# Optimisation Frameworks for Integrated Planning with Allocation of Transportation Resources for Industrial Gas Supply Chains

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### ABSTRACT

This work addresses the integrated optimisation of production-distribution planning and allocation of transportation resources for industrial gas supply chains. The production-distribution planning decisions include the production plan, purchasing plan for both a liquefied product and raw material from external suppliers, distribution plan by railcars and trucks, and demand allocation. In contrast, the allocating decisions of transportation resources involve the number of trucks and railcars at each plant, depot, and third-party supplier. First, we propose a mixedinteger nonlinear programming (MINLP) model, and then the MINLP model is reformulated as a mixed-integer linear fractional programming (MILFP) model. Furthermore, we present a multi-objective optimisation (MOO) model as an alternative approach. As solution strategies, we adopt Dinkelbach's algorithm and the reformulation-linearisation method for the MILFP model, whereas the  $\varepsilon$ -constraint method is used for the MOO model. Finally, industry-relevant case studies illustrate the applicability and performance of the proposed models and solution methods.

## 1. Introduction

Industrial gas supply chains involve domestic and/or international transportation between multi-site production plants, intermediate storage locations and several customers (Chima, 2007). Consequently, a large portion of supply chain costs come from transportation, and this has raised concerns about improving the transportation efficiency (Mason and Lalwani, 2006). Transportation efficiency can be improved by optimally allocating its resources. Furthermore, there is a need to consider not only the transportation efficiency but also the economic performance, such as total cost or profit, in an integrated manner. The system-wide approach where such multiple entities are coordinated can result in higher benefits to increase the overall profitability and supply chain performance (Barbosa-Póvoa, 2014; Pistikopoulos et al., 2021).

There are several studies on industrial gas supply chains, which concern with optimising the economic performance. An extensive review of literature focusing on the industrial gas supply chains was conducted by Barbosa-Povoa and Pinto (2020) and Ramaswamy et al. (2020). They provided an overview of the various components of supply chains in the industrial gas business and discussed the current contributions and challenges in supply chain scope representations, modelling and tractability, data management, and implementation.

Regarding production, Ierapetritou et al. (2002) studied a problem which considers the fluctuation of electricity prices to determine the optimal operation schedule of a production facility. First, they developed a two-stage stochastic mathematical framework resulting in an MINLP model. Then, they introduced a mixed-integer linear programming (MILP) approach to address the complexity of the MINLP model. Karwan and Keblis (2007) presented a mixedinteger programming (MIP) based optimisation framework to minimise the operation cost of an air separation unit that consumes a significant amount of electricity. The MIP model considers the hourly changed electricity price, which is known as the real time price (RTP). They identified the operating conditions that can take advantage of the RTP scheme via simulation studies. In work by Zhu et al. (2011), they focused on the operation of cryogenic air separation plants with a multiperiod nonlinear programming approach for uncertain power prices and product demands. Moreover, Mitra et al. (2012) developed a deterministic MILP model for optimal air separation planning under time-dependent

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electricity pricing. Cao et al. (2016) presented a dynamic model that can provide liquid storage, liquefaction, and vaporisation strategies for air separation units based on variations in electric prices and demand profiles. Caspari et al. (2019) proposed flexible operations of multiproduct air separation processes using an economic nonlinear model with a predictive control based strategy. Recently, Basán et al. (2020) studied a scheduling problem of air separation units by considering uncertainty in time-sensitive electricity prices. In the work, they presented an improved MILP formulation based on a mathematical model that was developed in their previous work (Basán et al., 2018). They also developed an efficient solution strategy combining a rolling horizon technique with an iterative solution method to solve industrial size instances.

From a distribution perspective, Campbell and Savelsbergh (2004b) maximised the total delivery volume on each route and developed a linear time algorithm for an optimal delivery schedule with a given order of customer visits. In Campbell and Savelsbergh (2004a), they addressed an inventory routing problem (IRP) that minimises long-term transportation costs for industrial gases. To efficiently solve large-scale, real-life instances, they also developed a solution strategy that relies on a decomposition approach. Dong et al. (2014) developed an MIP model for IRPs that considers the inventory management and distribution of industrial liquid products simultaneously. They formulated the model by considering driver-related regulations, time-varying customer consumption rates, and heterogeneous vehicles to obtain a practical solution. The computational difficulty of industrial-size instances was addressed by Dong et al. (2017), where the authors developed a two-level based iterative approach. Cóccola et al. (2018) investigated an IRP for several liquid products that are delivered by multi-compartment vehicles. To deal with the complexity of the problem, they proposed a decomposition strategy in which decisions on routes and delivery patterns are separately implemented using a nested column generation algorithm. In Subramanyam et al. (2021), they studied a multi-period vehicle routing problem (VRP) to minimise the cost of customer visit schedules under order uncertainty. An MIP model and branch-and-cut solution method were proposed for robust routing plans. A number of instances proved a solution quality from the developed model and approach.

Focusing on integrated production and distribution planning, Glankwamdee et al. (2008) developed an approximated production and distribution planning model; then, they extended the model into minimax and two-stage stochastic models to account for uncertainty in customer demand and product availability. Marchetti et al. (2014) proposed an MILP model to simultaneously determine operational production levels and distribution decisions in industrial gas supply chains at the minimum total cost. The production decisions are made by considering multi-site plants that operate at various production modes, while distribution decisions consider the combined vehicle routing and inventory management. This work was extended by Zamarripa et al. (2016) who proposed a rolling horizon based solution technique to deal with large-size industrial problems. You et al. (2011) developed an MILP model to integrate short-term and long-term distribution decisions and inventory planning. The short-term decisions are related to truck routing, while long-term decisions are related to tank sizing at customer sites. The objective was to minimise the total cost comprising the capital and operating costs. Zhang et al. (2017) introduced an MILP model and an interactive heuristic approach for a multi-scale routing problem that simultaneously considers production, distribution, inventory, and routing decisions. In addition, Misra et al. (2018) presented an enterprise-wide optimisation framework for integrated supply chain planning for the cryogenic air separation industry to minimise the total operating cost. Their work considered the cost of extra vehicles that can be hired or purchased to satisfy customer demand, but not vehicle efficiency nor vehicle allocation. In work by Malinowski et al. (2018), they developed a path-based integer programming model for a liquid helium global supply chain. The model was formulated by integrating supply contracts for sourcing, production, and routing of helium ISO containers. They also proposed a rolling horizon based solution strategy to address the complexity of the developed model. More recently, Lee et al. (2021) proposed an MILP model that simultaneously considers supply contracts, inventory management, production and distribution scheduling. They also developed a hierarchy based solution strategy to solve large-scale problems.

Despite the several research contributions on the industrial gas supply chains, to the best of our knowledge, no work has considered the integration of production-distribution decisions with transportation resource allocation decisions to improve both transportation efficiency and economic performance simultaneously. This work thus aims to incorporate the decisions on the allocation of transportation resources into our previous work (Lee et al., 2021), wherein the MILP models were proposed for the optimal production-distribution planning. An MINLP model is proposed, and then the model is reformulated as an MILFP model. Two different algorithms, Dinkelbach's algorithm (Dinkelbach, 1967) and the reformulation-linearisation method (Yue et al., 2013), are applied for the proposed MILFP model. Furthermore, an MOO model with the  $\varepsilon$ -constraint method (Haimes, 1971) is also presented as an alternative approach.

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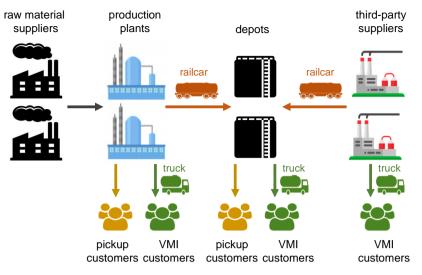


Figure 1: Industrial gas supply chain

The rest of this paper is organised as follows: Section 2 describes the problem and Section 3 presents the mathematical formulation of the MINLP, MILFP, and MOO models. Section 4 introduces the solution approaches for the proposed models. Section 5 presents and discusses the computational results of the case study. Finally, concluding remarks are provided in Section 6.

## 2. Problem statement

In this work, we address an integrated planning problem of industrial gas supply chains that includes decisions on the production, distribution, and allocation of trucks and railcars. The problem aims to simultaneously optimise the total operating cost and the number of allocated transportation resources. The industrial gas supply chain network is constructed with raw material suppliers, production plants, depots, third-party suppliers, and industrial customers, as illustrated in Fig. 1. The production at each plant involves the transformation, purification, and liquefaction of the raw material that is bought from an external supplier near the plant. The product can also be sourced from third-party suppliers, but this is considered only when it is more economical to source the product from such suppliers rather than producing at its production plants. In this problem, two types of customers, vendor managed inventory (VMI) and pickup customers, are considered. For VMI customers, the distribution decisions are made based on their inventory levels that are remotely monitored by instrumentation devices, while the distribution decisions are not considered for pickup customers. Each pickup customer collects the product at a designated plant or depot. The distribution of the liquefied product to the VMI customers is achieved by two transportation modes, railcars and trucks. Railcars undertake inter-plant transfers, that is, between plants or third-party suppliers and depots. In contrast, trucks are used for transportation between plants, depots, or third-party suppliers and customers.

The optimisation problem is fully described as follows:

#### Given are:

- locations of plants, depots, third-party suppliers, and customers;
- capacities of plants and limitations on raw material and product supplies;
- initial inventory and inventory limits of plants, depots, and customers;
- customer product consumptions;
- transportation times, quantities, and capacities of railcars and trucks;

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• cost data (i.e. unit and fixed production costs; plant start-up costs; unit transportation cost; raw material and product prices)

To determine:

- production plans including purchasing plans for the raw material and product from external suppliers;
- distribution plans of railcars and trucks;
- inventory levels;
- demand allocation to plants, depots, and third parties;
- allocation of truck resources;
- allocation of railcar resources

So as to:

minimise both total operating cost and number of allocated transportation resources, including trucks and railcars

# 3. Mathematical frameworks

In this section, we propose the MINLP, MILFP, and MOO models formulated based on the MILP model in Lee et al. (2021), for the integrated production-distribution planning with the truck and railcar allocation problem. A key difference between the proposed models and the previous work (Lee et al., 2021) lies in the capability to determine the optimal allocation of truck and railcar resources, together with the optimal production and distribution planning. Since a large number of constraints and variables are involved, only newly developed constraints, which are not included in the MILP model (Lee et al., 2021), are presented below. The other constraints are described in the Appendix A.

