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Stochastic Cyclic Inventory Routing with Supply Uncertainty: A Case in Green-Hydrogen Logistics

Umur Hasturk, Evrim Ursavas, Kees Jan Roodbergen
Department of Operations, Faculty of Economics and Business, University of Groningen, Groningen, the Netherlands
u.hasturk@rug.nl, e.ursavas@rug.nl, k.j.roodbergen@rug.nl

Albert H. Schrotenboer
Operations, Planning, Accounting & Control Group, School of Industrial Engineering, Eindhoven University of Technology, the Netherlands a.h.schrotenboer@tue.nl

Hydrogen can be produced from water, using electricity. The hydrogen can subsequently be kept in inventory in large quantities, unlike the electricity itself. This enables solar and wind energy generation to occur asynchronously from its usage. For this reason, hydrogen is expected to be a key ingredient for reaching a climate-neutral economy. However, the logistics for hydrogen are complex. Inventory policies must be determined for multiple locations in the network, and transportation of hydrogen from the production location to customers must be scheduled. At the same time, production patterns of hydrogen are intermittent, which affects the possibilities to realize the planned transportation and inventory levels. To provide policies for efficient transportation and storage of hydrogen, this paper proposes a parameterized cost function approximation approach to the stochastic cyclic inventory routing problem. Firstly, our approach includes a parameterized mixed integer programming (MIP) model which yields fixed and repetitive schedules for vehicle transportation of hydrogen. Secondly, buying and selling decisions in case of underproduction or overproduction are optimized further via a Markov decision process (MDP) model, taking into account the uncertainties in production and demand quantities. To jointly optimize the parameterized MIP and the MDP model, our approach includes an algorithm that searches the parameter space by iteratively solving the MIP and MDP models. We conduct computational experiments to validate our model in various problem settings and show that it provides near-optimal solutions. Moreover, we test our approach on an expert-reviewed case study at two hydrogen production locations in the Netherlands. We offer insights for the stakeholders in the region and analyze the impact of various problem elements in these case studies.

Key words: green hydrogen, stochastic cyclic inventory routing, static and dynamic decision making

1. Introduction

Renewable energy supply is known to be intermittent and uncertain (Anvari et al. 2016). For example, wind and solar energy generation depend on weather conditions (Drücke et al. 2021). A common way to maintain the balance between supply and demand in the electricity network is by means of conventional gas-fired power plants (Safari et al. 2019), which have an easily adjustable power output. The high market prices for natural gas, along with the desire of many countries to eliminate the use of fossil fuels (e.g., European Union 2012), stimulate the development and use of other mechanisms to balance supply and demand of energy in the network. The use of hydrogen as a storage medium for energy (Liu et al. 2010) is such an alternative balancing mechanism, which is expected to be deployed increasingly towards the future (Abe et al. 2019). Hydrogen can be produced emission-free from (renewable) electricity when supply exceeds demand. It can be stored and transported as a gas, and can be converted emission-free into electricity when needed (Oliveira, Beswick, and Yan 2021). Since conversions between hydrogen and electricity result in significant energy losses, direct use of hydrogen as a vehicle fuel, a heating source for households, and a feedstock for the industry is also considered attractive (Ball and Wietschel 2009).

A typical hydrogen-based energy network consists of a hydrogen producer and multiple hydrogen customers. The producer makes hydrogen from renewable energy sources, which yields a stochastic hydrogen supply per period. The producer is responsible for replenishing geographically dispersed customers, who generate electricity from hydrogen, or use it directly. Customers have stochastic demand for hydrogen per period. Although hydrogen can be transported via pipelines, this is for most applications not considered a likely scenario in the near future (Staffell et al. 2019). Hydrogen is therefore transported between locations via vehicles. The producer and the customers each have a storage facility to keep hydrogen in stock to buffer between deliveries. The capacities of these storage facilities are limited. There are two main challenges that arise in the planning for such a network.

Firstly, we need a transportation delivery schedule for transporting hydrogen from the producer to the customers. Similar to the cyclic inventory routing problem (CIRP, see Raa and Aghezzaf 2009, Rau, Budiman, and Widyadana 2018) this consists of: (1) a repetitive schedule with fixed time intervals between consecutive deliveries for each of the customers, (2) the routing for all vehicles, which determines which customers are delivered by which vehicle and in which sequence. The repetitive schedule and routing are decided upon at the beginning of the planning horizon and are subsequently used in all periods. This helps customers and the producer to align their dependent planning processes and associated resources as they will know exactly when the deliveries will occur.

Secondly, we need to manage hydrogen availability across all locations in response to stochastic supply at the producer and stochastic demand at the customers. As commonly deployed in the stochastic inventory routing problem (SIRP, see Raa and Aouam 2021, Sonntag, Schrotenboer, and Kiesmüller 2022), the producer determines the delivery quantity for each customer by using an

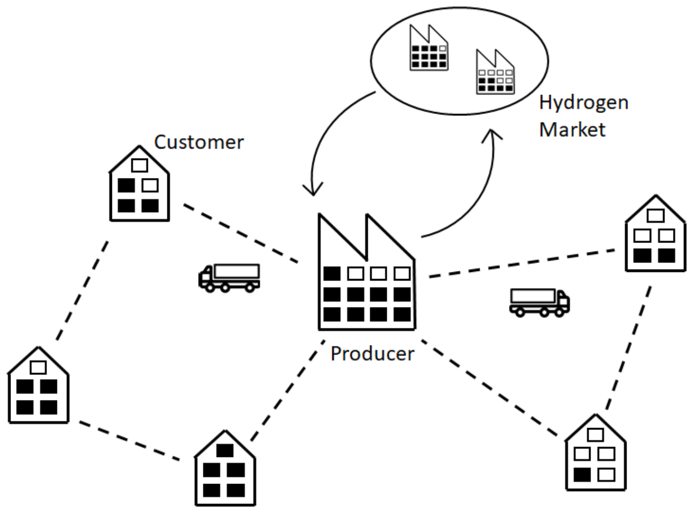


Figure 1 **Our paper considers a stochastic, cyclic, inventory routing problem with stochastic supply occurring in hydrogen logistics.**

