{y,s,p}E_{y,s,p}, \quad \forall y, s, p \quad (42)$$

$$E_{y,s,p} \in \{0,1\}, \quad F_{y,s,p} \geq 0, \quad \forall y, s, p \quad (43)$$

5.2. Branch-and-Refine Algorithm. To globally optimize the nonconvex MINLP problem, we can first solve the MILP lower-bounding problem, whose solution provides a valid lower bound to the global optimal solution, and then solve a reduced MINLP problem by fixing the binary variables $\mathrm{tru}_{j,y,s}$ and $\mathrm{Ix}_{k,y,s}$. Note that we do not fix the tank-sizing decisions, because in the MILP lower-bound problem, the safety stock levels are underestimated, and thus the optimal tank sizes might be underestimated. To avoid infeasibility, we fix only $\mathrm{tru}_{j,y,s}$ and $\mathrm{Ix}_{k,y,s}$ to solve the reduced MINLP.

The optimal solution of the reduced MINLP is also a feasible solution of the original stochastic continuous approximation model, so its objective value provides a valid global upper bound of the original MINLP problem. The remaining challenge is to iteratively refine and improve the solution so that the global optimal solution can be obtained after a finite number of iterations. If we use a sufficiently large number of intervals in the piecewise-linear lower bonding MILP problem, we obtain the global solution within a sufficiently small optimality margin, because the more intervals used, the better the approximation of the square-root function (see Figure 4). However, more intervals require additional variables and constraints in the lower-bounding MILP model. Similarly to our previous work,[22] in this case, we use an iterative branch-and-refine strategy based on successive piecewise-linear approximation to control the size of the problem.

In the first step of this algorithm, we consider a single linear approximation in the lower-bounding MILP; that is, we replace all of the square-root terms in the stochastic continuous approximation MINLP model with their corresponding secants as shown in Figure 5a. Thus, the optimal solution of the MILP problem provides the first lower bound, LB1. An upper bound can be obtained by fixing the values of the binary variables $\mathrm{tru}_{j,y,s}$ and $\mathrm{Ix}_{k,y,s}$ and then solving the stochastic continuous approximation model in the reduced variable space. Because of the presence of tank-sizing variables, the reduced problem is still an MINLP. As the lower-bounding MILP underestimates the tank sizes and the maximum tank size is fixed, it is possible that the reduced MINLP could be infeasible. In that case, we move on to the next iteration, and the upper bound is still the best upper bound provided in the previous iterations. Of course, the lower-bounding MILP could be infeasible as well, but this would imply that the original problem is infeasible, because the MILP is a relaxation of the original MINLP.

In the next step, we use the optimal solution of variable $\mathrm{LT}_{y,s}$ in the upper-bounding problem as the lower bound of a new interval and consider a two-interval linear approximation of the square-root terms, as shown in Figure 5b. If the optimal solution of the upper-bounding problem in the previous iteration lies at the bounds of some intervals, we do not add any new interval for the corresponding square-root term $(\mathrm{LT}_{y,s})^{1/2}$. After constructing the two-interval linear approximation MILP model, we can similarly obtain a lower bound and then an upper bound by solving the reduced MINLP.

Table 1. General Parameters Used in the Models

number of truck types	4
number of tank sizes	6
depreciation period (dep)	15 years
time duration of year y (Hz_y)	365 days
maximum number of working hours per day (hpd)	15 h/day
average truck speed in kilometers per hour (speed)	22 km/h
minimum tanker fraction unloaded (frac)	10%
product loss percentage per delivery (loss)	5%
safety stock as a percentage of tank size	15%

Table 2. Available Tank Sizes and Corresponding Capital and Service Costs

tank size, T_i^U (L)	service cost in terms of percentage of capital cost ($\mathrm{Cser}_i/\mathrm{Ccap}_i$, %)
1000	26.04
6000	16.34
10000	12.95
13000	13.44
16000	12.66
20000	11.92

Table 3. Network Structure of Each Scenario in Each Year for Case Study 1

scenario/year		customers in the network	TSP distance ($TSP_{y,s}$, km)	scenario probability ($prob_s$, %)
S1	year 1	N14, N15, N18, N21	4507	21
	year 2	N14, N15, N18, N21	4507	
	year 3	N14, N15, N18, N21	4507	
S2	year 1	N14, N18, N21	3007	9
	year 2	N14, N18, N21	3007	
	year 3	N14, N18, N21	3007	
S3	year 1	N14, N15, N18, N21	4507	14
	year 2	N14, N15, N21	4427	
	year 3	N14, N15, N21	4427	
S4	year 1	N14, N15, N18, N21	4507	21
	year 2	N14, N15, N18, N21	4507	
	year 3	N14, N15, N18	3281	
S5	year 1	N14, N15, N18, N21	4507	14
	year 2	N14, N15, N21	4427	
	year 3	N14, N15	2506	
S6	year 1	N14, N18, N21	3007	9
	year 2	N14, N18, N21	3007	
	year 3	N14, N18	1780	
S7	year 1	N14, N18, N21	3007	6
	year 2	N14, N21	2247	
	year 3	N14, N21	2247	
S8	year 1	N14, N18, N21	3007	6
	year 2	N14, N21	2247	
	year 3	N14	0	

As shown in Figure 5c, the number of intervals in the piecewise-linear model increases as the iteration number increases. Meanwhile, the best lower bound increases as the best upper bond decreases. The algorithm keeps iterating until the lower bound and upper bound are close enough to reach an optimality tolerance, such as 10^{-6}. Note that the number of intervals does not always equal the number of iterations, because the optimal solutions in some iterations might lie at the bounds of the intervals and, in that case, we do not increase new intervals for the corresponding square-root terms.

To summarize, the proposed branch-and-refine algorithm based on successive piecewise-linear approximation is as follows:

Step 1 (Initialization). Initialize iter = 1, LB = 0, and UB = $+\infty$. Set $NP_{y,s}^{iter} = 1$, $p \in P_{y,s} = \{0, 1, ..., NP_{y,s}^{iter}\}$. Use a single linear approximation (i.e., the secant) for the square-root terms. To achieve this, set $u_{y,s,0} = 0$ and $u_{y,s,1} = LT_{y,s}^{U}$, as well as $\alpha_{y,s,1} = [(u_{y,s,1})^{1/2} - (u_{y,s,0})^{1/2}]/(u_{y,s,1} - u_{y,s,0}) = 1/(LT_{y,s})^{1/2}$ and $\beta_{y,s,1} = (u_{y,s,1})^{1/2} - \alpha_{y,s,1}u_{y,s,1} = 0$.