## 3.1. Notation

Indices

i	production plant
j	depot
k	customer
т	third-party supplier
t	time period

Sets

- $K^V$  VMI customer set
- $K_i$  VMI customer set initially allocated to plant *i*
- $K_i$  VMI customer set initially allocated to depot j
- $K_m$  VMI customer set initially allocated to third party m

#### Parameters

γ	tuning parameter
$\Delta_t$	length of time period <i>t</i> (day)
$\theta_{ik}$	round trip time of trucks between plant $i$ and customer $k$ (day)
$\theta_{jk}$	round trip time of trucks between depot $j$ and customer $k$ (day)
$\theta_{mk}$	round trip time of trucks between third party $m$ and customer $k$ (day)
$AR^{max}$	maximum number of available railcar resources

$AT^{max}$	maximum number of available truck resources
$C^{OS}$	unit outsourcing cost (\$/ton)
$CAP^{TR}$	truck capacity (ton)
$D_{kt}$	product consumption of VMI customer $k$ in time period $t$ (ton/day)
$I_k^{ini}$	initial inventory level at customer $k$ (ton)
lr	maximum possible number of allocated railcars
lm	maximum possible number of allocated trucks at each plant, depot, and third party
Т	number of time periods

# Integer variables

$AR^{total}$	total number of allocated railcar resources
$AR_t$	number of railcars allocated to time period t
$AT^{total}$	total number of allocated truck resources to plants, depots, and third parties
$AT_i$	number of trucks allocated to plant <i>i</i>
$AT_j$	number of trucks allocated to depot <i>j</i>
$AT_m$	number of trucks allocated to third party m

# Binary variables

$ET_l$	1 if <i>l</i> th binary digit representation of the integer variable, $AT^{total}$ is equal to 1; 0, otherwise
$ER_l$	1 if <i>l</i> th binary digit representation of the integer variable, $AR^{total}$ is equal to 1; 0, otherwise

#### Continuous variables

$I_{kt}$	inventory level of customer $k$ at time period $t$ (ton)
$Q_{kt}^{OS}$	amount of outsourcing product served to customer $k$ in time period $t$ (ton)
$Q_{ikt}^{TR}$	product amount delivered by trucks from plant $i$ to customer $k$ (ton)
$Q_{jkt}^{TR}$ $Q_{mkt}^{TR}$	product amount delivered by trucks from depot $j$ to customer $k$ (ton)
$Q_{mkt}^{TR}$	product amount delivered by trucks from third party $m$ to customer $k$ (ton)
RUR	railcar utilisation (%)
$TC^{os}$	outsourcing product cost (\$)
$TC^{prod}$	production cost (\$)
$TC^{rail}$	railcar cost (\$)
$TC^{raw}$	raw material cost (\$)
$TC^{st}$	plant start-up cost (\$)
$TC^{third}$	third-party cost (\$)
$TC^{total}$	total operating cost (\$)
$TC^{truck}$	truck cost (\$)
TUR	tuck utilisation (%)
$UR_i$	utilisation of trucks allocated at plant $i$ (%)
$UR_{j}$	utilisation of trucks allocated at depot $j$ (%)
$UR_m$	utilisation of trucks allocated at third party $m$ (%)
UR <sup>trans</sup>	overall utilisation of transportation resources (%)
$\overline{RE_l}$	auxiliary variable, $\overline{RE_l} \equiv RUR \cdot ER_l$
$\overline{TE_l}$	auxiliary variable, $\overline{TE_l} \equiv TUR \cdot ET_l$

#### 3.2. MINLP model

In this section, the problem is formulated as an MINLP model (denoted as PD-MINLP). The MINLP model considers a fractional objective, of which the numerator is the total operating cost and of which the denominator is the transportation utilisation. The aim is to optimise the total operating cost and the number of trucks and railcars simultaneously:

$$\min \frac{TC^{total}}{UR^{trans}} \tag{1}$$

Since both the total operating cost and number of trucks and railcars are to be minimised in this problem, both can not be the denominator. Here, we introduce the overall utilisation of transportation resources,  $UR^{trans}$ , which is maximised as the total number of trucks and railcars is minimised.

The total operating cost comprises the raw material, production, plant start-up, third party, railcar, truck and outsourcing product costs:

$$TC^{total} = TC^{raw} + TC^{prod} + TC^{st} + TC^{third} + TC^{rail} + TC^{truck} + TC^{os}$$
(2)

Here, the last term  $TC^{os}$  is the outsourcing cost. The product can also be outsourced at high cost. Such outsourcing of the product is considered only when the VMI customer demand can not be fulfilled due to restrictions on the distribution.

The cost of outsourcing product is calculated by:

$$TC^{os} = \sum_{k \in K^V} \sum_{t} C^{OS} \cdot Q_{kt}^{OS}$$
(3)

where  $C^{OS}$  is the unit outsourcing cost and  $Q_{kt}^{OS}$  is the amount of outsourced product that VMI customer  $k \in K^V$  receives in time period *t*. For the unit outsourcing cost, a very high cost (1,000 \$/ton) is considered to disallow the product outsourcing when customer demands can be satisfied by either own production plants or third-party suppliers.

The utilisation of transportation resources is defined with the utilisation of trucks and railcars:

$$UR^{trans} = (TUR + RUR)/2 \tag{4}$$

where, TUR and RUR stand for the overall truck and railcar utilisations, respectively.

The truck utilisation is calculated based on the number of trucks at each plant, depot, and third-party supplier, which divided by the total number of allocated truck resources, and utilisation of trucks at each location:

$$TUR = \sum_{i} \frac{AT_{i}}{AT^{total}} \cdot UR_{i} + \sum_{j} \frac{AT_{j}}{AT^{total}} \cdot UR_{j} + \sum_{m} \frac{AT_{m}}{AT^{total}} \cdot UR_{m}$$
(5)

where  $AT_i$ ,  $AT_j$ , and  $AT_m$  are the integer variables that represent the number of allocated trucks to each location;  $AT^{total}$  is the total number of allocated trucks;  $UR_i$ ,  $UR_j$ , and  $UR_m$  are the utilisations of trucks allocated at each location, and it is defined as follows:

$$UR_{i} = 100 \cdot \sum_{t} \sum_{k \in K_{i}} \left( \frac{\gamma \cdot Q_{ikt}^{TR}}{CAP^{TR} \cdot AT_{i} \cdot \Delta_{t}} \cdot \theta_{ik} \right) / T \qquad \forall i$$
(6)

$$UR_{j} = 100 \cdot \sum_{t} \sum_{k \in K_{j}} \left( \frac{\gamma \cdot Q_{jkt}^{TR}}{CAP^{TR} \cdot AT_{j} \cdot \Delta_{t}} \cdot \theta_{jk} \right) / T \qquad \forall j$$
(7)

$$UR_{m} = 100 \cdot \sum_{t} \sum_{k \in K_{m}} \left(\frac{\gamma \cdot Q_{mkt}^{TR}}{CAP^{TR} \cdot AT_{m} \cdot \Delta_{t}} \cdot \theta_{mk}\right)/T \qquad \forall m$$
(8)

where  $Q_{ikt}^{TR}$ ,  $Q_{jkt}^{TR}$ , and  $Q_{mkt}^{TR}$  are the delivering amounts from each location to the customer in each period;  $\theta_{ik}$ ,  $\theta_{jk}$ , and  $\theta_{mk}$  are the round trip times between each plant, depot or third-party supplier and customer;  $CAP^{TR}$  is the truck capacity;  $\Delta_t$  is the length of each time period; and T is the number of time periods. In addition,  $K_i$ ,  $K_j$ , and  $K_m$  are the sets of VMI customers that are initially allocated to plant *i*, depot *j*, and third party *m*. The initial allocations are pre-determined based on the customers' geographical locations.

In addition, the total number of trucks to plant i, depot j, and third party m is as follows:

$$AT^{total} = \sum_{i} AT_{i} + \sum_{j} AT_{j} + \sum_{m} AT_{m}$$
(9)

Here,  $AT^{total}$  can be defined as either the integer or continuous variable. In both cases, the  $AT^{total}$  always return to a integer number based on its definition in Eq. 9.

The number of allocated trucks is constrained by the maximum number of available truck resources:

$$AT^{total} \le AT^{max} \tag{10}$$

The total travel time from plant i, depot j, and third-party supplier m to any customers executed by trucks is limited by the number of allocated trucks at each location and truck capacity:

$$\sum_{k \in K_i} \frac{\gamma \cdot Q_{ikt}^{TR}}{CAP^{TR}} \cdot \theta_{ik} \le AT_i \cdot \Delta_t \tag{11}$$

$$\sum_{k \in K_i} \frac{\gamma \cdot Q_{jkt}^{TR}}{CAP^{TR}} \cdot \theta_{jk} \le AT_j \cdot \Delta_t \qquad \qquad \forall j, t \qquad (12)$$

$$\sum_{k \in K_m} \frac{\gamma \cdot Q_{mkt}^{TR}}{CAP^{TR}} \cdot \theta_{mk} \le AT_m \cdot \Delta_t \qquad \qquad \forall m, t$$
(13)

where the delivering amount, from the plant, depot, and third party to the customer, divided by the truck capacity  $(Q_{ikt}^{TR}/CAP^{TR}, Q_{jkt}^{TR}/CAP^{TR})$ , and  $Q_{mkt}^{TR}/CAP^{TR})$ , estimates the number of trips each truck performs during each time period; then, it is multiplied by the transit time to calculate the total travelling time between the locations. Here,  $\gamma$  is the tuning parameter adopted to avoid underestimating the total travel time, which is 2 in this problem. The total travel time is restricted by the length of each time period and the number of allocated trucks. These constraints also set the limit on the delivery amount by truck capacity and availability of trucks at each location.

The railcar utilisation is defined based on the number of railcars allocated to time period *t*, total number of allocated railcar resources, and the number of time period:

$$RUR = \sum_{t} \frac{AR_{t}}{AR^{total} \cdot T}$$
(14)

where  $AR_t$  is the number of railcars allocated to time period t,  $AR^{total}$  represents the total number of allocated railcars that are used for transporting the product from plants/third parties to depots during the planning horizon, and T is the number of time period.

The number of railcars allocated to time period *t* is equal to the number of railcars that are travelling between the plant/third party and the depot during time period *t*:

$$AR_{t} = \sum_{i} \sum_{j \in J_{i}} \sum_{t'=0}^{2\tau_{ij}-1} NR_{ij\Omega(t-t')} + \sum_{m} \sum_{j \in J_{m}} \sum_{t'=0}^{2\tau_{mj}-1} NR_{mj\Omega(t-t')} \qquad \forall t$$
(15)

In Eq. 15, a cyclic operator,  $\Omega(\cdot)$ , is used, so that railcar deliveries ending after current planning horizon can be viewed as wrapping around to the beginning of the planning horizon and continuing from there. The cyclic operator was introduced by Shah et al. (1993), and it is defined as follows:

$$\begin{aligned} \Omega(t) &= t & if \ t \geq 1, \\ \Omega(t) &= \Omega(t+T) & if \ t \leq 0 \end{aligned}$$

The total number of allocated railcars must be greater than or equal to the maximum value of the number of railcars allocated to time period *t*:

$$AR_t \le AR^{total} \qquad \forall t \tag{16}$$

Here, as we minimise the total number of allocated railcar resources to maximise its utilisation, the value of  $AR^{total}$  returns to the maximum value of  $AR_t$ .

The number of allocated railcars is limited by the availability of railcar resources:

$$AR^{total} \le AR^{max} \tag{17}$$

Similar to  $AT^{total}$ ,  $AR_t$  and  $AR^{total}$  can also be defined as either the integer or continuous variable.

Finally, Eq. 18 calculates the inventory level for customer k at time period t. The inventory level at the end of time period t is equal to the inventory at the previous time period; incoming product transported by trucks from any plants, depots, and third-party suppliers; outsourced product, minus the customer's product consumption in each period:

$$I_{kt} = I_{k,t-1} \mid_{t>1} + I_k^{ini} \mid_{t=1} + \sum_{i:k \in K_i} Q_{ikt}^{TR} + \sum_{j:k \in K_j} Q_{jkt}^{TR} + \sum_{m:k \in K_m} Q_{mkt}^{TR} + Q_{kt}^{OS} - D_{kt} \Delta_t \quad \forall k \in K^V, t$$
(18)

In summary, the proposed MINLP model includes the objective function in Eq. 1, and the constraints in Eqs. 2-18, and A.1-A.34.

As presented, the developed model incorporates the production-distribution decisions by minimising the related operating costs given in 2 into the decisions regarding the allocation of transportation resources. Note that the allocating decisions for trucks and railcars are related to the utilisation rates as given in Eqs. 5-8 and Eq. 14.

#### 3.3. MILFP model

In the constraints of the proposed MINLP model, all nonlinearities come from the bilinear terms, which are formed as continuous variables multiplied or divided by discrete variables; thus, these can be linearised by introducing auxiliary variables, big M parameters, and additional constraints. Since only the objective function has the linear fractional form, it can be regarded as an MILFP model. In this section, the MINLP model is reformulated as an MILFP model by linearising the bilinear terms involved.

The constraints including the bilinear terms are Eqs. 5-8 and 14, which calculate the overall truck utilisation rate, the utilisation of trucks allocated to each plant, depot, and third-party suppliers, and the railcar utilisation, respectively. When Eqs. 6-8 are inserted to Eq. 5, Eq. 5 becomes:

$$TUR = \frac{TQ}{AT^{total}} \tag{19}$$

$$TQ = \sum_{i} \sum_{k \in K_{i}} \sum_{t} \frac{\gamma \cdot Q_{ikt}^{TR} \cdot \theta_{ik}}{CAP^{TR} \cdot \Delta_{t} \cdot T} + \sum_{j} \sum_{k \in K_{j}} \sum_{t} \frac{\gamma \cdot Q_{ijt}^{TR} \cdot \theta_{jk}}{CAP^{TR} \cdot \Delta_{t} \cdot T} + \sum_{m} \sum_{k \in K_{m}} \sum_{t} \frac{\gamma \cdot Q_{mkt}^{TR} \cdot \theta_{mk}}{CAP^{TR} \cdot \Delta_{t} \cdot T}$$
(20)

To linearise the bilinear term, TQ divided by  $AT^{total}$  in Eq. 19, the integer variable,  $AT^{total}$  is required to be expressed by a set of auxiliary binary variables at first:

$$AT^{total} = \sum_{l=1}^{lm} 2^{l-1} \cdot ET_l$$
(21)

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where  $ET_l$  is the binary variable and it is coded 1 when the *l*th binary digit representation is equal to 1. Here, *lm* is related to the maximum possible value of allocated trucks  $AT^{total}$ , i.e.,  $lm = log_2(AT^{max})$ .