inventory policy. Specifically, for each delivery period –as imposed by the transportation delivery schedule– we have a base-stock policy for each customer, given a required service level. The base-stock levels for a customer can differ between delivery periods. Furthermore, the limited size of the producers' storage facility, combined with the stochasticity in supply and demand, may lead to hydrogen shortages or surpluses at the producer's location. To guarantee that customers' service levels are met, the producer is connected to an external hydrogen market at which it can buy and sell hydrogen at market prices. Dynamic purchasing decisions at the producer determine when to buy and sell hydrogen, and in which quantity.

It is crucial that both the *static* transportation delivery schedule and the producer's *dynamic* purchasing decisions are optimized jointly to achieve long run global optimal solutions. This is complex, however, because the static transportation delivery schedule is decided upon only once, while the purchasing decisions are made dynamically in every period that follows. In isolation, these two decision problems are addressed in their own, natural way. Obtaining a static transportation delivery schedule is done using mixed integer programming (MIP) models and methods. On the other hand, the dynamic purchasing decisions are modeled naturally as a Markov decision process (MDP), thus requiring stochastic dynamic programming. In our hydrogen setting, the outcome of the MIP defines the size and timing of the stochastic demand faced by the producer, and thus defines the state, action, and transition space of the MDP. How to best combine this into a joint optimization problem is a yet unresolved fundamental question for which, to the best of the authors' knowledge, no generic solution approach exists.

In this paper, we consider a stochastic cyclic inventory routing problem (SCIRP) with supply uncertainty, as illustrated in Figure 1. Its goal is to find a long run, global optimal solution that minimizes the cost of the transportation delivery schedule, the inventory policies for the customers, and the dynamic purchasing decision for the producer. For this, we propose a generic solution approach that iteratively solves MIPs and MDPs utilizing ideas of parameterized cost function approximations (Powell and Ghadimi 2022). A parameterized cost function approximation is a method for solving stochastic dynamic decision problems by using a modified, parameterized deterministic policy so that it better anticipates future uncertainty. We apply this idea to our static transportation delivery schedule, i.e., we use a modified parameterized MIP to find a transportation delivery schedule that anticipates the impact of the dynamic purchasing decision. We evaluate the dynamic purchasing decision by solving the resulting MDP via value iteration. Our approach includes an efficient search method for setting the parameters in the modified parameterized MIP by iteratively solving the modified MIP and the MDP. To the best of the authors' knowledge, this is the first generic approach that combines such static and dynamic decisions.

This paper makes the following contributions to the literature. First, by introducing and solving the SCIRP with supply uncertainty, we consider a new and emerging application in hydrogen production and distribution that is relevant for an efficient transformation towards a green society. Second, we generalize the existing literature on the SCIRP by considering both a cyclic transportation delivery schedule and stochastic supply. The extant literature typically considers only demand uncertainty in non-cyclic settings (Adelman 2004, Kleywegt, Nori, and Savelsbergh 2004), supply uncertainty in non-cyclic settings (Alvarez et al. 2021), or do not consider supply uncertainty (Sonntag, Schrotenboer, and Kiesmüller 2022, Raa and Aouam 2021, Malicki and Minner 2021). Third, we introduce a generic solution approach based on jointly optimizing dependent static (MIP) and dynamic (MDP) decisions utilizing ideas from parameterized cost function approximations. Our generic approach finds high-quality solutions in low computation times. Fourth, we show on a set of new benchmark instances the importance of jointly optimizing static and dynamic decisions, as it can lead up to cost savings of 65%. Finally, we apply our approach to an extensive case study in the Northern Netherlands, where one of Europe's first Hydrogen Valleys (New Energy Coalition 2020) is realized, by analyzing how hydrogen should be distributed in expert-reviewed future scenarios.

The remainder of this paper is organized as follows. In Section 2, we provide a review of literature that relates to the SCIRP, such as the stochastic IRP, the cyclic IRP, and the production routing problem. In Section 3, the problem narrative is given, followed by a MIP and an MDP model definition for our joint optimization model. In Section 4, an example solution illustrates the joint optimization problem. In Section 5, the proposed solution approach is narrated including a new parameterized MIP model definition. In Section 6, the computational experiments are presented. In Section 7, an expert-reviewed case study demonstrates the impact of various problem elements for a number of future scenarios. In Section 8, we conclude our paper.

2. Literature Review

Our study contributes to the green hydrogen energy literature and several research streams of the inventory routing problem (IRP), which we will discuss one by one. First, we discuss the distribution of green hydrogen from an application perspective in Section 2.1. Next, we discuss the literature on the stochastic IRP and cyclic IRP in Sections 2.2 and 2.3, respectively. In our paper, we combine those elements into the stochastic cyclic IRP for which related work is presented in Section 2.4. Finally, we discuss how our work differs from other, related, settings in Section 2.5.

2.1. Green Hydrogen Energy Literature

Contributions in the green hydrogen literature typically take a high-level supply chain perspective. To the best of the authors' knowledge, there are no contributions that consider routing and supply uncertainty as in our study. In the following, we review the most-related works and refer the interested reader to the review by Sgarbossa et al. (2022).