Step 2. At iteration iter, solve the piecewise-linear approximation MILP model. If the MILP problem is infeasible, then the original problem is also infeasible, and the algorithm stops. If not, denote the optimal objective function value as φ^{iter} and the optimal solution of variables $tru_{j,y,s}$ and $Ix_{k,y,s}$ as $(tru_{j,y,s}^{*iter}, Ix_{k,y,s}^{*iter})$. If $\varphi^{iter} > LB$, then set LB = φ^{iter}.

Step 3. Fix the values of binary variables $tru_{j,y,s} = tru_{j,y,s}^{*iter}$ and $Ix_{k,y,s} = Ix_{k,y,s}^{*iter}$, and solve the original stochastic continuous approximation MINLP model in the reduced space, which is an MINLP with fewer binary variables, to obtain the *local* optimal solution.

If the reduced MINLP is feasible, denote the optimal value of the objective function as Φ^{iter} and the optimal solution as $LT_{y,s}^{iter}$. If Φ^{iter} < UB, then set UB = Φ^{iter}, and store the current optimal solution.

If the reduced MINLP is infeasible, denote the optimal solution of the lead times in the lower-bounding MILP as $LT_{y,s}^{iter}$.

Find $n_{y,s}^{iter}$ such that the optimal solution $LT_{y,s}^{iter}$ lies in the $n_{y,s}^{iter}$ interval, that is, $u_{y,s,n_{ci,y,s}^{iter}-1} \leq LT_{y,s} \leq u_{y,s,n_{ci,y,s}^{iter}}$. One approach to find the proper value of n_j^{iter} is to compute the product $(LT_{y,s}^{iter} - u_{y,s,p-1})(LT_{y,s}^{iter} - u_{y,s,p})$ for all $p = 2, 3, ..., NP_{y,s}^{iter}$ and then denote the first p that leads to a nonpositive value (zero or negative value) of the product as $n_{y,s}^{iter}$; that is, if $(LT_{y,s}^{iter} - u_{y,s,p-1})(LT_{y,s}^{iter} - u_{y,s,p}) \leq 0$, set $n_{y,s}^{iter} = p$.

If UB − LB $\leq \varepsilon$ (e.g., 10^{-9}), stop and output the optimal solution; otherwise, go to the next step.

Step 4. For those year−scenario pairs (y, s) such that $(LT_{y,s}^{iter})^{1/2} = \sum_p(\beta_{y,s,p}^{iter}E_{y,s,p}^{iter} + \alpha_{y,s,p}^{iter}F_{y,s,p}^{iter})$, set $NP_{y,s}^{iter+1} = NP_{y,s}^{iter}$, $\alpha_{y,s,p}^{iter+1} = \alpha_{y,s,p}^{iter}$, and $\beta_{y,s,p}^{iter+1} = \beta_{y,s,p}^{iter}$.

For other year−scenario pairs, set $NP_{y,s}^{iter+1} = NP_{y,s}^{iter} + 1$; update the set $P_{y,s}$ (i.e., $p \in P_{y,s} = \{0, 1, ..., NP_{y,s}^{iter+1}\}$); and update $u_{y,s,p}$, $\alpha_{y,s,p}$, and $\beta_{y,s,p}$ as follows:

- For $p < n_{y,s}^{iter}$ (i.e., $p = 0, 1, 2 ..., n_{y,s}^{iter}-1$), set $u_{y,s,p}^{iter+1} = u_{y,s,p}^{iter}$, $\alpha_{y,s,p}^{iter+1} = \alpha_{y,s,p}^{iter}$, and $\beta_{y,s,p}^{iter+1} = \beta_{y,s,p}^{iter}$.
- For $p = n_{y,s}^{iter}$, set $u_{y,s,n_j^{iter}}^{iter+1} = LT_{y,s}^{iter}$, $\alpha_{y,s,n_{y,s}^{iter}}^{iter+1} = [(LT_{y,s}^{iter})^{1/2} - (u_{y,s,n_{y,s}^{iter}-1})^{1/2}]/(LT_{y,s}^{iter} - u_{y,s,n_{y,s}^{iter}-1})$, and $\beta_{y,s,n_{y,s}^{iter}}^{iter+1} = (LT_{y,s}^{iter})^{1/2} - \alpha_{y,s,n_{y,s}^{iter}}^{iter+1}LT_{y,s}^{iter}$.
- For $p = n_{y,s}^{iter} + 1$, set $u_{y,s,n_{y,s}^{iter}+1}^{iter+1} = u_{y,s,n_{y,s}^{iter}}^{iter}$, $\alpha_{y,s,n_{y,s}^{iter}+1}^{iter+1} = [(u_{y,s,n_{y,s}^{iter}})^{1/2} - (LT_{y,s}^{iter})^{1/2}]/(u_{y,s,n_{y,s}^{iter}} - LT_{y,s}^{iter})$, and $\beta_{y,s,n_{y,s}^{iter}+1}^{iter+1} = (u_{y,s,n_{y,s}^{iter}})^{1/2} - \alpha_{y,s,n_{y,s}^{iter}}^{iter+1}u_{y,s,n_{y,s}^{iter}}$.
- For $p > n_{y,s}^{iter} + 1$ (i.e., $p = n_{y,s}^{iter} + 2, n_{y,s}^{iter} + 3, ..., NP_{y,s}^{iter}$), set $u_{y,s,p}^{iter+1} = u_{y,s,p-1}^{iter}$, $\alpha_{y,s,p}^{iter+1} = \alpha_{y,s,p-1}^{iter}$, and $\beta_{y,s,p}^{iter+1} = \beta_{y,s,p-1}^{iter}$. Then, set iter = iter + 1, and go to step 2.

6. CASE STUDIES

To illustrate the application of the proposed model and the performance of the proposed solution strategies, we consider three case studies. All computational experiments were performed on an IBM T400 laptop with an Intel 2.53 GHz CPU and 2 GB of RAM. The proposed solution procedure was coded in GAMS 23.2.1.[23] The MILP problems were solved using CPLEX 12, and the reduced MINLP problems in step 2 of the branch-and-refine algorithm were solved with the MINLP solver DICOPT. We used DICOPT as the convex MINLP solver and BARON 8.1.5 as the global optimizer in the computational experiments. The optimality tolerances of DICOPT, BARON, and the proposed branch-and-refine algorithm were all set to 10^{-3}, and the optimality margins of solving the piecewise-linear approximation MILP model (P4) and the reduced NLP model (P3) were both 10^{-6}.