Based on Eq. 21, Eq. 19 becomes:

$$TQ = \sum_{l=1}^{lm} 2^{l-1} \cdot TUR \cdot ET_l$$
(22)

Then, Eq. 22 can be rewritten by introducing an auxiliary variable,  $\overline{TE_l} \equiv TUR \cdot ET_l$ , a big-M parameter, and additional constraints:

$$TQ = \sum_{l=1}^{lm} 2^{l-1} \cdot \overline{TE_l}$$
<sup>(23)</sup>

$$\overline{TE_l} \le M^{TUR} \cdot ET_l \qquad \qquad \forall l = 1, ..., lm$$
(24)

$$\overline{TE}_{l} \le TUR \qquad \qquad \forall l = 1, ..., lm \tag{25}$$

$$TE_l \ge TUR - M^{TUR} \cdot (1 - ET_l) \qquad \qquad \forall l = 1, ..., lm$$
(26)

where  $M^{TUR}$  is a big number and an upper bound of variable TUR. Note that the symbol M with a superscript represents the big M value throughout the paper.

Similarly, Eq. 14, which is related to the railcar utilisation, is linearised with a set binary variables, an auxiliary variable, and additional constraints as follows:

$$AR^{total} = \sum_{l=1}^{l^{r}} 2^{l-1} \cdot ER_{l}$$
(27)

$$\sum_{l} AR_{l} = T \cdot \sum_{l=1}^{lr} 2^{l-1} \cdot \overline{RE_{l}}$$
(28)

$$\overline{RE_l} \le M^{RUR} \cdot ER_l \qquad \qquad \forall l = 1, ..., lr$$
(29)

$$\overline{RE_l} \le RUR \qquad \qquad \forall l = 1, ..., lr \tag{30}$$

$$RE_l \ge RUR - M^{RUR} \cdot (1 - ER_l) \qquad \qquad \forall l = 1, ..., lr$$
(31)

where  $\overline{RE_l}$  is the auxiliary variable which is defined as  $\overline{RE_l} \equiv RUR \cdot ER_l$ .  $ER_l$  is the binary variable and it is 1 when the *l*th binary digit representation is equal to 1. Here, *lr* is related to the maximum possible value of allocated railcars  $AR^{total}$ , i.e.,  $lr = log_2(AR^{max})$ .

As a result, the reformulated MILFP model consists of Eq. 1 for the objective function as well as Eqs. 2-4, 9-13, 15-18, 20-21, 23-31, and A.1-A.34.

#### 3.4. MOO model

As an alternative approach to solve the problem, we develop an MOO model that provides a set of Pareto-optimal solutions quantifying the trade-off between the total operating cost and utilisation of transportation resources. The MOO model includes the same constraints of the MILFP model except for the objective function. The MOO model is defined as follows:

min TC <sup>total</sup>	(32)
$max UR^{trans}$	(33)
s.t. Eqs. 2-4, 9-13, 15-18, 20-21, 23-31, and A.1-A.34.	

## 4. Solution approaches

## 4.1. Dinkelbach's algorithm

For the proposed MILFP model, we first adopt Dinkelbach's algorithm. Dinkelbach's algorithm (Dinkelbach, 1967) was developed to solve convex fractional programming by solving a sequence of nonlinear programming (NLP) subproblems. Dinkelbach's algorithm has been extended and applied by recent works (Bradley and Arntzen, 1999; Pochet and Warichet, 2008; Billionnet, 2010; Espinoza et al., 2010; Yue and You, 2013; Liu et al., 2014) for MILFP problems. The main idea of the algorithm is to transform the original MILFP problem into an MILP subproblem and then solve the MILP subproblem iteratively until a stopping criteria is met.

Given that, the proposed MILFP model presented above can be converted into the following model (denoted as PD-D):

min 
$$TC^{total} - f \cdot UR^{trans}$$
 (34)  
s.t. Eqs. 2-4, 9-13, 15-18, 20-21, 23-31, and A.1-A.34.

Moreover, the main procedure of the algorithm is illustrated in Fig 2 and summarised as follows:

Step 1. Initialise *f*;

- Step 2. Solve the PD-D model, and denote the optimal solution as  $TC^{total*}$  and  $UR^{trans*}$ ;
- **Step 3.** If  $|f \frac{TC^{total*}}{UR^{trans*}}|/|f| \le \delta$  (stopping criteria),

the optimal solution of the original MILFP model is  $TC^{total*}/UR^{trans*}$ ; otherwise, update  $f = TC^{total*}/UR^{trans*}$ , and go to Step 2.

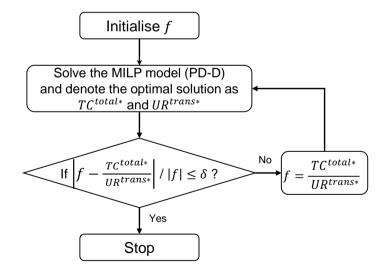


Figure 2: Flowchart of the Dinkelbach's algorithm

#### 4.2. Reformulation-linearisation method

Another method to solve the MILFP model is the reformulation-linearisation method (Yue et al., 2013). The method was developed by combining the Charnes-Cooper transformation method (Charnes and Cooper, 1959) and Glover's linearisation scheme (Glover, 1975) to address the limitation in the application of the Charnes-Cooper transformation. The Charnes-Cooper transformation method can be applied for only linear fractional programming (LFP) problems, wherein all variables in the constraints are continuous. However, incorporating the Glover's linearisation scheme allows us to solve MILFP problems involving discrete variables. Recently, use of the reformulation-linearisation strategy for solving MILFP problems has garnered attention. (Tong et al., 2014; Zhong and You, 2014; Yue et al., 2014; Chung et al., 2016)

In this section, we introduce the reformulation-linearisation method through the generalised model of the proposed MILFP model which is expressed as M0. The detailed model (denoted as PD-RL) for the problem considered in this work can be found in the Appendix B.

M0: min 
$$\frac{A0 + \sum_{i \in I} A1_i x_i + \sum_{j \in J} A2_j y_j}{B0 + \sum_{i \in I} B1_i x_i + \sum_{j \in J} B2_j y_j}$$
(35)

s.t. 
$$C0_k + \sum_{i \in I} C1_{ik} x_i + \sum_{j \in J} C2_{jk} y_j = 0$$
  $\forall k \in K$  (36)  
 $x_i \ge 0 \ \forall i \in I \text{ and } y_j \in \{0, 1\} \ \forall j \in J$ 

First, nonnegative auxiliary variables G and  $GX_i$ , such that  $G = \frac{1}{B0 + \sum_{i \in I} B1_i x_i + \sum_{j \in J} B2_j y_j}$ ,  $GX_i = G \cdot x_i$ ,

and  $GY_j = G \cdot y_j$  are introduced. With the introduction of these variables, the objective function and a set of constraints in M0 can be reformulated into Eqs. 37 and 38, respectively. Additionally, the nonlinear term in  $GY_j = G \cdot y_j$  can be linearised with additional constraints (Eqs. 40-42) based on the Glover's linearisation scheme. Therefore, the MILFP model (M0) can be transformed into the following MILP model (M1):

M1: min 
$$A0 \cdot G + \sum_{i \in I} A1_i \cdot GX_i + \sum_{j \in J} A2_j \cdot GY_j$$
(37)

s.t. 
$$C0_k \cdot G + \sum_{i \in I} C1_{ik} \cdot GX_i + \sum_{j \in J} C2_{jk} \cdot GY_j = 0$$
  $\forall k \in K$  (38)

$$B0 \cdot G + \sum_{i \in I} B1_i \cdot GX_i + \sum_{j \in J} B2_j \cdot GY_j = 1$$
(39)

$$GY_j \le G$$
  $\forall j \in J$  (40)

$$GY_j \le M \cdot y_j \qquad \qquad \forall j \in J \qquad (41)$$

$$GY_j \ge G - M \cdot (1 - y_j) \qquad \qquad \forall j \in J \qquad (42)$$

$$G \ge 0, \ GX_i \ge 0 \ \forall i \in I \text{ and } GY_i \ge 0, \ y_i \in \{0, 1\} \ \forall j \in J$$

Then, the solution of the original MILFP model (M0) is  $x_i^* = GX_i^*/G^*$  and  $y_j^* = GY_j^*/G^*$ , if the solution of the reformulated MILP model (M1) is  $GX_i^*$ ,  $y_i^*$ ,  $GY_j^*$ , and  $G^*$ .

The main advantage of this method compared with Dinkelbach's algorithm is that the model needs to solve the problem only once. The inclusion of new variables and constraints, however, increases the size of the problem. These properties are analysed when compared with the performance of Dinkelbach's algorithm in the case study.

#### 4.3. $\varepsilon$ -constrained method

To solve the developed MOO model, we apply the  $\varepsilon$ -constraint method, wherein one objective function is optimised, while the other objective function is converted into a constraint with a lower bound. The total operating cost ( $TC^{total}$ ) is kept as an objective function, and the utilisation of transportation resources ( $UR^{trans}$ ) is transformed into a constraint by setting a lower bound,  $\varepsilon$ . The resulting single-objective optimisation model (denoted as PD-MOO) is as follows:

min 
$$TC^{total}$$
 (43)  
s.t.  $\varepsilon \le UR^{trans}$  (44)  
Eqs. 2-4, 9-13, 15-18, 20-21, 23-31, and A.1-A.34

#### 5. Case study

In this section, we apply the developed models and solution approaches to an industrial case study, which was considered in our previous work (Lee et al., 2021), to demonstrate the applicability. In the problem, there are more than 25 plants, depots, and third-party suppliers; over 750 customers; hundreds of railcars; and more than 100 truck resources. The planning horizon is one month, which is divided into 30 days. The developed models are implemented in GAMS 34.3.0 on a desktop with an Intel 3.60 GHz CPU and 32.0 of RAM. Note that most of the input data used in this case study are not available due to confidentiality issues.

First, the problem is solved with the developed MINLP model, and then the computational performance of the MILFP model is investigated. For the MINLP model, five MINLP solvers, DICOPT, ALPHAECP, BARON, SBB and SCIP, are used. By contrast, three different solvers, Gurobi, Cplex, and SCIP are used for the MILP models (PD-D and PD-RL), which are transformed for Dinkelbach's algorithm and reformulation-linearisation method. The CPU time for each model is limited to 3 hr. In addition, the optimality gap is set to 1 % for the MINLP and PD-RL models, while 98 % with 0.01 of the stopping criteria ( $\delta$ ) are set for the PD-D model.

The model statistics and computational performance are presented in Table 1 and 2, respectively. As observed, the MILFP model, which uses Dinkelbach's algorithm (PD-D), shows the best performance, and it obtains the optimal solution of 57.26 k\$/% within 3,120 s. The reformulation-linearisation method (PD-RL) is terminated after 10,800 s due to the time limit, and it obtains a 6.56 % worse solution (61.76 k%/%) compared with the solution from Dinkelbach's algorithm. It is noticeable that the problem size is increased when the reformulation-linearisation method is employed due to the introduction of auxiliary variables and constraints. It should also be noted that the number of discrete variables is almost doubled. This is because the integer variables related to the railcars and the number of trucks at each plant, depot, and third-party supplier have been expressed by the binary representation to adopt the reformulation-linearisation method as presented in Appendix B.