Almaraz et al. (2014) consider a case in France and minimize environmental and safety objectives while deciding about centralized or decentralized production and storage of hydrogen and different transportation modes. Welder et al. (2018) focus on multiple production technologies of green hydrogen, providing a comparison of these technologies for a case study in Germany. However, none of these works consider inventory routing optimization as in our work.

Instead of considering multiple green-hydrogen production technologies, Woo et al. (2016) study the green hydrogen supply chain by focusing solely on biomass production. They are concerned with deciding the allocation of land for yielding multiple crops, which are then used as biomass to produce hydrogen. The authors consider uncertainty in both supply and demand of hydrogen, and touch upon transportation decisions too. They assume a fixed cost of using a transportation mode and of operating it between two locations. Clearly, this does not grasp the importance of routing optimization as the IRP does, and thus does not realistically represent green hydrogen distribution costs as in our study.

2.2. Stochastic Inventory Routing Problem

The stochastic IRP (SIRP) is a collective name for IRPs considering at least one stochastic element. Most often this concerns demand uncertainty, but some recent works also incorporate supply uncertainty and lead time uncertainty. Another important distinction between SIRP models is whether decisions are made dynamically or statically. Dynamic models are built typically upon dynamic programming (DP) and Markov decision process (MDP) techniques, providing real-time operational-level decisions. Static models typically focus on integer programming (IP) techniques, utilizing chance constraints to guarantee some operational performance metric, while focusing on optimizing tactical-level decisions. Our work considers static and dynamic decisions while considering both supply and demand uncertainty. In the following, we only touch upon the most related works, and otherwise refer the interested reader to the excellent review by Coelho, Cordeau, and Laporte (2014b).

Some seminal works on dynamic SIRP models exist. Adelman (2004) models the SIRP as an MDP by using approximated value functions with the aim to provide dynamic policies. They formulate two primal-dual formulations, in which the dual feasible solutions are implemented to achieve lower bounds on true value function values and to solve the optimality equations of the MDP model. Kleywegt, Nori, and Savelsbergh (2002) also considers a dynamic SIRP and model it as an MDP. The MDP model is provided for the general case where a route may consist of multiple customers. Then, the model is solved by a dynamic programming approximation method for only the direct delivery case, where a single customer is served within a route. Later, Kleywegt, Nori, and Savelsbergh (2004) extend this work and solve the general case to near optimality by a decomposition and an approximation of the value function. Bertazzi et al. (2013) study a SIRP with demand uncertainty where each customer has to have a base-stock level equaling their inventory capacity. The authors permit stock-outs with a penalty cost. They model the problem dynamically for a finite time horizon and derive two solution methods. The first is a hybrid rollout algorithm that combines a rollout approach with a deterministic MILP. The second is a branch-and-cut algorithm with additional valid inequalities to solve the problem to optimality. A similar approach is given in Coelho, Cordeau, and Laporte (2014a) in which short-term forecasts are injected in a MILP, which is then solved on a rolling horizon basis.

Using integer programming techniques, some authors focus on static models of the SIRP. Yu et al. (2012) model the SIRP with demand uncertainty with chance constraints to achieve a service level while respecting a limited inventory capacity. They present a hybrid solution approach by simplifying the model, linearizing nonlinear elements, and decomposing decisions. They show that a large-scale problem of 200 customers may be solved to near optimality by their approach. Another SIRP under demand uncertainty with service levels is studied by Crama et al. (2018), where the product is assumed to be perishable. Unlike most other IRPs, the authors assume no holding cost but provide the formulation for the case with a holding cost. They create four solution methods for their formulation of the problem with a finite time horizon and discuss the impact of each element of the problem such as information, storage capacity, and shelf life.

Only recently, supply uncertainty has started to gain attention in the SIRP. To the best of our knowledge, Alvarez et al. (2021) is the only SIRP paper considering supply uncertainty. The authors modeled the problem as a two-stage integer programming recourse for a finite time horizon with discrete probabilistic supply and demand distributions. In this model, a routing decision is selected at the first step. Then, the optimal transportation delivery schedule is derived for all possible combinations of supply and demand scenarios at the second step. Thus, the delivery decisions may be given after the realization of a scenario, assuming that the decision maker knows the exact amounts of supply and demand for all the periods in the time horizon. Our approach does not rely on generating scenarios and utilizes a chance-constrained model instead. This allows us to guarantee exact service levels for the customers.

2.3. Cyclic Inventory Routing Problem

The cyclic IRP (CIRP) is the branch of IRPs where the proposed routing solutions are cyclic, and can thus be executed repetitively in an infinite planning horizon. The majority of this research area provides fixed transportation delivery schedules to be implemented repetitively, which helps both customers and producers to plan their (dependent) operations. Most of the literature considers deterministic settings (see, e.g., Michel and Vanderbeck 2012, Diabat, Archetti, and Najy 2021).

Gaur and Fisher (2004) study a cyclic IRP to provide a weekly transportation delivery schedule for a well-known supermarket chain in the Netherlands; Albert Heijn. The authors limit the number of customers in each vehicle route by two, which is then improved by a heuristic that allows for more customers in a single route. Their proposed solutions reduced costs by 4% during the first year of implementation. Raa and Aghezzaf (2009) work on a CIRP by considering some real-life constraints such as minimal cycle times and daily driving time restrictions. Their column generation-based heuristic includes two main steps; clustering and assigning stock levels, and an insertion heuristic for the routes.