6.1. Case Study 1: Four-Customer Case. In the first case study, we consider a four-customer cluster of an industrial gas supply chain, of which the network structure and the monthly mean demand rates for the first year are given in Figure 6. All of the customers need to size their tanks. In the three-year horizon, we consider a 15% annual demand growth rate for all customers, and the standard deviation of uncertain daily demand is considered as one-third of the daily mean demand. Other major input data for this case study are given in Tables 1 and 2.

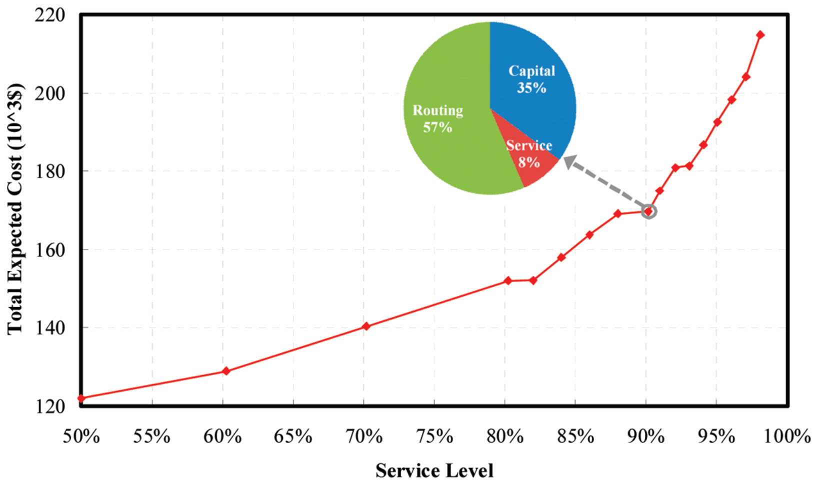


Figure 7. Pareto curve for case study 1 (total expected cost vs service level).

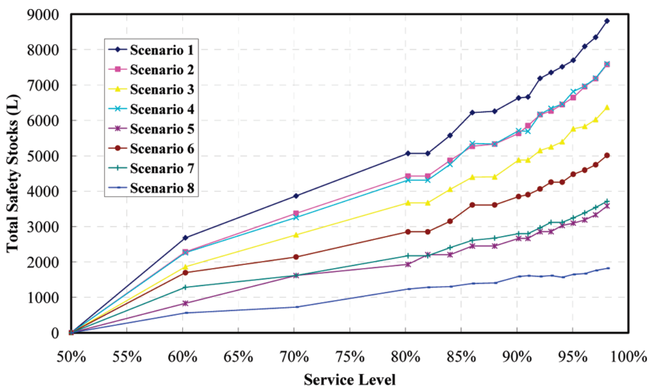


Figure 8. Scenario total safety stocks of the third year under different service levels for case study 1.

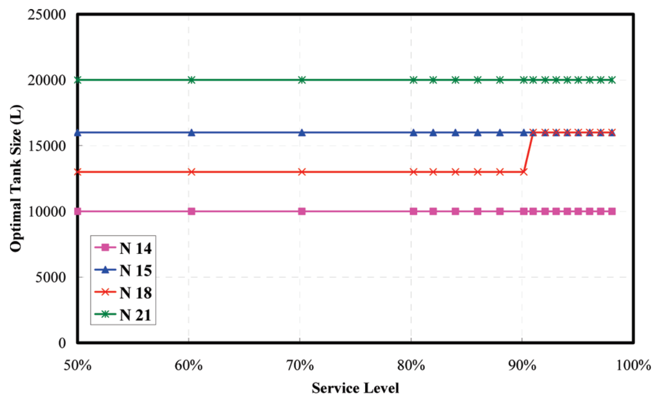


Figure 9. Optimal tank-sizing decisions under different service levels for case study 1.

Although all four customers are included in the network at time zero, some of them might terminate the contract in a certain future year as follows:

- N14 will not terminate the contract by the end of year 3.
- N15 has a 30% chance of terminating the contract in year 1.
- N18 has a 40% chance of terminating the contract in year 2.
- N21 has a 50% chance of terminating the contract in year 3.

We assume that each event is independent of the others, so eight scenarios are generated for this case study. The detailed network structure and TSP distances to visit all customers once for each scenario in each year and the probability of each scenario are given in Figure 1 and Table 3.

We consider 17 instances with service level α ranging from 50% to 98% for all customers and the corresponding service level parameter z_α ranging from 0 to 2.07, where z_α is a standard normal deviate such that $\Pr(z \leq z_\alpha) = \alpha$. We note that all the 17 instances have similar problem structures; the only difference among them is the service level parameter. As these instances are solved sequentially with service levels ranging from 50% to 98%, an instance's solution provides a good starting point for solving the next instance. We solved these 17 instances with DICOPT, BARON, and the proposed branch-and-refine algorithm (CPLEX + DICOPT). The original MINLP model for stochastic continuous approximation includes 264 binary variables, 3300 continuous variables, and 4344 constraints. DICOPT returned "infeasible" for all of the instances, presumably because of the numerical difficulty arising from the square-root terms. One way to overcome this issue is to add a sufficiently small number ε to each square-root term; see our earlier work[22] for details. The global optimizer BARON took 70354 CPU s to solve all 17 instances (on average, 4138 CPU s/instance) to an optimality gap of 10^{-6}. With the proposed branch-and-refine algorithm using CPLEX and DICOPT, we solved all 17 instances to global optimality in a total of 285 CPU s (on average, 17 CPU s/instance). Clearly, the proposed global optimization algorithm demonstrated much better performance than the general-purpose commercial MINLP solvers.

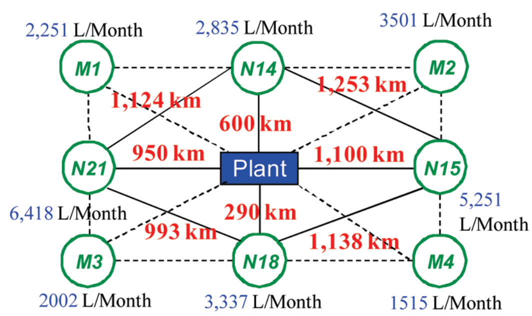


Figure 10. Case study 2: Eight-customer industrial gas supply chain.