Comparing the computational performance of the algorithms for the MINLP solvers with the MILFP model, all are not satisfactory. The DICOPT solver returns almost the same optimal solution as Dinkelbach's algorithm but requires longer CPU time, which is more than three times that of Dinkelbach's algorithm. The SBB solver cannot find any feasible solution within the time limit. After the time limit, ALPHAECP, BARON, and SCIP get the optimal solutions of 62.27 k\$/%, 62.48 k\$/%, and 93.85 k\$/% respectively, but the values are not as good as the optimal solution from Dinkelbach's algorithm.

In addition, we also compare the computational performance of the MILP solvers for the MILFP model, and the results are presented in Table 3. As can be seen, Gurobi is the most efficient solver for both Dinkelbach's algorithm and the reformulation-linearisation method. In Dinkelbach's algorithm, Gurobi takes 3,120 s to get the optimal solution of 57.26 k\$/%, whereas Cplex gets a 0.78 % higher solution after the time limit. Concerning the reformulation-linearisation method, the solution of Cplex obtained after 3 hr is far from the solution gained by Dinkelbach's algorithm with Gurobi. The SCIP solver shows the worst performance for both Dinkelbach's algorithm and the reformulation-linearisation method. For Dinkelbach's algorithm, SCIP cannot reach the solution obtained by Gurobi within the time limitation, whereas no solution is returned for the reformulation-linearisation method.

#### Table 1

Model statistics of the MINLP and MILFP models

Mode	Equationa	Continuous D		
wode	Equations	variables	variables	
PD-MINLP	140,907	160,143	5,455	
$PD-D^{a}$	149,957	160,159	5,471	
PD-RL <sup>b</sup>	237,916	169,786	9,487	
	2 1 11			

a Dinkelbach's algorithm

b Reformulation and linearisation method

#### Table 2

Computational performance of the MINLP and MILFP models

Model	Algorithm	Unit cost (k\$/%)	Total operating cost (\$)	Truck utilisation (%)	Railcar utilisation (%)	Total no. of trucks	Total no. of railcars	CPU time (s)
PD-MINLP	DICOPT	57.31	5,302 k	85.10	99.72	60	65	10,800 <sup>c</sup>
	ALPHAECP	62.27	5,366 k	84.69	87.66	60	74	10,800 <sup>c</sup>
	BARON	62.48	5,273 k	72.27	94.49	68	69	10,800 <sup>c</sup>
	SBB	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$10,800^{c}$
	SCIP	93.85	8,570 k	83.70	98.94	58	69	$10,800^{c}$
$PD\text{-}D^a$	Gurobi	57.26	5,317 k	85.92	99.79	59	65	3,120
PD-RL <sup>b</sup>	Gurobi	61.76	5,520 k	80.52	98.23	63	64	$10,800^{c}$

a Dinkelbach's algorithm

b Reformulation and linearisation method

c Computation was terminated due to the time limit (3 hr)

d A feasible solution has not been found within the time limit (3 hr)

#### Table 3

Computational performance of MILP solvers for the MILFP model

Model	Algorithm	Unit cost (k\$/%)	Total operating cost (\$)	Truck utilisation (%)	Railcar utilisation (%)	Total no. of trucks	Total no. of railcars	CPU time (s)
$PD\text{-}D^a$	Gurobi	57.26	5,317 k	85.92	99.79	59	65	3,120
	Cplex	57.71	5,362 k	85.97	99.85	59	63	$10,800^{c}$
	SCIP	62.86	5,634 k	80.09	99.17	80	63	$10,800^{c}$
PD-RL <sup>b</sup>	Gurobi	61.76	5,520 k	80.52	98.23	63	64	$10,800^{c}$
	Cplex	82.03	5,693 k	39.23	99.58	128	63	10,800 <sup>c</sup>
	SCIP	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$10,800^{c}$

a Dinkelbach's algorithm

b Reformulation and linearisation method

c Computation was terminated due to the time limit (3 hr)

d A feasible solution has not been found within the time limit (3 hr)

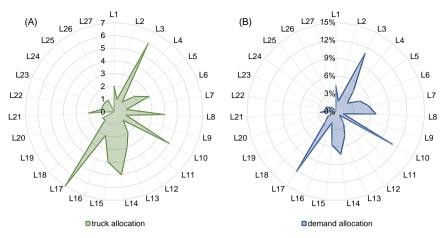


Figure 3: (A) The number of allocated trucks and (B) optimal demand allocation from the MILFP model

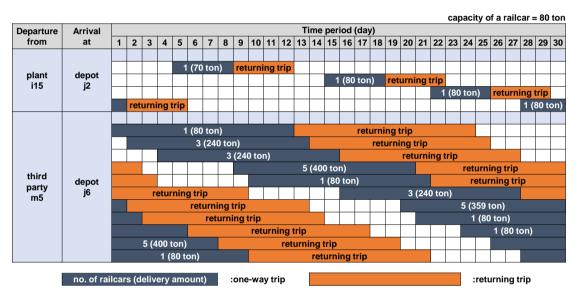


Figure 4: Optimal railcar schedule from the MILFP model

Next, we investigate the solution gained from the MILFP model. Since Dinkelbach's algorithm was identified as the most efficient approach, only the result from that approach is presented in the remainder of the paper. Fig. 3 presents the number of allocated trucks and percentage of allocated demand to each plant, depot, and third-party supplier. As observed, the number of allocated trucks varies between 0 to 7 and it is determined by considering the optimal demand allocation to each location. At location L17, which has the largest demand allocation, 7 trucks are allocated. On the contrary, at locations, L20 and L27, which have no demand allocation, no trucks are allocated. This result shows that the proposed MILFP model is capable of allocating truck resources by taking into account the optimal demand allocation that is determined by considering production and distribution costs. Fig. 4 illustrates the optimal schedule of railcars that depart from two different plants. In the figure, the grey and orange bars represent one-way and returing trips, respectively. The values in the each grey bar show the delivering amount and number of railcars used for the delivery. As depicted, the MILFP model can also provide the railcar schedule by optimally allocating railcar resources. Fig. 5 shows the total cost breakdown. The truck cost constitutes the highest percentage (41 %), while approximately one-fourth and one-fifth of the total operating cost are allocated to the raw material and production costs, respectively. The remaining portion is allocated to railcar cost (7 %), third party cost (3 %), outsourcing product cost (1 %) and plant start-up cost (1 %).

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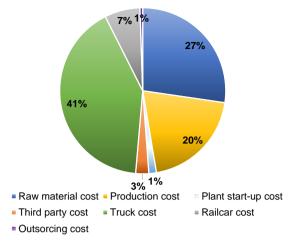


Figure 5: Cost breakdown of total operating cost obtained from the MILFP model

# Table 4Comparison of optimal solutions from the $M^R$ and MILFP models

Model	$M^R$	$PD\text{-}D^a$	Improvement
Total operating cost (\$), TC <sup>total</sup>	5,274 k	5,317 k	-0.82 %
Truck utilisation, TUR	37.64 <sup>b</sup> %	85.92 %	56.19 %
Railcar utilisation, RUR	84.95 <sup>b</sup> %	99.79 %	14.87 %
Transportation utilisation, UR <sup>trans</sup>	61.30 <sup>b</sup> %	92.86 %	33.99 %
Total no of trucks, AT <sup>total</sup>	135	59	-
Total no. of railcars, AR <sup>total</sup>	74 <sup>c</sup>	65	-

a MILFP model with Dinkelbach's algorithm

b Post-processing utilisation calculated based on the optimal solution gained from the model  $M^R$  (Lee et al., 2021) and Eqs.4-8, 14-16

c Post-processing total number of railcars calculated based on the optimal solution gained from the model  $M^R$  (Lee et al., 2021) and Eqs.15-16

Furthermore, we investigate the impact of the proposed MILFP model, which simultaneously considers the optimal allocation of the transportation resources and economic aspect (i.e. total operating cost). To evaluate the impact, we compare the solution of the MILFP model with the solution from the model (denoted as  $M^R$ ) provided by Lee et al. (2021). The difference of the model  $M^R$  from the proposed MILFP is that it optimises the total operating cost without considering the optimal transportation resource allocation and utilisation. The comparison is presented in Table 4. Note that the values regarding the number of railcars, truck utilisation and railcar utilisation for the model  $M^R$  are calculated based on Eqs.15-16, 4-8, and 14-16, respectively, using the optimal values obtained by the model. As reported, there are significant differences in utilisation rates of trucks and railcars. When the model considers only the economic aspect, it results in low transportation efficiency. The model  $M^R$  obtains a solution with 37.64 % of truck utilisation and 84.95 % of railcar utilisation. On contrary, the MILFP model can improve the transportation efficiency dramatically by considering optimal cost and transportation resource allocation in an integrated manner. The truck, railcar, and overall transportation resource utilisations show 56.19 %, 14.87 %, and 33.99 % of improvements, respectively, by showing only 0.82 % of the increase in the total operating cost. In addition, the number of transportation resources (135 vs. 59) and railcars (74 vs. 65).

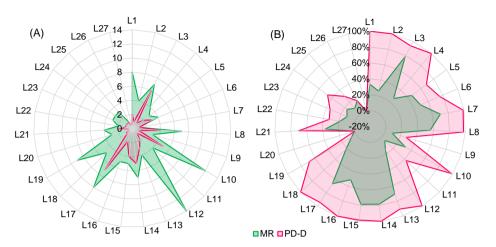


Figure 6: Comparison of (A) truck allocation and (B) truck utilisation from the M<sup>R</sup> (Lee et al., 2021) and MILFP models

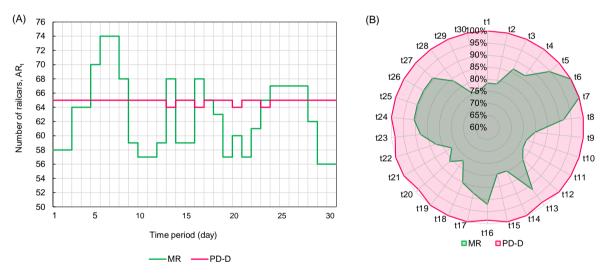


Figure 7: Comparison of (A) railcar allocation and (B) railcar utilisation from the M<sup>R</sup> (Lee et al., 2021) and MILFP models

Figs. 6-7 depict more detailed comparison of truck and railcar utilisations gained from the models. In Fig. 6, the radar graphs compare the truck allocation and its utilisation at each location. As observed, the MILFP model can improve not only the truck utilisation but also the number of trucks at each location. In Fig. 7, the left line graph shows the number of railcars that perform the product delivery from plants to depots during a time period. The number of railcars used in each time period is the optimal value of  $AR_t$ , which is in Eq. 15. On the other hand, the right radar graph in Fig. 7 shows the railcar utilisation in each time period. Before optimally allocating the railcar resources, the number of railcars used is almost evenly distributed (see the solution from the MILFP model, i.e., PD-D), and it results in a high railcar utilisation.

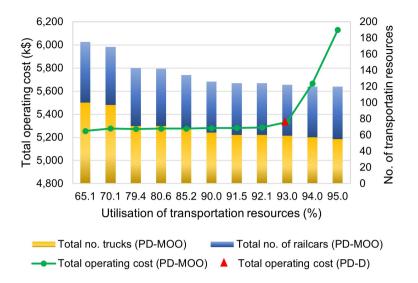


Figure 8: Pareto profile with the total operating cost and utilisation of transportation resources

Finally, we examine the solutions from the multi-objective optimisation model (PD-MOO). The lower bound for the transportation resource utilisation ( $\varepsilon$ ) is fixed to 11 values from 65 to 95 %. The optimality gap and time limit are set to 1 % and 10,800 s, respectively. The resulting model includes 149,957 equations, 160,158 continuous variables, and the same number of discrete variables as that of the PD-D model (5,417). The entire process to get the Pareto-optimal solutions with different values of  $\varepsilon$  takes 31,885 s of CPU time.