Several studies provide heuristic approaches. Vansteenwegen and Mateo (2014) consider a single vehicle CIRP. The aim is to maximize profits obtained from serving customers. Thus, not all customers need to be delivered. Since the vehicle may do more than one trip at a period, the routing structure is similar to multi-vehicle IRPs. The authors propose an iterative local search metaheuristic for the problem. Another heuristic approach is discussed in Rau, Budiman, and Widyadana (2018) for the CIRP with multiple objectives, minimizing costs and the emission of vehicles. The authors consider both the distance and the weight of the vehicle to calculate emission levels. They propose a variant of the particle swarm optimization algorithm to solve the problem, which reduces the costs and the emission levels by 20% in their instances. In Bertazzi et al. (2020), the authors solve a finite-time CIRP with a three-phase approach; combining heuristics with branch-and-cut. The first phase applies a branch-and-cut algorithm. If the optimal solution has not been reached within a preset time limit, a lower bound is taken and the second phase of the heuristic approach is solved so that an upper bound is determined. Using the valid inequalities defined by the first two phases, branch-and-cut is again applied to solve the problem to optimality in the third phase.

2.4. Stochastic Cyclic Inventory Routing Problem

The variant of the IRP that relates most closely to our work is the stochastic cyclic IRP (SCIRP), where both customer demand uncertainty is considered while cyclic routing solutions are required. Sonntag, Schrotenboer, and Kiesmüller (2022) work on a SCIRP with infinite supply and stochastic demand with known stationary distributions. Their aim is to provide a cyclic replenishment policy with a fixed number of periods in-between consecutive deliveries, where it is guaranteed that each customer is replenished up to their base-stock level. They reformulate the chance-constrained model into an integer programming model by using a Dantzig–Wolfe decomposition. Then, this model is solved to near optimality for mid- and large-size instances using branch-and-price. Our static (transportation delivery schedule) decisions generalize the approach by Sonntag, Schrotenboer, and Kiesmüller (2022) by adhering to a cyclic pattern of a finite number of days (for example a week). Moreover, they do not consider supply uncertainty. Raa and Aouam (2021) study a similar problem as Sonntag, Schrotenboer, and Kiesmüller (2022), and propose a population-based metaheuristic approach, by decomposing the problem into route design and fleet design stages. Finally, Malicki and Minner (2021) address a SCIRP with a finite planning horizon. They allow variable safety stocks and replenishment intervals for the first time in the SCIRP literature. This helps to address non-stationary demand patterns. They model the problem as a mixed-integer chance constraint problem, which is then solved with an adaptive large neighborhood search algorithm that smartly utilizes lot-sizing heuristics.

Our study is the first study that addresses a SCIRP including supply uncertainty. In addition, we detail dynamic purchasing decisions on how to mitigate supply uncertainty using an operational-level MDP to include the associated costs in the design of our cyclic inventory routing design. For this, we propose a generic, new solution approach based on parameterized cost function approximation. To the best of the author's knowledge, the work of Mulder, van Jaarsveld, and Dekker (2019) is the only work that relates to our approach. They consider a maritime shipping setting for which a specialized and tailored solution approach is feasible depending on the structure of the cost function. Our approach is generic and does not rely on such assumptions.

2.5. Other Related Research

The production routing problem (PRP) concerns jointly optimizing lot sizing and vehicle routing. Unlike IRPs with stochastic supply (as in our problem), PRPs plan the supply (i.e., the lot sizing) based on the routing policy so that supply, inventory holding, and transportation costs are minimized. Studies are mostly based on heuristic multi-phase approaches, but there are a few exact methods available. Due to PRP's focus on discrete scheduling of production processes, we only review the most important contributions in this area and refer the interested reader to Adulyasak, Cordeau, and Jans (2015b) and Neves-Moreira et al. (2019) for an overview of the complete field.

Regarding the multi-phase approaches, Adulyasak, Cordeau, and Jans (2014) work on a deterministic PRP under a finite time horizon and propose an adaptive large neighborhood search heuristic. This decomposition-based heuristic has two phases; initialization and improvement, where a network flow subproblem is solved in the improvement phase. Adulyasak, Cordeau, and Jans (2015a) use a similar two-phase construction to solve a stochastic PRP with demand uncertainty. Benders decomposition is used to solve this problem to optimality, enhanced with additional valid inequalities. Neves-Moreira et al. (2019) consider a multi-product PRP with time delivery windows. The authors' heuristic approach adds one more phase, thus having three phases named as; size reduction, initial solution, and improvement. This decomposition method is tested in a case study in a meat industry company, achieving a 20% cost reduction compared to the company's policy.

Schenekemberg et al. (2021) introduce the two echelon PRP. The authors provide two exact solution methods; branch-and-cut and a parallel algorithm. The parallel algorithm provides previously unknown optimal solutions for large-sized PRP instances with 50 customers, and is also found to be efficient for the deterministic two-echelon multi-depot inventory routing problem.

3. Model

This section introduces the mathematical model for the stochastic cyclic inventory routing problem (SCIRP) with supply uncertainty. For readability, we refer to our problem as the SCIRP. We start with the problem narrative, where on a high-level the system elements, the decisions to be taken, and the associated costs are explained. Afterward, we introduce a MIP for the static, tactical-level inventory routing decisions and an MDP for the dynamic, operational-level purchasing decisions. We end with the joint optimization problem that formalizes the goal of the SCIRP.

3.1. Problem Narrative

We consider a joint green hydrogen production and distribution system over an infinite discrete time horizon $\mathcal{T}$ that consists of cyclic repetitions of T periods (e.g., a week). Every period $\tau \in \mathcal{T}$ corresponds to a cycle period $t \in \mathscr{T} := \{1, \dots T\}$. A green hydrogen producer receives a stationary stochastic supply from a renewable energy source at each period $\tau \in \mathcal{T}$. The producer uses the stochastic supply to replenish a given set of geographically dispersed customers that each face stationary stochastic demand at each period $\tau \in \mathcal{T}$. We define the node set $\mathscr{N}^0 := \{0\} \cup \mathscr{N}$, where 0 represents the producer and $\mathscr{N} := \{1, 2, \dots, N\}$ represents the customers.