Table 4. Network Structure of Each Scenario in Each Year for Case Study 2

scenario/year		customers in the network	TSP distance ($TSP_{y,s}$, km)	scenario probability ($prob_s$, %)
S1	year 1	N14, N15, N18, N21	4507	16.1446
	year 2	N14, N15, N18, N21	4507	
S2	year 1	N14, N15, N18, N21	4507	6.9191
	year 2	N14, N15, N18	3281	
S3	year 1	N14, N15, N18, N21	4507	1.7938
	year 2	N14, N15, N21	4427	
S4	year 1	N14, N15, N18, N21	4507	4.0361
	year 2	N14, N15	2505	
S5	year 1	N14, N18, N21	3007	0.4485
	year 2	N14, N18, N21	3007	
S6	year 1	N14, N18, N21	3007	1.7298
	year 2	N14, N18	1780	
S7	year 1	N14, N18, N21	3007	0.7688
	year 2	N14, N21	2247	
S8	year 1	N14, N18, N21	3007	0.1922
	year 2	N14	0	
S9	year 1	N14, N15, N18, N21	4507	5.3815
	year 2	N14, N15, N18, N21, M1	4934	
S10	year 1	N14, N15, N18, N21	4507	2.3064
	year 2	N14, N15, N18, M1	4642	
S11	year 1	N14, N15, N18, N21	4507	0.5979
	year 2	N14, N15, N21, M1	4934	
S12	year 1	N14, N15, N18, N21	4507	1.3454
	year 2	N14, N15, M1	4339	
S13	year 1	N14, N18, N21	3007	0.1495
	year 2	N14, N18, N21, M1	3433	
S14	year 1	N14, N18, N21	3007	0.5766
	year 2	N14, N18, M1	3142	
S15	year 1	N14, N18, N21	3007	0.2563
	year 2	N14, N21, M1	2674	
S16	year 1	N14, N18, N21	3007	0.0641
	year 2	N14, M1	1900	
S17	year 1	N14, N15, N18, N21	4507	8.6932
	year 2	N14, N15, N18, N21, M2	4954	
S18	year 1	N14, N15, N18, N21	4507	3.7257
	year 2	N14, N15, N18, M2	3728	
S19	year 1	N14, N15, N18, N21	4507	0.9659
	year 2	N14, N15, N21, M2	4874	
S20	year 1	N14, N15, N18, N21	4507	2.1733
	year 2	N14, N15, M2	2953	
S21	year 1	N14, N18, N21	3007	0.2415
	year 2	N14, N18, N21, M2	4632	
S22	year 1	N14, N18, N21	3007	0.9314
	year 2	N14, N18, M2	3405	
S23	year 1	N14, N18, N21	3007	0.4140
	year 2	N14, N21, M2	4360	
S24	year 1	N14, N18, N21	3007	0.1035
	year 2	N14, M2	2200	
S25	year 1	N14, N15, N18, N21	4507	4.0361
	year 2	N14, N15, N18, N21, M3	4754	
S26	year 1	N14, N15, N18, N21	4507	1.7298
	year 2	N14, N15, N18, M3	4642	
S27	year 1	N14, N15, N18, N21	4507	0.4485
	year 2	N14, N15, N21, M3	4737	

Table 4. Continued

scenario/year		customers in the network	TSP distance ($TSP_{y,s}$, km)	scenario probability ($prob_s$, %)
S28	year 1	N14, N15, N18, N21	4507	1.0090
	year 2	N14, N15, M3	4625	
S29	year 1	N14, N18, N21	3007	0.1121
	year 2	N14, N18, N21, M3	3254	
S30	year 1	N14, N18, N21	3007	0.4324
	year 2	N14, N18, M3	3142	
S31	year 1	N14, N18, N21	3007	0.1922
	year 2	N14, N21, M3	2715	
S32	year 1	N14, N18, N21	3007	0.0480
	year 2	N14, M3	2604	
S33	year 1	N14, N15, N18, N21	4507	16.1446
	year 2	N14, N15, N18, N21, M4	4760	
S34	year 1	N14, N15, N18, N21	4507	6.9191
	year 2	N14, N15, N18, M4	3533	
S35	year 1	N14, N15, N18, N21	4507	1.7938
	year 2	N14, N15, N21, M4	4737	
S36	year 1	N14, N15, N18, N21	4507	4.0361
	year 2	N14, N15, M4	2958	
S37	year 1	N14, N18, N21	3007	0.4485
	year 2	N14, N18, N21, M4	4632	
S38	year 1	N14, N18, N21	3007	1.7298
	year 2	N14, N18, M4	3405	
S39	year 1	N14, N18, N21	3007	0.7688
	year 2	N14, N21, M4	4609	
S40	year 1	N14, N18, N21	3007	0.1922
	year 2	N14, M4	2830	

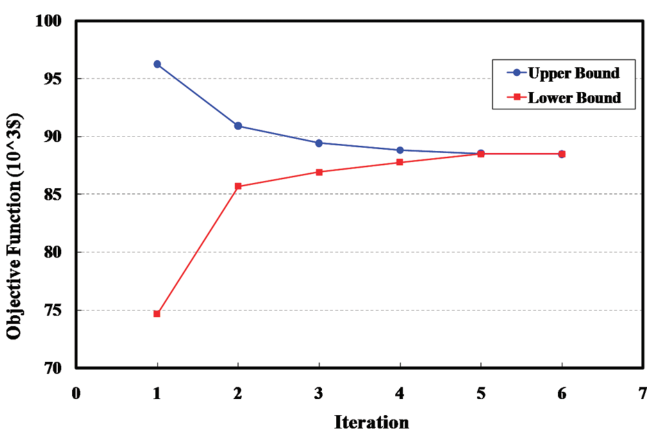


Figure 11. Bounds of each iteration of the proposed branch-and-refine algorithm for case study 2 under an 82% service level.

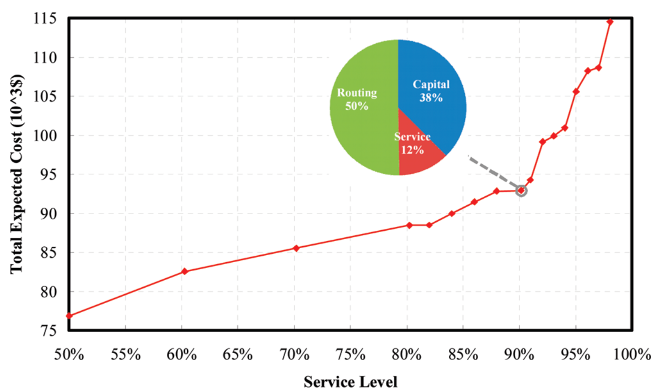


Figure 12. Pareto curve for case study 2 (total expected cost vs service level).