Fig. 8 shows the trade-offs between the two objectives. The bar chart represents the total number of allocated trucks and railcars, while the green line indicates the Pareto frontier that is approximated by the Pareto-optimal solutions. With 65.1 % of the utilisation of transportation resources, the total operating cost is 5,253 k\$. The cost slightly increases to 5,276 k\$ when we aim at 70 % of the utilisation and maintains the almost same level until the utilisation reaches 90.0 %. After that point, significant trade-offs are observed. As the utilisation increases from 91.5 to 95.0 %, the total cost increases from 5,282 to 6,129 k\$. Moreover, the total number of trucks and railcars is decreased gradually as the utilisation increments, and a considerable increase in total cost is observed when the number goes below 122. Looking at the solution from the MILFP model (see the red point in Fig. 8), that is on the Pareto curve and yields a good balance between the two objectives. From the results, we can see that the MILFP approach could directly lead to the solution that a reasonable trade-off is achievable between the total cost and utilisation, while the multi-objective optimisation method produces multiple solutions that support the decision-making.

Instance	No. of plants/ third	No. of depots	No. of customers	AT <sup>max</sup>	AR <sup>max</sup>	Model	Equations	Continuous variables	Discrete variables
D1	parties	1	40		20		4.000	c 177	100
Ρ1	1	T	48	30	30	PD-MINLP	4,938	6,177	193
						PD-D <sup>a</sup>	4,970	6,187	203
						PD-RL <sup>b</sup>	9,779	6,521	328
Ρ2	3	1	92	30	30	PD-MINLP	9,232	11,567	428
						$PD-D^{a}$	9,264	11,577	438
						$PD-RL^{b}$	17,975	12,278	688
P3	6	2	197	50	50	PD-MINLP	24,311	29,481	977
						$PD\text{-}D^a$	24,349	29,493	989
						$PD-RL^{b}$	41,997	31,004	1,486
P4	12	2	468	70	70	PD-MINLP	53,491	66,084	1,964
						$PD\text{-}D^a$	53,535	66,108	1,968
						$PD-RL^{b}$	91,931	68,992	2,840
P5	18	3	653	100	100	PD-MINLP	106,693	124,091	3,934
						$PD\text{-}D^a$	106,737	124,105	3,948
						PD-RL <sup>b</sup>	166,251	130,174	5,977

Table 5Model statistics of five additional instances

a Dinkelbach's algorithm

b Reformulation and linearisation method

## 5.1. Additional computational studies

For more reliable and conclusive insights into the general performance in particular of the MINLP and MILFP models, additional computational tests are conducted. Five problems with different numbers of plants, depots, third parties, customers, and transportation resources are considered. The problem sizes and results are given in Table 5 and 6, respectively.

As can be seen, the CPU times vary from one approach to the other in each instance, and it is increased significantly as the problem size increases. Specifically, Dinkelbach's algorithm requires up to 2,681 s, and it is faster than using the MINLP solvers and reformulation-linearisation method. For small instances, P1 and P2, Dinkelbach's algorithm obtains the solutions within 201 s, whereas DICOPT and the reformulation-linearisation method require slightly longer CPU times. For medium-size instance P3, the CPU times of DICOPT and reformulation-linearisation method have been increased dramatically (6,589 s and 4902 s, respectively), while Dinkelbach's algorithm can still get the solution within 441 s. For P4 and P5 having thousands of discrete variables, the performance of the reformulation-linearisation is not satisfactory. In both instances, it cannot reach 1 % of optimality gap within the time limit, while Dinkelbach's approach and DICOPT take up to 9,973 s and 2,681 s, respectively. This is due to the binary representation for the integer variables, as well as the introduction of additional constraints and variables regarding the Glover's linearisation scheme. These two facts result in a much larger model size when using the reformulation-linearisation method. As for the comparison between the MINLP solvers, DICOPT is much faster than ALPHAECP, BARON, SBB, and SCIP, especially for large-size instances. In case of P4 and P5, DICOPT can get the solutions within 3 hr of the time limit, but other MINLP solvers are terminated before reaching the optimality tolerance. Overall, for this planning problem, of which the objective is the minimisation of the total cost divided by the utilisation of transportation resources, Dinkelbach's algorithm is shown to be much more efficient than the MINLP solvers and reformulation-linearisation method.

able 6	
omputational performance of the MINLP and MILFP models for five additional instanc	es

			Unit	Total	Truck	Railcar	Tota	Total	CPU
nstance	Model	Algorithm	cost	operating	utilisation	utilisation	no. of	no. of	time
			(k\$/%)	cost (k\$)	(%)	(%)	trucks	railcars	(s)
P1	PD-MINLP	DICOPT	2.90	226	57.64	98.52	3	9	33
		ALPHAECP	2.90	226	57.64	98.52	3	9	65
		BARON	2.90	226	57.64	98.52	3	9	139
		SBB	2.90	226	57.64	98.52	3	9	205
		SCIP	2.90	226	57.64	98.52	3	9	267
	$PD-D^{a}$	Gurobi	2.90	226	57.64	98.52	3	9	21
	$PD-RL^{b}$	Gurobi	2.90	226	57.64	98.52	3	9	51
P2	PD-MINLP	DICOPT	8.47	778	83.69	100.00	9	7	337
		ALPHAECP	8.47	778	83.69	100.00	9	7	963
		BARON	8.47	778	83.69	100.00	9	7	2,49
		SBB	8.47	778	83.69	100.00	9	7	2,00
		SCIP	8.47	778	83.69	100.00	9	7	3,14
	$PD-D^{a}$	Gurobi	8.47	778	83.69	100.00	9	7	201
	PD-RL <sup>b</sup>	Gurobi	8.47	778	83.69	100.00	9	7	736
P3	PD-MINLP	DICOPT	17.28	1,627	88.33	100.00	14	14	6,58
		ALPHAECP	17.28	1,623	87.85	100.00	15	18	6,83
		BARON	17.46	1,606	83.97	100.00	15	17	10,80
		SBB	17.70	1,608	81.68	100.00	15	17	10,80
		SCIP	17.28	1,623	87.85	100.00	15	18	10,07
	$PD-D^{a}$	Gurobi	17.28	1,623	87.85	100.00	15	18	441
	PD-RL <sup>b</sup>	Gurobi	17.28	1,623	87.85	100.00	15	18	4,90
P4	PD-MINLP	DICOPT	41.68	4,007	92.29	100.00	52	19	2,03
		ALPHAECP	42.14	4,008	91.72	98.52	52	18	10,80
		BARON	42.58	4,019	90.55	98.24	52	19	10,80
		SBB	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	10,80
		SCIP	44.46	4,232	92.47	97.90	52	19	10,80
	$PD\text{-}D^a$	Gurobi	41.61	4,000	92.28	100.00	52	19	1,28
	$PD-RL^{b}$	Gurobi	41.95	4,043	93.07	99.67	52	20	10,80
Ρ5	PD-MINLP	DICOPT	64.49	6,159	91.11	99.91	79	74	9,97
		ALPHAECP	65.15	6,164	91.08	98.17	79	75	10,80
		BARON	68.27	6,567	92.93	99.47	76	76	10,80
		SBB	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	$N/A^d$	10,80
		SCIP	73.14	6,953	91.49	98.65	75	75	10,80
	$PD\text{-}D^a$	Gurobi	64.06	6,158	92.35	99.92	78	76	2,68
	PD-RL <sup>b</sup>	Gurobi	64.59	6,165	91.08	99.82	79	74	10,80

a Dinkelbach's algorithm

b Reformulation and linearisation method

c Computation was terminated due to the time limit (3 hr)

d A feasible solution has not been found within the time limit (3 hr)

## 6. Concluding remarks

This work addressed an integrated planning problem for industrial gas supply chains extended from our previous work (Lee et al., 2021). The problem considered both transportation efficiency, which is related to an optimal allocation of trucks and railcars, and the economic aspect (i.e. total operating cost) simultaneously. First, we formulated the problem as an MINLP model that accounts for the total operating cost divided by the utilisation as an objective. Then, the developed MINLP model was reformulated as an MILFP model. Two algorithms, Dinkelbach's algorithm and reformulation-linearisation method, were embedded for the MILFP model. Real-world industrial case studies investigated the computational performance of the proposed models. The computational results revealed that the MILFP model with the Dinkelbach's algorithm was the most efficient compared with the reformulation-linearisation method and commercial MINLP solvers. The case studies also proved the applicability of the proposed models and approaches to determine an optimal allocation of transportation resources, together with production and distribution plans. As an alternative approach, we also proposed a multi-objective optimisation model. The model treated the total operating cost and the utilisation of transportation resources as two separate objective functions. To solve the model, we adopted the  $\varepsilon$ -constraint method where one of the objective functions is introduced as a constraint. We tested the developed model with the same case study considered for the MILFP model. The obtained set of Pareto-optimal solutions illustrated the relationship between the two objectives. Based on the Pareto-optimal solutions, a reasonable trade-off between the objectives was identified. Further work could be directed at addressing the uncertainty of input parameters such as customer demand and transportation time and treating the robustness of the models

# Abbreviations

IRP	inventory routing problem
LFP	linear fractional programming
MILP	mixed-integer linear programming
MINLP	mixed-integer nonlinear programming
MILFP	mixed-integer linear fractional programming
MOO	multi-objective optimisation
NLP	nonlinear programming
RTP	real time electricity price
VRP	vehicle routing problem
VMI	vendor managed inventory

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## A. Appendix A. Integrated planning of industrial gas supply chains model

The MILP model proposed by (Lee et al., 2021) is presented as follows:

#### A.1. Costs

The purchasing cost of raw material from external suppliers is calculated based on the discount type of supply contract:

$$TC^{raw} = \sum_{i} \sum_{n} C^{raw}_{in} \cdot F_{in}$$
(A.1)

$$\sum_{n} F_{in} = \sum_{t} R_{it} \qquad \forall i \qquad (A.2)$$

$$(\lambda_{in} - \lambda_{i,n-1} \mid_{n>1}) \cdot Y_{i,n+1} \le F_{in} \le (\lambda_{in} - \lambda_{i,n-1} \mid_{n>1}) \cdot Y_{in} \qquad \qquad \forall i, n < N$$

$$(A.3) \qquad \qquad \forall i, n < N \qquad \qquad (A.4)$$

$$F_{in} \leq M^F \cdot Y_{in}$$

$$\forall i, n \in \mathbb{N}$$

$$\forall i, n = N$$

$$(A.5)$$

The production cost is determined by the operating mode and the production amount:

$$TC^{prod} = \sum_{i} \sum_{t} \mu_{i} \cdot P_{i}^{max} \cdot W_{it} + \sum_{i} \sum_{t} v_{i} \cdot P_{it}$$
(A.6)

The plant start-up cost occurs when each plant start to produce the product:

$$TC^{st} = \sum_{i} \sum_{t} C_i^{st} \cdot U_{it}$$
(A.7)

The purchasing product cost from third-party suppliers is given by:

$$TC^{third} = \sum_{m} \sum_{n} C_{mn}^{third} \cdot S_{mn}$$
(A.8)

$$\sum_{n} S_{mn} = \sum_{t} O_{mt} \qquad (A.9)$$

$$\begin{aligned} (\lambda_{mn} - \lambda_{m,n-1} \mid_{n>1}) \cdot Z_{m,n+1} &\leq S_{mn} \leq (\lambda_{mn} - \lambda_{m,n-1} \mid_{n>1}) \cdot Z_{mn} & \forall i, n < N \\ Z_{mn} \geq Z_{m,n+1} & \forall i, n < N \end{aligned}$$
(A.10)

$$S_{mn} \le M^S \cdot Z_{mn} \qquad \qquad \forall m, n = N \qquad (A.12)$$

Total railcar cost is calculated based on the number of railcars used for delivery:

$$TC^{rail} = \sum_{i} \sum_{j \in J_i} \sum_{t} C_{ij}^{RC} \cdot NR_{ijt} + \sum_{m} \sum_{j \in J_m} \sum_{t} C_{mj}^{RC} \cdot NR_{mjt}$$
(A.13)

and truck cost is given as follows:

$$TC^{truck} = \sum_{i} \sum_{k \in K_{i}} \sum_{t} \frac{Q_{ikt}^{TR}}{CAP^{TR}} \cdot L_{ik} \cdot C^{TR}$$

$$+ \sum_{j} \sum_{k \in K_{j}} \sum_{t} \frac{Q_{jkt}^{TR}}{CAP^{TR}} \cdot L_{jk} \cdot C^{TR}$$

$$+ \sum_{m} \sum_{k \in K_{m}} \sum_{t} \frac{Q_{mkt}^{TR}}{CAP^{TR}} \cdot L_{mk} \cdot C^{TR}$$
(A.14)