The decisions comprise two dependent parts. Firstly, a tactical-level inventory routing decision is made in the form of a periodic, routing solution that repeats itself every T periods over the infinite time horizon. These routes are used for the replenishment of hydrogen from the producer to the customers using capacitated vehicles. To design such a so-called transportation delivery schedule, customers are grouped into fixed clusters with an associated vehicle route and a delivery schedule over the T periods. The delivery schedule encodes on which of the T periods the associated vehicle route is performed. Customers are delivered at most once every period. We assume that customers' inventory is replenished according to a base-stock policy subject to a service level constraint on each delivery day. Note, the base-stock level set for each delivery period is part of our decision. As a consequence, the amount of inventory on each vehicle route is stochastic. From the perspective of the producer, the proposed clustering of customers and associated transportation delivery schedule transforms individual stochastic customer demands into T independent demand distributions for each cycle period. See Section 3.2 for the details.

Secondly, the producer faces a dynamic, operational-level purchasing problem to manage, at each period, the inflow of stochastic hydrogen supply to ensure the feasibility of the outflow of demand as depicted by the transportation delivery schedule outlined above. At each period τ, the producer observes how much demand needs to be replenished by the customers. The producer has access to a capacitated storage unit to keep hydrogen in stock to anticipate the fulfillment of demand in later periods. Furthermore, the producer is connected to a hydrogen market at which it can buy hydrogen to meet customer demand, and sell hydrogen for an extra profit. We ensure in this way that the producer always replenishes inventory up to the decided base-stock policies (as part of the tactical-level decision) at the customers. See Section 3.3 for the details.

The goal of the SCIRP is to minimize the total expected cycle costs of the combined tactical-level and operational-level decisions. This includes transportation costs (fixed and variable), inventory holding costs at customers, emergency shipment costs (in case of insufficient vehicle capacity), and hydrogen buying and selling costs. In the following, we first give the details of the tactical-level decisions after which we describe the operational-level decisions. An overview of all notation is given in Table 9 in Appendix A.

3.2. The Tactical-Level Inventory Routing

We propose a set-partitioning model for the tactical-level inventory routing decisions. We consider a set of clusters $\mathscr{R}$, where each cluster $r \in \mathscr{R}$ describes a set of customers, the shortest vehicle route among these customers, the delivery periods in the cycle $\{1,\dots,T\}$, and a base-stock level at each delivery period for each customer. We refer to these delivery periods and the associated base-stock levels as a *transportation delivery schedule* of a cluster. Then, the tactical-level inventory routing decision boils down to selecting clusters with mutually exclusive customers that jointly partition the customer set. In the following, we first describe the cost and feasibility of these clusters for general stochastic customer demand and provide the set partitioning model afterward.

3.2.1. Customer cluster cost and feasibility. Let $\mathscr{N}_r \subseteq \mathscr{N}$ be the set of customers in cluster $r \in \mathscr{R}$. The cyclic cluster cost c_r of cluster r consists of the deterministic fixed and variable transportation costs (c_r^{T}), the expected inventory holding costs at its customers (c_r^{H}), and the expected costs of emergency shipments (c_r^{E}). The cluster cost c_r is then defined by

$$
\begin{aligned}
c_r &= c_r^{\mathrm{T}} + c_r^{\mathrm{H}} + c_r^{\mathrm{E}} && (1)\\
&= \sum_{t=1}^{T} \left[\theta_r^t (W + w \cdot d_r) + h \sum_{i \in \mathscr{N}_r} \mathbb{E}\left[IL_{it}^+(\vec{S}_r^i) \right] + e \cdot \theta_r^t \mathbb{E}\left[\left(\sum_{i \in \mathscr{N}_r} D_r^{it}\left(\vec{S}_r^i\right) - Q \right)^+ \right] \right]. && (2)
\end{aligned}
$$

The first term of Equation (2) is the transportation cost of a cluster for a cycle. Parameter θ_r^t denotes whether the transportation delivery schedule of cluster r includes delivery period t. The fixed transportation cost is W, and the variable transportation costs equal $w \cdot d_r$, where d_r is the length of the shortest route among the customers in cluster r. The second term of Equation (2) comprises the expected holding costs of cluster r for each cycle. The holding cost equals h per unit of inventory. For each customer $i \in \mathscr{N}_r$, $IL_{it}^+(\vec{S}_r^i)$ denotes the expected on-hand inventory at period t for base-stock policy $\vec{S}_r^i = \{S_r^{it}\}_{t=1}^T$. Here S_r^{it} denotes the base-stock level of customer i if t is a delivery period of cluster r and equals 0 otherwise. The third term denotes the expected cyclic emergency shipment costs. As the amount replenished in each delivery period of a cluster r is stochastic, the vehicle capacity might be insufficient and emergency shipments may occur at the cost of e per unit shipped outside the capacity of our vehicle. Let $D_r^{it}\left(\vec{S}_r^i\right)$ denote the demand to be shipped to customer i on period t assuming base-stock policy $\vec{S}_r^i$ is being implemented. We denote the vehicle capacity by Q. Thus, $\left(\sum_{i \in \mathscr{N}_r} D_r^{it}\left(\vec{S}_r^i\right) - Q\right)^+$ represents the amount of hydrogen which exceeds the vehicle capacity for cluster r on delivery period t.