The optimal solutions of these 17 instances are given in Figures 7–9. Figure 7 shows the Pareto optimal curve between the total expected cost and the service level. As the service level increases from 50% to 98%, the total expected cost increases from \$121,965 to \$214,866. Thus, a higher service level implies a higher total expected cost. In particular, when the service level increases from 80% to 82% and from 88% to 90%, the total expected cost increases by only \$40 and \$170, respectively. Therefore, setting the service level to 82% or 90% might be good choices in terms of balancing economics and service level.

The cost breakdown for the 90% service level case is also given in Figure 7. One can see that the sum of the capital and service costs is close to the estimated routing cost. The pie chart reveals the tradeoff between distribution costs and costs for installing and maintaining the storage tanks.

Figure 8 shows the total safety stock levels (sum of the safety stocks of all customers) for the third year under different specifications of the service level. One can see a similar trend that the higher the service level maintained, the greater the cost for each scenario. Because of different network structures and different numbers of customers, different scenarios have different

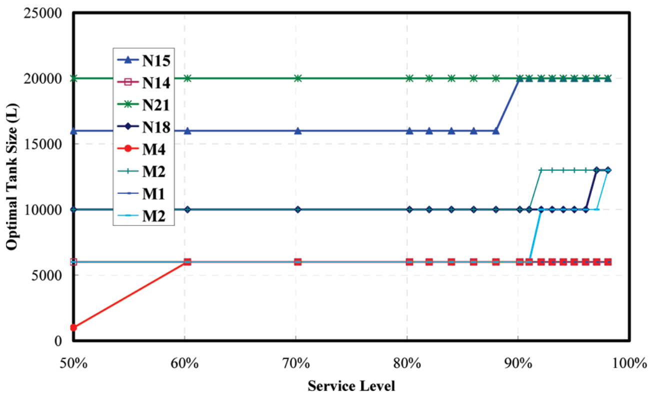


Figure 13. Optimal tank-sizing decisions under different service levels for case study 2.

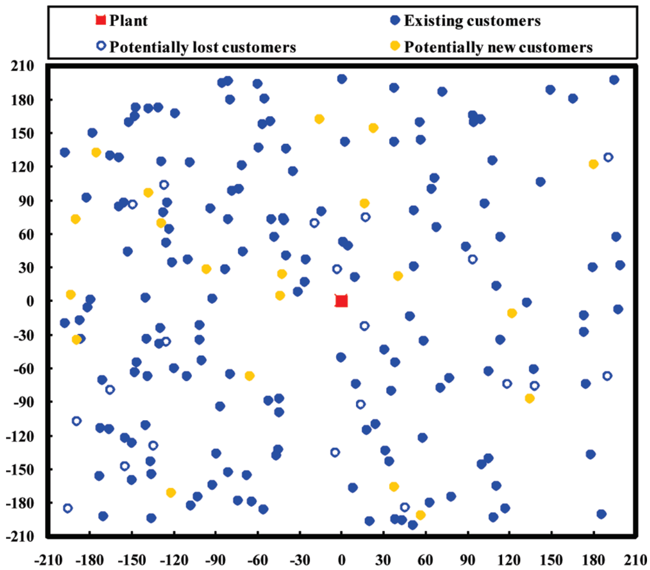


Figure 14. Location map of the 200 customers in the industrial gas supply chain of case study 3.

costs, and they can be generally classified into four groups: Scenario 1 includes all four customers in all three years, so it has the highest scenario cost; scenario 8 has the fewest customers throughout the planning horizon, so it has the lowest scenario cost; scenarios 2−4 have more customers than scenarios 5−7, so their costs are between those for scenarios 1 and 8.

Figure 9 depicts how the optimal tank-sizing decisions, which are first-stage decisions that are independent of scenario, change as the service level increases from 50% to 98%. It is interesting to see that the optimal tank-sizing decisions for all customers do not change when the service level increases from 50% to 90%. This result suggests, in turn, that optimal tank-sizing decisions are relatively robust in terms of service level. When the service level increases above 90%, the optimal tank size for customer N18 increases from 13000 to 16000 L. This is because higher service level requires more safety stocks, and thus, a larger tank is needed.

6.2. Case Study 2: Eight-Customer Case. In the second case study, we consider an eight-customer cluster of an industrial gas supply chain as shown in Figure 10. Customers N14, N15, N18, and N21 are existing customers, and customers M1−M4 are potentially new customers that could join the network in year 2. All of the customers need to size their tanks. The monthly demand rates in the first year for all customers are also given in Figure 10. We consider a 15% annual demand growth rate for all customers throughout the planning horizon, and the standard deviation of uncertain daily demand is considered as one-third of the daily mean demand. Other major input data for this case study are the same as those given in Tables 1 and 2.

Although all four customers are included in the network at time zero, some of them might terminate the contract in a future year as follows:

- N14 will not terminate the contract by the end of year 2.
- N15 has a 30% chance of terminating the contract in year 1.
- N18 has a 10% chance of terminating the contract in year 2.
- N21 has a 20% chance of terminating the contract in year 2.
- M1 has a 25% chance of signing a new contract starting in year 2.
- M2 has a 35% chance of signing a new contract starting in year 2.
- M3 has a 20% chance of signing a new contract starting in year 2.
- M4 has a 50% chance of signing a new contract starting in year 2.
- At most one customer among M1, M2, M3, and M4 will sign a contract.

We assume that each event is independent of the others, so 40 scenarios are generated for this case study. (Note that at most one new customer will join the network.) The detailed network structure for each scenario in each year and the probabilities of scenarios are given in Table 4.