#### A.2. Production constraints

The production amount at each plant is constrained by the minimum and maximum production capacities:

$$P_i^{\min} \cdot W_{it} \le P_{it} \le P_i^{\max} \cdot W_{it} \tag{A.15}$$

and the following constraint determined whether the each plant changes its operating model from off- to on-mode.

$$W_{it} - W_{i,t-1} \mid_{t>1} \le U_{it} \tag{A.16}$$

The amount of raw material that can be purchased at each plant in each period is restricted:

$$R_{it} \le R_i^{max} \qquad \qquad \forall i, t \tag{A.17}$$

The relationship between the amount of the raw material and production amount is given as:

$$R_{it} = \alpha_i P_{it} \qquad \qquad \forall i, t \qquad (A.18)$$

#### A.3. Third-party supplier constraints

The amount of purchasing product from each third-party supplier in each period is also limited:

$$O_{mt} \le O_m^{max}$$
  $\forall m, t$  (A.19)

and the product flow coming out from third parties is calculated by:

$$O_{mt} = \sum_{j \in J_m} Q_{mjt}^{RC} + \sum_{k \in K_m} Q_{mkt}^{TR} \qquad \forall m, t$$
(A.20)

#### A.4. Transportation constraints

The delivery amount by railcars is bounded based on the capacity and the number of used railcars:

$$Q_{ijt}^{RC} \le CAP^{RC} \cdot NR_{ijt} \qquad \qquad \forall i, j \in J_i, t \tag{A.21}$$

$$Q_{mjt}^{RC} \le CAP^{RC} \cdot NR_{mjt} \qquad \qquad \forall m, j \in J_m, t \tag{A.22}$$

#### A.5. Inventory mass balance

$$I_{it} = I_{i,t-1} |_{t>1} + I_i^{ini} |_{t=1} + P_{it} - \sum_{j \in J_i} Q_{ijt}^{RC} - \sum_{k \in K_i} Q_{ikt}^{TR} - \sum_{k \in K_i^P} DP_{ikt} \Delta_t \qquad \forall i, t \quad (A.23)$$

$$I_{jt} = I_{j,t-1} |_{t>1} + I_{j}^{ini} |_{t=1} + \sum_{i:j \in J_i} Q_{ij,\Omega(t-\tau_{ij})}^{RC} + \sum_{m:j \in J_m} Q_{mj,\Omega(t-\tau_{mj})}^{RC} - \sum_{k \in K_j} Q_{jkt}^{TR} - \sum_{k \in K_j^P} DP_{jkt} \Delta_t \quad \forall j, t \quad (A.24)$$

Note that the mass balance for VMI customer  $k \in K^V$  is give in Eq. 18.

The following inventory constraints set maximum and minimum levels, and the inventory level at the end of the time horizon:

$$I_i^{min} \le I_{it} \le I_i^{max} \qquad \qquad \forall i, t \tag{A.25}$$

$$I_j^{min} \le I_{jt} \le I_j^{max} \qquad \qquad \forall j, t \tag{A.26}$$

$$\begin{split} I_k^{min} &\leq I_{kt} \leq I_k^{max} & \forall k \in K^V, t \\ I_{it} &= I_i^{ini} & \forall i, t = T \end{split} \tag{A.27}$$

$$\forall i, t = T \tag{A.28}$$

$$I_{jt} = I_j^{ini} \qquad \qquad \forall j, t = T \tag{A.29}$$

$$I_{kt} = I_k^{ini} \qquad \forall k \in K^V, t = T \tag{A.30}$$

#### A.6. Multiple sourcing constraints

The multiple sourcing constraints limit the number of plants, depots, and third parties that each customer can be served the product:

$$\sum_{i:k \in K_i} X_{ik} + \sum_{j:k \in K_j} X_{jk} + \sum_{m:k \in K_m} X_{mk} \le NS \qquad \forall k \in K^V$$
(A.31)

$$Q_{ikt}^{TR} \le M^Q \cdot X_{ik} \qquad \qquad \forall i, k \in K_i, t \qquad (A.32)$$

$$Q_{jkt}^{TR} \le M^Q \cdot X_{jk} \qquad \qquad \forall j, k \in K_j, t \qquad (A.33)$$

$$\forall j, k \in K_j, t \qquad (A.34)$$

$$Q_{mkt}^{TR} \le M^Q \cdot X_{mk} \qquad \qquad \forall m, k \in K_m, t \tag{A.34}$$

## Notation

#### Indices

*n* cost region

#### Sets

- $J_i$  set of depots allocated to plant i
- $J_m$  set of depots allocated to third parties m
- $K_i^P$  set of pickup customers designated to plant *i*
- $K_i^P$  set of pickup customers designated to depot j

#### Parameters

- $\alpha_i$  coefficient relates amount of raw material and product produced by plant *i*
- $\lambda_{in}$  amount of raw material corresponding to plant *i* and cost region *n* (ton)
- $\mu_i$  unit fixed production cost of plant *i*, (\$/ton)
- $v_i$  unit production cost of plant *i* (\$/ton)
- $\sigma_{mn}$  amount of product corresponding to third party *m* and cost region *n* (ton)
- $\tau_{ij}$  transportation time of railcars between plant *i* and depot *j* based on one-way trip (day)
- $\tau_{ij}$  transportation time of railcars between third party *m* and depot *j* based on one-way trip (day)
- $C^{TR}$  unit transportation cost for trucks, (\$/mile)
- $C_{ij}^{RC}$  transportation cost for each railcar between plant *i* and depot *j* (\$)
- $C_{in}^{raw}$  unit cost for raw material purchased by plant *i* corresponding to cost region *n* (\$/ton)
- $C_i^{st}$  plant start-up cost of plant *i* (\$)
- $C_{mj}^{RC}$  transportation cost for each railcar between third party *m* and depot *j* (\$)
- $C_{mn}^{third}$  unit cost for product purchased from third party *m* corresponding to cost region *n* (\$/ton)

*CAP<sup>RC</sup>* loading capacity for each railcar (ton)

- $DP_{ikt}$  product consumption at plant *i* of pickup customer *k* in time period *t*(ton/day)
- $DP_{ikt}$  product consumption at depot *j* of pickup customer *k* in time period *t*(ton/day)
- $I_i^{ini}$  initial inventory level at plant *i* (ton)
- $I_i^{ini}$  initial inventory level at depot *j* (ton)
- $I_i^{max}$ ,  $I_i^{min}$  maximum and minimum inventory levels at plant *i* (ton)
- $I_i^{max}$ ,  $I_i^{min}$  maximum and minimum inventory levels at depot j (ton)
- $I_k^{max}$ ,  $I_k^{min}$  maximum and minimum inventory levels at customer k (ton)
- $L_{ik}$  round-trip distance between plant *i* and customer *k* (mile)
- $L_{ik}$  round-trip distance between depot *j* and customer *k* (mile)
- $L_{mk}$  round-trip distance between third-party *m* and customer *k* (mile)
- NS maximum number of sources each customer can be served over a time horizon
- $O_m^{max}$  maximum availability of product at third party *m* in each time period (ton)
- $P_i^{max}$ ,  $P_i^{min}$  maximum and minimum production capacities of plant *i* in each time period (ton)
- $R_i^{max}$  maximum availability of raw material for plant *i* in each time period (ton)

#### **Integer Variables**

- $NR_{iit}$  number of railcars departing plant *i* to depot *j* in time period *t*
- $NR_{mit}$  number of railcars departing third-party *m* to depot *j* in time period *t*

#### **Binary Variables**

- $U_{it}$  1 if production mode of plant *i* is switched from the off-mode to the on-mode at time period *t*; 0, otherwise
- $W_{it}$  1 if production mode of plant *i* is the on-mode in time period *t*; 0, otherwise
- $X_{ik}$  1 if customer k is served the product from plant i; 0, otherwise
- $X_{jk}$  1 if customer k is served the product from depot j; 0, otherwise
- $X_{mk}$  1 if customer k is served the product from third party m; 0, otherwise
- $Y_{in}$  1 if total amount of raw material purchased by plant *i* is in cost region *n*; 0, otherwise
- $Z_{mn}$  1 if total amount of product purchased from third party *m* is in cost region *n*; 0, otherwise

#### **Continuous Variables**

- $F_{in}$  amount of raw material purchased by plant *i* corresponding to cost region *n* (ton)
- $I_{it}$  inventory level of plant *i* at time period *t* (ton)
- $I_{jt}$  inventory level of depot *j* at time period *t* (ton)
- $O_{mt}$  product amount purchased from third party *m* during time period *t* (ton)
- $P_{it}$  production amount at plant *i* during time period *t* (ton)
- $Q_{iit}^{RC}$  product amount delivered from plant *i* to depot *j* by railcars during time period *t* (ton)
- $Q_{mit}^{RC}$  product amount delivered from third party *m* to depot *j* by railcars during time period *t* (ton)
- $R_{it}$  amount of raw material purchased by plant *i* during time period *t* (ton)
- $S_{mn}$  amount of product purchased from third party *m* corresponding to cost region *n* (ton)

#### **B.** Appendix B. Reformulated MILFP model

Reformulation-linearisation is a method to reformulate an MILFP model into an equivalent MILP form, by introducing additional continuous variables and constraints. The first step of the reformulation is to introduce a new variable G, such that  $G = 1/UR^{trans}$ . In the following formulation, variables which have a capital G in front of the original variables that methods are multiply by G.

The corresponding MILP model (PD-RL) is given below:

#### **B.1.** Transformation for integer variables

To reformulate the proposed MILFP model to an equivalent MILP model using reformulation-linearisation method, integer variables should be expressed by a number of binary variables at first. The integer variables involved in the MILFP model are the number of allocated trucks at plants/depots/third-party suppliers  $(AT_i, AT_j, \text{ and } AT_m)$  and the number of railcars used for the product delivery between plants/third-party suppliers and depots in time period t ( $NR_{ijt}$  and  $NR_{mit}$ ). These integer variables are replaced by its binary representation:

$$AT_{i} = \sum_{q=1}^{qm} 2^{q-1} \cdot XI_{iq}$$
(B.1)

$$AT_{j} = \sum_{q=1}^{qm} 2^{q-1} \cdot XJ_{jq}$$
(B.2)

$$AT_m = \sum_{q=1}^{qm} 2^{q-1} \cdot XM_{mq}$$
(B.3)

where  $XI_{iq}$ ,  $XJ_{jq}$  and  $XM_{mq}$  are binary variables which indicate whether the *q*th digit of the binary representation of the variables are equal to 1 or not. Here,  $qm = log_2 AT^{max}$ 

$$NR_{ijt} = \sum_{h=1}^{hm} 2^{h-1} \cdot B_{ijth}$$
(B.4)

$$NR_{mjt} = \sum_{h=1}^{hm} 2^{h-1} \cdot B_{mjth}$$
(B.5)

where  $B_{ijth}$  and  $B_{mjth}$  are binary variables which are 1 when the *h*th digit of the binary representation of the variables are equal to 1 and  $hm = log_2 A R^{max}$ 