Each cluster $r \in \mathscr{R}$ is subject to three constraints. First, each customer has only a limited capacity U for the storage of hydrogen, so $S_r^{it} \leq U$ for all $i \in \mathscr{N}_r, t \in \mathscr{T}$. Second, Constraint (3) imposes a service level α. Meaning that the probability of having a positive inventory level is at least α for each customer i in cluster r at period t.

$$
\mathbb{P}\left\{ IL_{it}^+(\vec{S}_r^i) > 0 \right\} \geq \alpha \qquad \forall r \in \mathscr{R}, i \in \mathscr{N}_r, t \in \mathscr{T}. \tag{3}
$$

Furthermore, Constraint (4) limits the probability that vehicle capacity is not sufficient (i.e., the probability an emergency shipment occurs) with at most $1-\gamma$ for each delivery of each cluster r. The chance constraint helps to limit the size of the cluster set $\mathscr{R}$, which is computationally convenient.

$$
\mathbb{P}\left\{ \sum_{i \in \mathscr{N}_r} D_r^{it}\left(\vec{S}_r^i\right) \leq Q \right\} \geq \gamma \qquad \forall r \in \mathscr{R}, t \in \mathscr{T}. \tag{4}
$$

For each cluster r with a given transportation delivery schedule (i.e., we know at what periods we deliver customers $\mathcal{N}_r$), we assume a base-stock policy at delivery period t covering the demand until the next delivery period. In other words, we set the base-stock level as if we have a classic single-item inventory system with backorders and lead time equal to the number of periods that we need to cover till the next replenishment, and we act as if this repeats continuously. In case the number of periods between deliveries is equal, this is optimal (see also Lemmas 1-3 in Sonntag, Schrotenboer, and Kiesmüller (2022)). However, in practice, this is often not possible. For example, if the cycle $\{1,\ldots,T\}$ resembles a week and two delivery days are selected, the number of days between consecutive deliveries is not equal.

Explicitly, for a delivery period t and a cluster r, let n_{tr} be the number of periods until the next delivery and let m_{tr} be the number of periods since the last delivery. We set the base-stock level S_r^{it} equal to $I_{in}^{-1}(\alpha)$, i.e., the critical fraction of demand distribution over the next n periods at customer $i \in \mathcal{N}_r$ until the next delivery. Here I_{in} denotes the cumulative demand distribution faced by customer i during n periods. For example, if demand is normally distributed with mean μ_i and standard deviation σ_i, $I_{in}^{-1}(\alpha)$ equals $n\mu_i + z_\alpha \sigma_i \sqrt{n}$ where z_α is the z-score associated with the $(1-\alpha)$ quantile.

As stated above, this approximation is not optimal if n_{tr} and m_{tr} differ. The following remarks make this explicit.

Remark 1 (Order-size distribution). Let $t \in \{1,\ldots,T\}$ be a delivery period of customer i, assume $m_{tr} >> n_{tr}$ and T is sufficiently large, and assume only 2 delivery periods are selected for customer i within the cycle $\{1,\ldots,T\}$. In such a case, it is non-negligible that the observed inventory level at period t exceeds the set base-stock policy S_r^{it}, and accordingly, no order will be placed at the producer. That is, the order size distribution at time t will have a significant probability mass at 0.

Remark 2 (Optimality of base-stock policy). Remark 1 deduces that setting base-stock levels as we do might result in overshooting the set base-stock levels. If this is the case, it will result in a too-high service level (i.e., exceeding α) at a customer. This follows trivially by realizing that the total safety stock increases if we replenish more often (i.e., demand pooling) during the cycle. Thus, in our experiments, Constraint 3 is respected but not necessarily binding. However, preliminary experiments have shown that these effects were not significant from a computational perspective. That is, it will not lead to different routing decisions. We, therefore, ignore this phenomenon in the remainder of this paper.

In what follows, we detail the calculation of holding and emergency shipment costs. In line with the previous remarks, these expressions are thus approximations of the actual cost, but preliminary experiments also show that the approximations are good enough.

The holding cost is calculated by the average end inventory over the cycle periods. On $(t+\ell)^{th}$ period ($\ell \le n_{tr}$) after the last delivery on cycle period t, the end inventory on customer i with the base-stock policy is

$$\mathbb{E}\left[\left(S_r^{it} - I_{i\ell}\right)^+\right]. \tag{5}$$

For the example of normally distributed demand, we have $S_r^{it} - I_{i\ell} \sim N\left(\left(n_{tr}-\ell\right)\mu_i\right) + z_\alpha \sigma_i \sqrt{n_{tr}}, \ell\sigma_i^2)$. From this, we can easily calculate the expected holding cost for each period.[1]

For the replenishment of cluster r on delivery period t, the expected amount of emergency shipment would be

$$\mathbb{E}\left[\left(\sum_{i\in\mathcal{N}_r}\left(S_r^{it} - \left(S_r^{i(t-m_{tr})} - I_{i(m_{tr})}\right)\right) - Q\right)^+\right], \tag{6}$$

where $\sum_{i\in\mathcal{N}_r}\left(S_r^{it} - \left(S_r^{i(t-m_{tr})} - I_{i(m_{tr})}\right)\right) - Q \sim N(\sum_{i\in\mathcal{N}_r}\left[n_{tr}\mu_i + z_\alpha\sigma_i\left(\sqrt{n_{tr}} - \sqrt{m_{tr}}\right)\right] - Q, \sum_{i\in\mathcal{N}_r} m_{tr}\sigma_i^2)$ for the normal distribution case. This random variable shall not be positive with a probability of γ in order to satisfy Constraint (4).