Similarly, we consider 17 instances with service level α ranging from 50% to 98% and the corresponding service level parameter z_α ranging from 0 to 2.07. All 17 instances were solved with DICOPT, BARON, and the proposed branch-and-refine algorithm (CPLEX + DICOPT). The original MINLP model for stochastic continuous approximation includes 816 binary variables, 12516 continuous variables, and 16236 constraints. DICOPT returned infeasible for all instances, and the global optimizer BARON could not return any feasible solution after running for 7 days. With the proposed branch-and-refine algorithm using CPLEX and DICOPT, we solved all 17 instances to global optima in a total of 1770 CPU s (on average, 104 CPU s/instance) under an optimality tolerance of 10^{-6}. At most six iterations were required to solve each instance. As an example, the instance under 82% service level needed six iterations to reach the optimality tolerance. The upper and lower bounds of each iteration for this instance are shown in Figure 11. As the iteration number increases, the upper bound decreases, and the lower bound increases until the optimality margin is reached. The lower-bounding MILP problem in the last iteration has the maximum problem size, including 1296 binary variables, 12996 continuous variables, and 167356 constraints. The computational results show that, for this problem, the proposed global optimization algorithm is much more computationally efficient than the general-purpose commercial MINLP solvers.

The optimal solutions of these 17 instances are given in Figures 12 and 13. Figure 12 shows the Pareto optimal curve between the total expected cost and the service level. One can see that, as the service level increases from 50% to 98%, the total expected cost increases from \$76,861 to \$114,515. Thus, a higher service level implies a higher total expected cost. Figure 13 shows

Table 5. Network Structure of Each Scenario in Each Year for Case Study 3

scenario	customers in the network	total number of customers	TSP distance ($TSP_{y,s}$, km)	probability ($prob_s$, %)
S1	existing customers and potentially lost customers	180	3914	40
S2	only existing customers	160	3083	30
S3	existing customers, potentially lost customers, and potentially new customers	200	4335	30

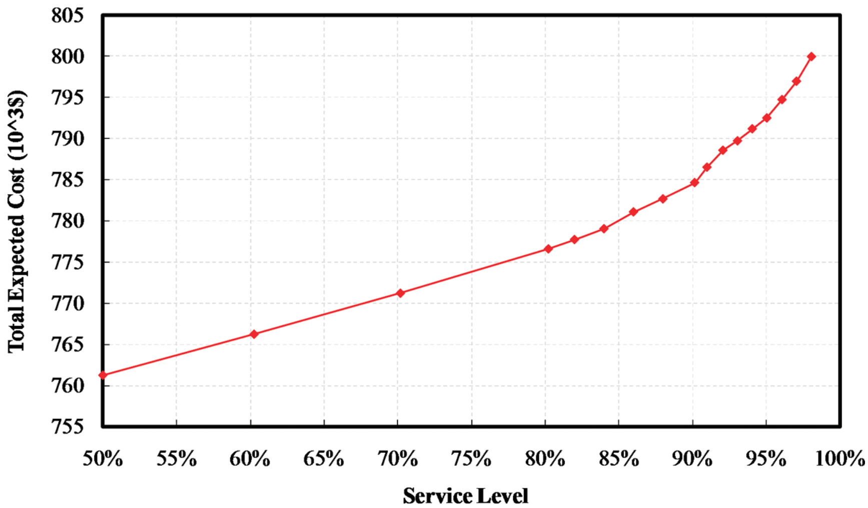


Figure 15. Pareto optimal curves for the 200-customer industrial gas supply chain in case study 3.

how the optimal tank-sizing decisions, which are first-stage decisions that are independent of scenario, change as the service level increases from 50% to 98%. One can see that the optimal tank sizes mainly depend on the customer demands and locations. As the service level increases, the required amount of safety stocks also increases, and thus, the optimal tank sizes might stay unchanged or increase. The cost breakdown for the 90% service level case is also given in Figure 12. The pie chart also reveals the tradeoff between the distribution costs and the costs for installing and maintaining the storage tanks.

6.3. Case Study 3: Large-Scale Instances with 200 Customers. In the last case study, we consider a large-scale industrial gas supply chain with 200 customers. A one-year planning horizon is considered, and all of the customers are new and need to size their tanks. As one can see from the previous two case studies, the proposed branch-and-refine algorithm is more efficient for this problem than the commercial general-purpose MINLP solvers. Thus, we use only the proposed global optimization algorithm for this case study.

The data provided in Tables 1 and 2 were used for the three instances in this case study. Because of the large number of customers, we randomly generated their locations and demand rates. All of the customer locations were generated in a 400 km × 400 km square following a uniform distribution, with the plant located in the center of this square. The detailed locations of the customers and plant are given in Figure 14. The TSP distances to visit all customers once (not including the plant) for different scenarios and years were obtained with Concorde TSP Solver[24] through its NEOS interface[25] with CPLEX 12. The Concorde TSP solver is quite computationally effective: for a 200-customer case that will be discussed later, it took less than 2 s to obtain the global optimal solution for the TSP values.

The monthly demand rates of customers in the first year ($demc_{n,y}$, L/month) were generated using normal distributions as follows

$$demc_{n,y} = 100 + 100|N[0, 15]|$$

Note that we took the absolute values of the normal distribution so that the monthly demand rates were always higher than 100 L/month. Although the normal distribution was unbounded, the maximum monthly demand rate obtained from the sampling was 5783 L/month. We considered a 15% annual demand growth rate for all customers throughout the planning horizon, and the standard deviation of uncertain daily demand was considered as one-third of the daily mean demand.

This example was designed for the case that a group of customers belonging to the same organization that will decide to terminate the existing contract or signing a contract for the entire group, that is, a group of customers might join or leave the network at the same time in some situation. We consider three organizations that have master contracts with the vendor and have branches in different locations. If any of the organizations decides to terminate the contract with the vendor, all of its locations will have their supplies finished and tanks removed. Hence, we consider three scenarios in this case study. Their probabilities and network structures are given in Table 5. Specifically, we consider 160 customers as existing customers that will not terminate the contract in the coming year; another 20 customers as potentially lost customers that might terminate the contract in year 1; and the last 20 customers as potentially new

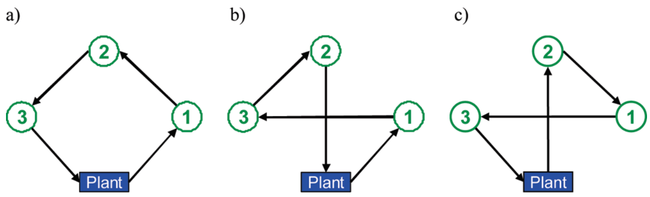


Figure 16. All possible routes for the delivery for a three-customer cluster.