#### **B.2.** Objective function

#### **B.3.** Costs

$$GTC^{total} = GTC^{raw} + GTC^{prod} + GTC^{st} + GTC^{third} + GTC^{rail} + GTC^{truck} + GTC^{os}$$
(B.7)

$$GTC^{os} = \sum_{k \in K^V} \sum_{t} C^{OS} \cdot GQ_{kt}^{OS}$$
(B.8)

$$GTC^{raw} = \sum_{i} \sum_{n} C^{raw}_{in} GF_{in}$$
(B.9)

$$\sum_{n} GF_{in} = \sum_{t} GR_{it} \qquad \qquad \forall i \qquad (B.10)$$

$$(\lambda_{in} - \lambda_{i,n-1} \mid_{n>1}) \cdot GY_{i,n+1} \le GF_{in} \le (\lambda_{in} - \lambda_{i,n-1} \mid_{n>1}) \cdot GY_{in} \qquad \qquad \forall i, n < N \quad (B.11)$$

$$\begin{aligned} GY_{in} \geq GY_{i,n+1} & \forall i, n < N \quad (B.12) \\ GF_{in} \leq M^{GF} \cdot GY_{in} & \forall i, n = N \quad (B.13) \end{aligned}$$

$$GTC^{prod} = \sum_{i} \sum_{t} \mu_{i} P_{i}^{max} \cdot GW_{it} + \sum_{i} \sum_{t} v_{i} \cdot GP_{it}$$
(B.14)

$$GTC^{st} = \sum_{i} \sum_{t} C_{i}^{st} \cdot GU_{it}$$
(B.15)

$$GTC^{third} = \sum_{m} \sum_{n} C_{mn}^{third} \cdot GS_{mn}$$
(B.16)

$$\sum_{n} GS_{mn} = \sum_{t} GO_{mt} \qquad \forall m \qquad (B.17)$$

$$\begin{aligned} & (\lambda_{mn} - \lambda_{m,n-1} \mid_{n>1}) \cdot GZ_{m,n+1} \leq GS_{mn} \leq (\lambda_{mn} - \lambda_{m,n-1} \mid_{n>1}) \cdot GZ_{mn} \\ & GS_{mn} \leq M^{GS} \cdot GZ_{mn} \\ \end{aligned} \qquad \qquad \forall i, n < N \quad (B.18) \\ & \forall m, n = N \end{aligned}$$

$$GZ_{mn} \ge GZ_{m,n+1}$$
  $\forall i, n < N$  (B.20)

$$GTC^{rail} = \sum_{i} \sum_{j \in J_{i}} \sum_{t} C_{ij}^{RC} \cdot (\sum_{h=1}^{hm} 2^{h-1} \cdot GB_{ijth}) + \sum_{m} \sum_{j \in J_{m}} \sum_{t} C_{mj}^{RC} (\sum_{h=1}^{hm} 2^{h-1} \cdot GNR_{mjth})$$
(B.21)  
$$GTC^{truck} = \sum_{i} \sum_{k \in K_{i}} \sum_{t} \frac{GQ_{ikt}^{TR}}{CAP^{TR}} \cdot L_{ik} \cdot C^{TR} + \sum_{j} \sum_{k \in K_{j}} \sum_{t} \frac{GQ_{jkt}^{TR}}{CAP^{TR}} \cdot L_{jk} \cdot C^{TR}$$

$$+\sum_{m}\sum_{k\in K_{m}}\sum_{t}\frac{GQ_{mkt}^{TR}}{CAP^{TR}}\cdot L_{mk}\cdot C^{TR}$$
(B.22)

## **B.4.** Production constraints

$$P_i^{min} \cdot GW_{it} \le GP_{it} \le P_i^{max} \cdot GW_{it} \tag{B.23}$$

$$GW_{it} - GW_{i,t-1} \mid_{t>1} \le GU_{it} \qquad \qquad \forall i,t \qquad (B.24)$$

$$\begin{array}{ll} GR_{it} \leq G \cdot R_i^{max} & \forall i,t & (B.25) \\ GR_{it} = \alpha_i \cdot GP_{it} & \forall i,t & (B.26) \end{array}$$

$$GO_{mt} \le G \cdot O_m^{max} \qquad \forall m, t \qquad (B.27)$$

$$GO_{mt} = \sum_{k} GQ_{mit}^{RC} + \sum_{k} GQ_{mit}^{TR} \qquad \forall m, t \qquad (B.28)$$

$$CO_{mt} = \sum_{j \in J_m} GQ_{mjt}^{RC} + \sum_{k \in K_m} GQ_{mkt}^{TR} \qquad \forall m, t$$
(B.28)

# **B.6.** Transportation capacity constraints

$$\sum_{k \in K_i} \frac{GQ_{ikt}^{TR}}{CAP^{TR}} \cdot \theta_{ik} \le \sum_{q=1}^{qm} 2^{q-1} \cdot GXI_{iq} \cdot \Delta_t \qquad \qquad \forall i, t \qquad (B.30)$$

$$\sum_{k \in K_j} \frac{GQ_{jkt}^{TR}}{CAP^{TR}} \cdot \theta_{jk} \le \sum_{q=1}^{qm} 2^{q-1} \cdot GXJ_{jq} \cdot \Delta_t \qquad \qquad \forall j,t \qquad (B.31)$$

$$\sum_{k \in K_m} \frac{GQ_{mkt}^{TR}}{CAP^{TR}} \cdot \theta_{mk} \le \sum_{q=1}^{qm} 2^{q-1} \cdot GXM_{mq} \cdot \Delta_t \qquad \qquad \forall m, t$$
(B.32)

(B.19)

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$$GQ_{ijt}^{RC} \le CAP^{RC} \cdot \sum_{h=1}^{hm} 2^{h-1} \cdot GB_{ijth} \qquad \qquad \forall i, j \in J_i, t$$
(B.33)

$$GQ_{mjt}^{RC} \le CAP^{RC} \cdot \sum_{h=1}^{hm} 2^{h-1} \cdot GB_{mjth} \qquad \qquad \forall m, j \in J_m, t$$
(B.34)

# **B.7.** Inventory mass balance

$$GI_{it} = GI_{i,t-1} \mid_{t>1} + G \cdot I_i^{ini} \mid_{t=1} + GP_{it} - \sum_{j \in J_i} GQ_{ijt}^{RC} - \sum_{k \in K_i} GQ_{ikt}^{TR} - \sum_{k \in K_i^P} G \cdot DP_{ik} \quad \forall i, t$$
(B.35)

$$GI_{jt} = GI_{j,t-1} \mid_{t>1} + G \cdot I_{j}^{ini} \mid_{t=1} + \sum_{i: j \in J_{i}} GQ_{ij,\Omega(t-\tau_{ij})}^{RC} + \sum_{m: j \in J_{m}} GQ_{mj,\Omega(t-\tau_{mj})}^{RC} - \sum_{k \in K_{j}} GQ_{jkt}^{TR} - \sum_{k \in K_{j}^{P}} G \cdot DP_{jk} \qquad \forall j, t$$
(B.36)

$$GI_{kt} = GI_{k,t-1} |_{t>1} + G \cdot I_k^{ini} |_{t=1} + \sum_{i:k \in K_i} GQ_{ikt}^{TR} + \sum_{j:k \in K_j} GQ_{jkt}^{TR} + \sum_{m:k \in K_m} GQ_{mkt}^{TR} + GQ_{kt}^{OS} - G \cdot D_k \qquad \forall k \in K^V, t \quad (B.37)$$

$$\begin{array}{ll} G \cdot I_i^{min} \leq GI_{it} \leq G \cdot I_i^{max} & \forall i, t \\ G \cdot I_i^{min} \leq GI_{jt} \leq G \cdot I_i^{max} & \forall j, t \end{array}$$
 (B.38)

$$G \cdot I_k^{min} \le G I_{kt} \le G \cdot I_k^{max} \qquad \forall k \in K^V, t \tag{B.40}$$

$$GI_{it} = G \cdot I_i^{ini}$$
  $\forall i, t = T$  (B.41)

$$\begin{aligned} GI_{jt} &= G \cdot I_j^{ini} & & \forall j, t = T \\ GI_{kt} &= G \cdot I_k^{ini} & & \forall k \in K^V, t = T \end{aligned} \tag{B.42}$$

## **B.8.** Multiple sourcing constraints

$$\sum_{i:k\in K_i} GX_{ik} + \sum_{j:k\in K_i} GX_{jk} + \sum_{m:k\in K_m} GX_{mk} \le G \cdot NS \qquad \forall k \in K^V$$
(B.44)

$$GQ_{ikt}^{TR} \le M^{GQ} \cdot GX_{ik} \qquad \qquad \forall i, k \in K_i, t \qquad (B.45)$$

$$\begin{array}{ll} GQ_{jkt}^{TR} \leq M^{GQ} \cdot GX_{jk} & & \forall j,k \in K_j,t & (B.46) \\ GQ_{mkt}^{TR} \leq M^{GQ} \cdot GX_{mk} & & \forall m,k \in K_m,t & (B.47) \end{array}$$

$$\forall m, k \in K_m, t \tag{B.47}$$

#### **B.9.** Truck utilisation constraints

$$GTQ = \sum_{i} \sum_{k \in K_{i}} \sum_{t} \frac{\gamma \cdot GQ_{ikt}^{TR} \cdot \theta_{ik}}{CAP^{TR} \cdot \Delta_{t} \cdot T} + \sum_{j} \sum_{k \in K_{j}} \sum_{t} \frac{\gamma \cdot GQ_{ijt}^{TR} \cdot \theta_{jk}}{CAP^{TR} \cdot \Delta_{t} \cdot T} + \sum_{m} \sum_{k \in K_{m}} \sum_{t} \frac{\gamma \cdot GQ_{mkt}^{TR} \cdot \theta_{mk}}{CAP^{TR} \cdot \Delta_{t} \cdot T}$$
(B.48)

$$GAT^{total} = \sum_{l=1}^{lm} 2^{l-1} \cdot \overline{GTE_l}$$
(B.49)

$$\overline{GTE_l} \le M^{GTUR} \cdot GET_l \quad \forall l = 1, ..., lm$$
(B.50)

$$\overline{GTE_l} \le GTUR \quad \forall l = 1, ..., lm \tag{B.51}$$

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$$\overline{GTE_l} \ge GTUR - M^{GTUR} \cdot (G - GET_l) \quad \forall l = 1, ..., lm$$
(B.52)

$$GAT^{total} = \sum_{i} \sum_{q=1}^{qm} 2^{q-1} \cdot GXI_{iq} + \sum_{j} \sum_{q=1}^{qm} 2^{q-1} \cdot GXJ_{jq} + \sum_{m} \sum_{q=1}^{qm} 2^{q-1} \cdot GXM_{mq}$$
(B.53)

$$GAT^{total} \le G \cdot AT^{max} \tag{B.54}$$

# **B.10.** Railcar utilisation constraints

$$GAR^{total} = \sum_{l=1}^{lr} 2^{l-1} \cdot GER_l$$
 (B.55)

$$\sum_{l} GAR_{l} = T \cdot \sum_{l=1}^{lr} 2^{l-1} \cdot \overline{GRE_{l}}$$
(B.56)

$$\overline{GRE_l} \le M^{GRUR} \cdot GER_l \qquad \qquad \forall l = 1, ..., lr$$
(B.57)

$$\overline{GRE_l} \le GRUR \qquad \qquad \forall l = 1, ..., lr \tag{B.58}$$

$$\overline{GRE_l} \ge GRUR - M^{GRUR} \cdot (G - GER_l) \qquad \qquad \forall l = 1, ..., lr$$
(B.59)

$$GAR_{t} = \sum_{i} \sum_{j \in J_{i}} \sum_{t'=0}^{2\tau_{ij}-1} (\sum_{h=1}^{hm} 2^{h-1} \cdot GB_{ij\Omega(t-t'),h}) + \sum_{m} \sum_{j \in J_{m}} \sum_{t'=0}^{2\tau_{mj}-1} (\sum_{h=1}^{hm} 2^{h-1} \cdot GB_{mj\Omega(t-t'),h}) \quad \forall t$$
(B.60)  
$$GAR^{total} \ge GAR_{t} \qquad \forall t$$
(B.61)

$$GAR^{total} \le G \cdot AR^{max} \tag{B.62}$$

# **B.11.** Transportation utilisation

$$GUR^{trans} = (GTUR + GRUR)/2 \tag{B.63}$$

## **B.12.** Glover's linearisation scheme

$GU_{it} \leq G$	$\forall i, t$	(B.64)
$GU_{it} \leq M^G \cdot U_{it}$	$\forall i, t$	(B.65)
$GU_{it} \ge G - M^G \cdot (1 - U_{it})$	$\forall i, t$	(B.66)
$GW_{it} \leq G$	$\forall i, t$	(B.67)
$GW_{it} \leq M^G \cdot W_{it}$	$\forall i, t$	(B.68)
$GW_{it} \ge G - M^G \cdot (1 - W_{it})$	$\forall i, t$	(B.69)
$GX_{ik} \leq G$	$\forall i, k$	(B.70)
$GX_{ik} \le M^G \cdot X_{ik}$	$\forall i, k$	(B.71)
$GX_{ik} \ge G - M^G \cdot (1 - X_{ik})$	$\forall i, k$	(B.72)
$GX_{jk} \leq G$	$\forall j,k$	(B.73)
$GX_{jk} \le M^G \cdot X_{jk}$	$\forall j,k$	(B.74)
$GX_{jk} \ge G - Mv \cdot (1 - X_{jk})$	$\forall j,k$	(B.75)
$GX_{mk} \leq G$	$\forall m, k$	(B.76)