The tactical-level inventory routing decision is then obtained by solving a set partitioning model. Let β_r^i be equal to 1 if cluster r contains customer i, and 0 otherwise. Let x_r be a binary decision variable equaling 1 if cluster r is selected and 0 otherwise. The tactical-level inventory routing decision is then obtained by solving:

$$\min \sum_{r\in\mathscr{R}} c_r x_r \tag{7}$$

$$\text{s.t} \sum_{r\in\mathscr{R}} \beta_r^i x_r = 1 \qquad \forall i \in \mathcal{N}, \tag{8}$$

$$x_r \in \{0,1\} \qquad \forall r \in \mathscr{R}. \tag{9}$$

The objective is to minimize the expected cyclic cluster cost. Constraints (8) ensure each customer is contained in exactly one cluster. This model relies on a full enumeration of the cluster set $\mathscr{R}$. We detail how we do this in Section 5. Furthermore, this model completely ignores supply uncertainty faced by the producer. The next section will introduce a dynamic purchasing model to ensure the feasibility of tactical-level inventory routing decisions in operational settings.

[1] Note our calculation is exact. This is very close to the often assumed calculation for high service levels, in which it is assumed that the average inventory level during the cycle equals the safety stock plus half the cycle stock.

3.3. The Operational-Level Purchasing

At each period, the producer needs to ensure that enough hydrogen is available to satisfy customer demand as imposed by the transportation delivery schedules of the selected clusters. The producer has a maximum capacity to store hydrogen, and it can buy and sell hydrogen at fixed market prices at the hydrogen market. We model this dynamic purchasing decision of how much hydrogen to buy and sell at each period, and thus how much hydrogen to keep in stock at the producer, as an MDP. We first define the order of events at each period, after which we provide the MDP formulation.

3.3.1. The order of events. At each period, we first observe the current hydrogen inventory level (as a result of the last period's supply) and the customer demand within the clusters that are delivered in that period (as given by the tactical-level decision). Hereafter, the producer buys or sells hydrogen from the market, and we assume this arrives instantaneously (e.g., overnight) at the producer. Finally, the customers are replenished. A graphical overview is presented in Figure 2.

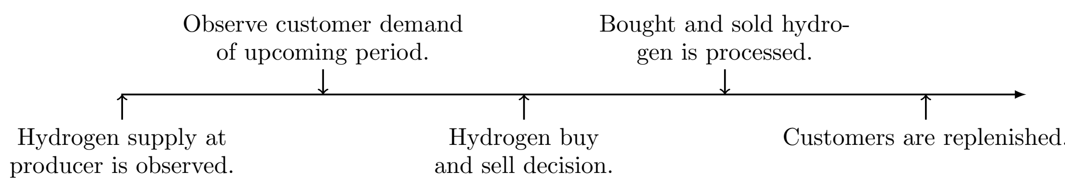


Figure 2 **Timeline of a period.**

3.3.2. Markov decision process. Let D_0 be the probability distribution function of hydrogen supply at the producer. The MDP takes as input the tactical-level replenishment planning $\mathbf{x}$, which imposes on each period t a demand distribution D_t. For readability, we omit dependency on $\mathbf{x}$ in our notation.

We consider two states in the dynamic purchasing decision problem. The state s_1 is observed before the realization of uncertain supply and demand and comprises of the period $t \in \{1, \ldots, T\}$ and the inventory level $\omega \in \mathbb{N}_{\geq 0}$. The state s_2 is observed after the realization of uncertain supply and demand, and consists of the period $t \in \{1, \ldots, T\}$ and the inventory position $\omega^* \in \mathcal{N}$.

We consider a net-demand distribution D_t^* for each period t that resembles the sum of customer demand minus the hydrogen supply. The state $s_1 = (t, \omega)$ transitions to the state $s_2 = (t^*, \omega^*)$ according to D_t^*, where $t^* = t$. State s_2 transitions to state $s_1 = (t+1 \mod T, \omega)$ by taking hydrogen buy (q_1) and sell (q_2) decisions. We formalize this in the remainder of this section.

We define two value functions. Let $v(s_1)$ and $y(s_2)$ be the expected future cost of being in state s_1 and s_2, respectively. The transition from state s_1 to s_2, and vice versa, is recursively defined by the following set of equations:

$$v(t, \omega) = \sum_{\omega^* \in \mathcal{R}} \mathbb{P}\left[(t, \omega^*) | (t, \omega), D_t^*\right] \cdot y(t, \omega^*), \tag{10}$$

$$y(t,\omega^*) = \min_{(q_1,q_2)\in\mathscr{A}(s_2)} \left\{ c(\omega^*, q_1, q_2) + v(t+1 \mod T, \omega^* + q_1 - q_2) \right\}. \tag{11}$$

In Equation (10), we let the value $v(t,\omega)$ being in state $s_1 = (t,\omega)$ be the expected value of transitioning to states $s_2 = (t,\omega^*)$ under the probability measure $\mathbb{P}$ based on the net demand distribution D_t^*. Note that ω^* can take a negative value, as it reflects the inventory position before buying or selling hydrogen.

In Equation (11), we take cost minimizing buying (q_1) and selling (q_2) decisions. The set of admissible buying and selling decisions is defined for all $s_2 \in \mathscr{A}(s_2)$ by

$$\mathscr{A}(t,\omega^*) = \{(q_1,q_2) | -\omega^* \le q_1 - q_2 \le C - \omega^*, q_1 \ge 0, q_2 \ge 0\}. \tag{12}$$

This resembles that we cannot sell more than our current inventory, and we cannot buy more than fits in our storage facility. Buying hydrogen comes at a unit price of c_1, and selling hydrogen comes at a unit price of $c_2 < c_1$. Next to these costs, the producer incurs a fixed ordering cost each time they decide to buy from the external source (K_1) and a so-called fixed emergent purchase cost (K_2). The latter cost reflects the case when the current inventory is insufficient to meet today's customer demand, i.e. when $\omega^* < 0$. The difference with the fixed ordering cost is that the producer may choose to keep a safety-stock, to ensure that there is sufficient inventory to meet today's customer demand with a higher probability. According to these costs, the costs of taking decision (q_1, q_2) is defined as:

$$c(\omega^*, q_1, q_2) = K_1\delta_1 + K_2\delta_2 + c_1 q_1 - c_2 q_2, \tag{13}$$

where $\delta_1 = 1$ if $q_1 > 0$ and 0 otherwise, and $\delta_2 = 1$ if $\omega^* < 0$ and 0 otherwise.