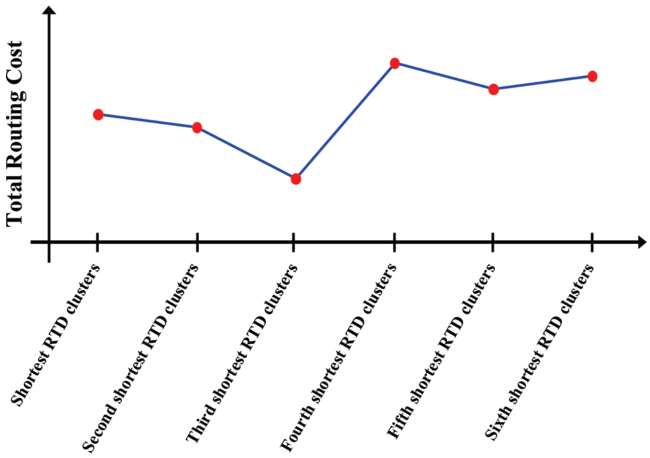


Figure 17. Total cost changes as the combination of clusters changes.

customers, who might sign a contract and join the distribution network in year 1. Scenario 1, with 40% probability, includes a network consisting of existing customers and potentially lost customers; scenario 2, with 30% probability, is for a network consisting of only existing customers (i.e., the potentially lost customers terminate their contract in year 1); and scenario 3, with 30% probability, has a distribution network with all of the customers (i.e., the potentially new customers sign the contract and join the distribution network in year 1).

We consider 17 instances with service level α ranging from 50% to 97% and the corresponding service level parameter z_α ranging from 0 to 1.89. All 12 instances were solved with the proposed branch-and-refine algorithm (CPLEX + DICOPT). It took 19783 CPU s to solve all 12 instances (on average, 1649 CPU s/instance). Each instance required four to six iterations depending on the specified service level. The maximum size of the lower-bounding MILP problem (at the sixth iteration) included 2439 discrete variables, 12623 continuous variables, and 14150 constraints.

The Pareto curve for this case is given in Figure 15. Because of the one-year planning horizon and the relatively small customer demand standard deviations, the total expected costs increase by only around \$40,000 as the service level increases from 50% to 97%. One can see a similar trend as in the previous case studies that higher service level requires higher total expected cost.

This case study illustrates the application of the proposed stochastic continuous approximation method and the effectiveness of the branch-and-refine algorithm for solving large-scale problems.

7. CONCLUSIONS

In this work, we have developed a computational framework to deal with industrial gas inventory-distribution planning under uncertain demand and customer presence. The framework consists of an upper-level stochastic continuous approximation model and a lower-level detailed routing model. The stochastic continuous approximation model is an MINLP problem that captures the uncertainty in demand fluctuation and customer presence by incorporating a stochastic inventory model and a two-stage stochastic programming framework. This model simultaneously optimizes the tank-sizing decisions, safety stock levels, and estimated vehicle routing costs. To efficiently solve this stochastic MINLP problem for large-scale problems, we have proposed an efficient branch-and-refine algorithm based on successive piecewise-linear approximations. Detailed operational decisions in inventory-distribution planning can be obtained by solving the lower-level routing model after fixing the solutions from the stochastic continuous approximation model. Three case studies were presented to demonstrate the applicability of the proposed model. Computational experiments on large-scale industrial gas supply chains with up to 200 customer showed that the proposed algorithm is much more efficient than commercial MINLP solvers for solving stochastic continuous approximation problems.

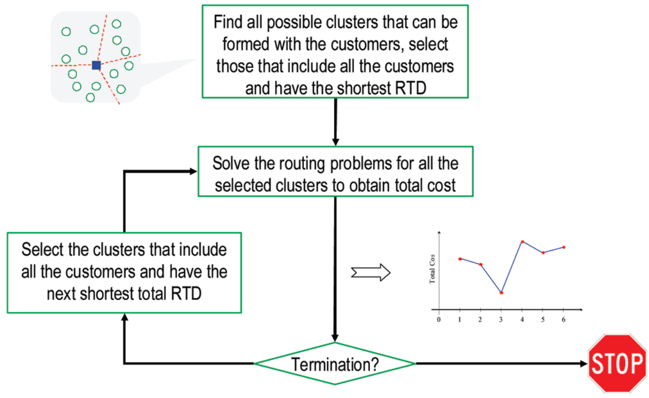


Figure 18. Algorithmic framework of the clustering-based heuristic for solving the detailed routing problem.

APPENDIX: CLUSTERING-BASED HEURISTIC FOR DETAILED ROUTING PROBLEM

A number of methods can be used to improve the computational efficiency of solving detailed vehicle routing problems.[15] In this appendix, we present a clustering-based heuristic that is easy to implement in practice.

In the first step, we create all possible clusters such that the maximum number of customers allowed in a cluster is four. Note that the maximum number of customers included in a cluster is problem-dependent. For the problem addressed in this work, we found that each truck trip visits at most four customers in most cases. Thus, we consider that each cluster has at most four customers.

For example, if there are seven customers {1, 2, 3, 4, 5, 6, 7} and customers 1−5 cannot be clustered with customers 6 and 7, then we have the following clusters: {1}, {2}, {3}, {4}, {5}, {6}, {7}, {1, 2}, {1, 3}, {1,4}, {1, 5}, {2, 3}, {2, 4}, {2, 5}, {3, 4}, {3, 5}, {4, 5}, {6, 7}, {1, 2, 3}, {1, 2, 4}, {1, 2, 5}, {1, 3, 4}, {1, 3, 5}, {1, 4, 5}, {2, 3, 4}, {2, 3, 5}, {2, 4, 5}, {3, 4, 5}, {1, 2, 3, 4}, {1, 2, 3, 5}, {1, 2, 4, 5}, {1, 3, 4, 5}, and {2, 3, 4, 5}.

The round-trip distances (RTDs) for each cluster can be calculated by the traveling salesman distance between the plant and all of the customers included in the cluster. For instance, assume that a delivery is made to all customers in the cluster {1, 2, 3}. Figure 16 shows all possible ways to travel:

If the shortest RTD is obtained by routing b, then for the cluster {1, 2, 3}, we can assume that the RTD is the one calculated by method b.

From the set of all possible clusters formed, we select the clusters that include all of the customers and lead to the shortest RTDs from the plants. Therefore, for customers 1−7 described above, a set of clusters that includes all of the customers and is the shortest RTD could be: {1, 4, 5}, {2, 3}, {6, 7}.