$GX_{mk} \le M^G \cdot X_{mk}$	$\forall m, k$	(B.77)
$GX_{mk} \ge G - M^G \cdot (1 - X_{mk})$	$\forall m, k$	(B.78)
$GY_{in} \leq G$	$\forall i, n$	(B.79)
$GY_{in} \leq M^G \cdot Y_{in}$	$\forall i, n$	(B.80)
$GY_{in} \ge G - M^G \cdot (1 - Y_n i)$	$\forall i, n$	(B.81)
$GZ_{mn} \leq G$	$\forall m, n$	(B.82)
$GZ_{mn} \leq M^G \cdot Z_{mn}$	$\forall m, n$	(B.83)
$GZ_{mn} \ge G - M^G \cdot (1 - Z_{mn})$	$\forall m, n$	(B.84)
$GET_l \leq G$	$\forall l$	(B.85)
$GET_l \leq M^G \cdot ET_l$	$\forall l$	(B.86)
$GET_l \ge G - M^G \cdot (1 - ET_l)$	$\forall l$	(B.87)
$GER_l \leq G$	$\forall l$	(B.88)
$GER_l \leq M^G \cdot ER_l$	$\forall l$	(B.89)
$GER_l \ge G - M^G \cdot (1 - ER_l)$	$\forall l$	(B.90)
$GXI_{iq} \leq G$	$\forall i, q$	( <b>B</b> .91)
$GXI_{iq} \le M^G \cdot XI_{iq}$	$\forall i, q$	(B.92)
$GXI_{iq} \ge G - M^G \cdot (1 - XI_{iq})$	$\forall i, q$	(B.93)
$GXJ_{jq} \leq G$	$\forall j, q$	(B.94)
$GXJ_{jq} \le M^G \cdot XJ_{jq}$	$\forall j, q$	(B.95)
$GXJ_{jq} \ge G - M^G \cdot (1 - XJ_{jq})$	$\forall j, q$	(B.96)
$GXM_{mq} \le G$	$\forall m, q$	(B.97)
$GXM_{mq} \le M^G \cdot XM_{mq}$	$\forall m, q$	(B.98)
$GXM_{mq} \ge G - M^G \cdot (1 - XM_{mq})$	$\forall m, q$	(B.99)
$GB_{ijth} \leq G$	$\forall i, j, t, h$	(B.100)
$GB_{ijth} \leq M^G \cdot B_{ijth}$	$\forall i, j, t, h$	(B.101)
$GB_{ijth} \ge G - M^G \cdot (1 - B_{ijth})$	$\forall i, j, t, h$	(B.102)
$GB_{mjth} \leq G$	$\forall m, j, t, h$	(B.103)
$GB_{mith} \leq M^G \cdot B$	$\forall m, j, t, h$	(B.104)
$GB_{mith} \ge G - M^G \cdot (1 - B_{mith})$	$\forall m, j, t, h$	(B.105)
Time II.		

Finally,

$$GUR^{trans} = 1$$

(B.106)

## References

- Barbosa-Póvoa, A.P., 2014. Process supply chains management-where are we? where to go next? Frontiers in Energy Research 2, 23.
- Barbosa-Povoa, A.P., Pinto, J.M., 2020. Process supply chains: Perspectives from academia and industry. Computers & Chemical Engineering 132, 106606.
- Basán, N.P., Cóccola, M.E., Dondo, R.G., Guarnaschelli, A., Schweickardt, G.A., Méndez, C.A., 2020. A reactive-iterative optimization algorithm for scheduling of air separation units under uncertainty in electricity prices. Computers & Chemical Engineering 142, 107050.
- Basán, N.P., Grossmann, I.E., Gopalakrishnan, A., Lotero, I., Méndez, C.A., 2018. Novel milp scheduling model for power-intensive processes under time-sensitive electricity prices. Industrial & Engineering Chemistry Research 57, 1581–1592.
- Billionnet, A., 2010. Optimal selection of forest patches using integer and fractional programming. Operational Research 10, 1-26.
- Bradley, J.R., Arntzen, B.C., 1999. The simultaneous planning of production, capacity, and inventory in seasonal demand environments. Operations Research 47, 795–806.
- Campbell, A.M., Savelsbergh, M.W., 2004a. A decomposition approach for the inventory-routing problem. Transportation Science 38, 488-502.
- Campbell, A.M., Savelsbergh, M.W., 2004b. Delivery volume optimization. Transportation Science 38, 210-223.
- Cao, Y., Swartz, C.L., Flores-Cerrillo, J., 2016. Optimal dynamic operation of a high-purity air separation plant under varying market conditions. Industrial & Engineering Chemistry Research 55, 9956–9970.
- Caspari, A., Pérez, Y.M., Offermanns, C., Schäfer, P., Ecker, A.M., Peschel, A., Schliebitz, F., Zapp, G., Mhamdi, A., Mitsos, A., 2019. Economic nonlinear model predictive control of multi-product air separation processes, in: Computer Aided Chemical Engineering. Elsevier. volume 46, pp. 1–6.
- Charnes, A., Cooper, W.W., 1959. Chance-constrained programming. Management Science 6, 73-79.
- Chima, C.M., 2007. Supply-chain management issues in the oil and gas industry. Journal of Business & Economics Research (JBER) 5.
- Chung, H., Ahn, H.S., Jasin, S., 2016. On (re-scaled) multi-attempt approximation of customer choice model and its application to assortment optimization. Ross School of Business Paper.
- Cóccola, M.E., Méndez, C.A., Dondo, R.G., 2018. Optimizing the inventorying and distribution of chemical fluids: An innovative nested column generation approach. Computers & Chemical Engineering 119, 55–69.
- Dinkelbach, W., 1967. On nonlinear fractional programming. Management Science 13, 492-498.
- Dong, Y., Maravelias, C.T., Pinto, J.M., Sundaramoorthy, A., 2017. Solution methods for vehicle-based inventory routing problems. Computers & Chemical Engineering 101, 259–278.
- Dong, Y., Pinto, J.M., Sundaramoorthy, A., Maravelias, C.T., 2014. Mip model for inventory routing in industrial gases supply chain. Industrial & Engineering Chemistry Research 53, 17214–17225.
- Espinoza, D., Fukasawa, R., Goycoolea, M., 2010. Lifting, tilting and fractional programming revisited. Operations Research Letters 38, 559-563.
- Glankwamdee, W., Linderoth, J., Shen, J., Connard, P., Hutton, J., 2008. Combining optimization and simulation for strategic and operational industrial gas production and distribution. Computers & Chemical Engineering 32, 2536–2546.
- Glover, F., 1975. Improved linear integer programming formulations of nonlinear integer problems. Management Science 22, 455–460.
- Haimes, Y., 1971. On a bicriterion formulation of the problems of integrated system identification and system optimization. IEEE Transactions on Systems, Man, and Cybernetics 1, 296–297.
- Ierapetritou, M., Wu, D., Vin, J., Sweeney, P., Chigirinskiy, M., 2002. Cost minimization in an energy-intensive plant using mathematical programming approaches. Industrial & Engineering Chemistry Research 41, 5262–5277.
- Karwan, M.H., Keblis, M.F., 2007. Operations planning with real time pricing of a primary input. Computers & Operations Research 34, 848-867.
- Lee, Y., Carrero-Parreno, A., Ramaswamy, S., Pinto, J.M., Papageorgiou, L.G., 2021. Hierarchical approach to integrated planning of industrial gas supply chains. Industrial & Engineering Chemistry Research 60, 5207–5219.
- Liu, S., Simaria, A.S., Farid, S.S., Papageorgiou, L.G., 2014. Optimising chromatography strategies of antibody purification processes by mixed integer fractional programming techniques. Computers & Chemical Engineering 68, 151–164.
- Malinowski, E., Karwan, M.H., Pinto, J.M., Sun, L., 2018. A mixed-integer programming strategy for liquid helium global supply chain planning. Transportation Research Part E: Logistics and Transportation Review 110, 168–188.
- Marchetti, P.A., Gupta, V., Grossmann, I.E., Cook, L., Valton, P.M., Singh, T., Li, T., André, J., 2014. Simultaneous production and distribution of industrial gas supply-chains. Computers & Chemical Engineering 69, 39–58.
- Mason, R., Lalwani, C., 2006. Transport integration tools for supply chain management. International Journal of Logistics: Research and Applications 9, 57–74.
- Misra, S., Saxena, D., Kapadi, M., Gudi, R.D., Srihari, R., 2018. Short-term planning framework for enterprise-wide production and distribution network of a cryogenic air separation industry. Industrial & Engineering Chemistry Research 57, 16841–16861.
- Mitra, S., Grossmann, I.E., Pinto, J.M., Arora, N., 2012. Optimal production planning under time-sensitive electricity prices for continuous powerintensive processes. Computers & Chemical Engineering 38, 171–184.
- Pistikopoulos, E.N., Barbosa-Povoa, A., Lee, J.H., Misener, R., Mitsos, A., Reklaitis, G.V., Venkatasubramanian, V., You, F., Gani, R., 2021. Process systems engineering-the generation next? Computers & Chemical Engineering 147, 107252.
- Pochet, Y., Warichet, F., 2008. A tighter continuous time formulation for the cyclic scheduling of a mixed plant. Computers & Chemical Engineering 32, 2723–2744.
- Ramaswamy, S., Madan, T., Thyagarajan, K., Pinto, J.M., Laínez-Aguirre, J.M., 2020. Advanced decision-support technologies for the design and management of industrial gas supply chains, in: Smart Manufacturing. Elsevier, pp. 387–421.
- Shah, N., Pantelides, C.C., Sargent, R., 1993. Optimal periodic scheduling of multipurpose batch plants. Annals of Operations Research 42, 193–228.
- Subramanyam, A., Mufalli, F., Laínez-Aguirre, J.M., Pinto, J.M., Gounaris, C.E., 2021. Robust multiperiod vehicle routing under customer order uncertainty. Operations Research 69, 30–60.

- Tong, K., You, F., Rong, G., 2014. Robust design and operations of hydrocarbon biofuel supply chain integrating with existing petroleum refineries considering unit cost objective. Computers & Chemical Engineering 68, 128–139.
- You, F., Pinto, J.M., Capón, E., Grossmann, I.E., Arora, N., Megan, L., 2011. Optimal distribution-inventory planning of industrial gases. i. fast computational strategies for large-scale problems. Industrial & Engineering Chemistry Research 50, 2910–2927.
- Yue, D., Guillén-Gosálbez, G., You, F., 2013. Global optimization of large-scale mixed-integer linear fractional programming problems: a reformulation-linearization method and process scheduling applications. AIChE Journal 59, 4255–4272.
- Yue, D., Slivinsky, M., Sumpter, J., You, F., 2014. Sustainable design and operation of cellulosic bioelectricity supply chain networks with life cycle economic, environmental, and social optimization. Industrial & Engineering Chemistry Research 53, 4008–4029.
- Yue, D., You, F., 2013. Sustainable scheduling of batch processes under economic and environmental criteria with minlp models and algorithms. Computers & Chemical Engineering 54, 44–59.
- Zamarripa, M., Marchetti, P.A., Grossmann, I.E., Singh, T., Lotero, I., Gopalakrishnan, A., Besancon, B., André, J., 2016. Rolling horizon approach for production–distribution coordination of industrial gases supply chains. Industrial & Engineering Chemistry Research 55, 2646–2660.
- Zhang, Q., Sundaramoorthy, A., Grossmann, I.E., Pinto, J.M., 2017. Multiscale production routing in multicommodity supply chains with complex production facilities. Computers & Operations Research 79, 207–222.
- Zhong, Z., You, F., 2014. Globally convergent exact and inexact parametric algorithms for solving large-scale mixed-integer fractional programs and applications in process systems engineering. Computers & Chemical Engineering 61, 90–101.
- Zhu, Y., Legg, S., Laird, C.D., 2011. A multiperiod nonlinear programming approach for operation of air separation plants with variable power pricing. AIChE Journal 57, 2421–2430.