After the clustering, we solve the detailed routing problem for each of the clusters formed above, i.e., consider the routing for some or all of the customers in {1, 4, 5}, {2, 3}, and {6, 7} separately. In this way, we are able to capture the location and volume synergies for large-scale routing problems.

The clusters were selected on the basis of the shortest total RTD. However, note that the shortest RTD does not necessarily mean that the lower total distribution costs are lower than those of any other clusters. Hence, we have to solve the routing problem for another combination of clusters that includes all seven customers. This analysis must be continued until the clusters that lead to the lowest total costs have been found. For example, the plot of total cost versus combination of clusters in Figure 17 indicates that the third set of clusters leads to the smallest total cost. It is also clear that other clusters lead to higher costs, and, hence we do not need to evaluate more than six clusters in this example. Figure 18 summarizes the entire heuristic method.

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ACKNOWLEDGMENT

The authors acknowledge financial support from Praxair, Inc.; the Pennsylvania Infrastructure Technology Alliance, and the National Science Foundation under Grants DMI-0556090 and OCI-0750826. F.Y. is partially supported by the U.S. Department of Energy under Contract DE-AC02-06CH11357.

NOMENCLATURE

Sets/Indices

i = set of tank sizes
j = set of truck sizes
k = set for binary representations of integers
n = set of customers
$n \in N_{y,s}$ = subset of customers included in the network of scenario s and year y
s = set of scenarios
y = set of years

Parameters

Ccap_i = capital cost of tank of size i
Cd_j = delivery cost of truck j
$\mathrm{Cout}_{n,y}$ = outage cost for customer n in year y
Cser_i = service cost of tank of size i
ck_j = delivery cost per kilometer traveled of truck j
$\mathrm{dem}_{n,y}$ = demand of customer n in year y
$\mathrm{demc}_{n,y}$ = monthly demand rate of customer n in year y
dep = depreciation period in years
espace_n = 1 if there is extra space for installing another tank at customer n; 0 otherwise
frac = minimum tanker fraction unloaded
FT_load = loading time for each customer
FT_del = loading time for each delivery from the plant
hpd = maximum number of working hours per day
Hz_y = time duration of year y
loss = product loss percentage per delivery
new_n = 1 if customer n is new; 0 otherwise
$\mathrm{ot}_{i,n}$ = 1 if tank size i originally installed at customer n; 0 otherwise
prob_s = probability of scenario s
rr_n = distance between the plant and customer n
$\sigma_{n,y}$ = standard deviation of daily demand
speed = average truck traveling speed in kilometers per hour
T_i^{L}, T_i^{U} = lower and upper bounds, respectively, for tank of size i
tsize_n = 1 if tank of customer n is sized; 0 otherwise
$\mathrm{TSP}_{y,s}$ = traveling salesman distance of all customers (excluding the plant) included in the distribution network of scenario s in year y
Vtruck_j = full transportation capacity of truck j
wacc = working capital discount factor
$\mathrm{winv}_{n,y,s}$ = upper bound of working inventory
z_α = service-level parameter, standard normal deviate of α

Binary Variables (0−1)

$\mathrm{et}_{i,n}$ = 1 if customer n has a tank of size i installed in extra space; 0 otherwise
$\mathrm{Ix}_{k,y,s}$ = 0−1 variable for the binary representation of the number of replenishments in scenario s and year y ($x_{y,s}$)
$\mathrm{tru}_{j,y,s}$ = 1 if truck j is selected for replenishmsnt in scenario s and year y; 0 otherwise
$\mathrm{yt}_{i,n}$ = 1 if customer n has a tank of size i installed; 0 otherwise

Continuous Variables (0 to +∞)

$\mathrm{capcost}_s$ = capital cost of scenario s
$\mathrm{ccapic}_{y,s}$ = effective capacity of a truck for the replenishments in scenario s, year y
$\mathrm{crot}_{y,s}$ = approximated routing cost of scenario s, year y
$\mathrm{cunit}_{y,s}$ = unit transportation cost of scenario s, year y
$\mathrm{distcost}_s$ = distribution cost of scenario s
E[cost] = total expected cost
$\mathrm{LT}_{y,s}$ = replenishment lead time of scenario s, year y
$\mathrm{mrt}_{y,s}$ = minimum routing distance to visit all customers in scenario s, year y
$\mathrm{servcost}_s$ = service cost of scenario s
$\mathrm{safety}_{n,y,s}$ = safety stock level in scenario s and year y for customer n
$\mathrm{seg}_{y,s}$ = auxiliary variable, for groups of customers
$\mathrm{Tccapic}_{y,s}$ = reciprocal of $\mathrm{ccapic}_{y,s}$
$\mathrm{Trp}_{n,y,s}$ = total delivery amount from plant to customer n in scenario s and year y
$\mathrm{Vend}_{n,y,s}$ = inventory level of customer n at the end of scenario s, year y
Vl_n,Vu_n = minimum and maximum volumes, respectively, of the tank at customer n
$\mathrm{Vm}_{n,y,s}$ = maximum inventory level of customer n in scenario s, year y
$\mathrm{Vzero}_{n,y,s}$ = initial volume at customer n in scenario s and year y
$\mathrm{winv}_{n,y,s}$ = maximum working inventory of customer n in scenario s, year y
$x_{y,s}$ = number of replenishment in year y in scenario s

Auxiliary Variables (0 to $+\infty$)

$LTIx_{k,y,s}$ = auxiliary variable for the product of $Ix_{k,y,s}$ and $LT_{y,s}$
$LTIx1_{k,y,s}$ = auxiliary variable for linearization
$mrIx_{k,y,s}$ = auxiliary variable for the product of $Ix_{k,y,s}$ and $mrt_{y,s}$
$mrIx1_{k,y,s}$ = auxiliary variable for linearization
$mrItru_{j,k,y,s}$ = auxiliary variable for the product of $tru_{,j,y,s}$ and $mrIx_{k,y,s}$
$mrItru1_{j,k,y,s}$ = auxiliary variable for linearization
$TruSeg_{j,y,s}$ = auxiliary variable for the product of $tru_{,j,y,s}$ and $seg_{y,s}$
$TruSeg1_{j,y,s}$ = auxiliary variable for linearization
$wIx_{n,k,y,s}$ = auxiliary variable for the product of $Ix_{k,y,s}$ and $winv_{n,y,s}$
$wIx1_{n,k,y,s}$ = auxiliary variable for linearization

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