Depending on the tactical solution $\mathbf{x}$, we define $\Pi(\mathbf{x})$ as the set of all feasible dynamic policies of the MDP. The actions that yield the minimum values of $y(t,\omega^*)$ define the optimal dynamic policy for the purchasing decisions of the producer, denoted as $\pi^*(\mathbf{x})$. Upon that, we compute $C(\pi^*(\mathbf{x}))$ as the expected cycle costs of the producer's buying and selling decisions.

In order to obtain the optimal policy, we use value iteration to solve the system of equations (10) and (11). This requires discretization of the inventory levels and net-demand distribution, as detailed in Section 5.3.

3.4. The Joint Optimization Problem

The goal of the SCIRP is to determine both a transportation delivery schedule and a dynamic policy for the producer's purchasing decisions that minimizes total expected cost. The following optimization problem reflects these joint decisions:

$$\min \sum_{r\in\mathscr{R}} c_r x_r + C(\pi^*(\mathbf{x})) \tag{14}$$

$$\text{s.t} \sum_{r\in\mathscr{R}} \beta_r^i x_r = 1 \qquad \forall i \in \mathscr{N}, \tag{15}$$

$$\pi^*(\mathbf{x}) \in \Pi(\mathbf{x}), \tag{16}$$

$$x_r \in \{0,1\} \qquad \forall r \in \mathscr{R}, \tag{17}$$

where Constraint 15 ensures that the customer clusters are selected in such a way that each customer is assigned to exactly one cluster. The next section provides an illustrative problem instance of the SCIRP and a feasible solution, which details all the aforementioned elements of our problem.

4. An Example Solution

To gain insight into the dependency between the tactical-level and operational-level decisions, we discuss an example instance in this section. The location and corresponding distances of 3 customers are given in Figure 3a, where 0 represents the producer location. The daily demands of customers $1-3$ are normally distributed with mean values of $100, 250, 500$ and standard deviations of $25, 50, 75$, respectively. The daily supply of the producer is also normally distributed with a mean of 850 and a standard deviation of 120.

(a) The locations and distances of example instance. (b) Routing and clustering of the example solution.

Figure 3 Locations (3a) and the associated routing (3b) for the illustrative SCIRP example.

The tactical-level decision is displayed in Figure 3b. It shows two clusters being selected: A cluster comprising customers 1 and 2, and a cluster consisting of customer 3 solely. The transportation delivery schedules and associated costs are displayed in Table 1. The transportation costs may be verified by the first element of Equation (2) with parameters $W = 100$ and $w = 20$. Secondly, the holding costs are computed by Equation (5) with $h = 0.2$ and $\alpha = 0.95$. Finally, one may verify the emergency shipment costs with Equation (6) with $e = 25$ and $Q = 1200$. This solution satisfies the emergency shipment chance constraint with $\gamma = 0.9$.

Upon the transportation delivery schedule, we need to base our dynamic purchasing decisions. We discretize the continuous inventory levels in steps of 5 units. We set $K_1 = 1000$, $K_2 = 2500$,

Table 1 The transportation delivery schedule and the costs of the illustrative solution.

(a) The transportation delivery schedule of clusters.

Cluster	Mo	Tu	We	Th	Fr	Sa	Su
{1,2}	✓			✓		✓	
{3}		✓	✓		✓		✓

(b) The cycle costs of clusters.

Cluster	Transport	Holding	Emergency
{1,2}	1020	863	72.2
{3}	880	885	77.4

$c_1 = 10$, and $c_2 = 2$. The resulting expected cyclic buying and selling costs, obtained by value iteration, is found to be 782. We observe that the optimal purchase policy is similar to a period-dependent (s, S) policy, i.e., if the inventory drops below a corresponding s, the policy buys up to S. The (s, S) values for each day of the week are provided in Table 2.

Table 2 The optimal (s, S) policies of the example solution.

	Mo	Tu	We	Th	Fr	Sa	Su
s	0	340	30	315	70	350	330
S	385	795	605	805	670	820	640

Unlike in a classic stationary (s, S) policy, the producer's inventory may exceed S for particular periods, for example, when the supply is more than the demand outflow on the next day of making a purchase. Moreover, this may occur consecutively for multiple periods and accumulate the producer's inventory up to its capacity. In the ranges of $[s, C]$ for each day of the week, the policy implies no buy or sell for the producer in the illustrative example. If the inventory is above C, the optimal policy is only to sell the part that is in excess of the capacity.

Now, consider an alternative tactical-level solution where the only change occurs on the transportation delivery schedule of the clusters, given in Table 3. In this solution, the transportation delivery schedule of customer 3 is postponed for 5 days. For example, the base-stock policy on Tuesday in the first solution is used as the base-stock policy on Sunday in the alternative solution. Thus, by only postponing the transportation delivery schedule, the expected cost of the tactical-level decision does not change. However, we observe that the expected cost of the dynamic purchasing decisions increases to 2025, which is more than double the expected cost of the dynamic purchasing decision in the original solution. This results in a 27% increase in the total expected cycle cost of the SCIRP.

Table 3 The transportation delivery schedule of the alternative tactical-level solution.

Cluster	Mo	Tu	We	Th	Fr	Sa	Su
{1,2}	✓			✓		✓	
{3}	✓		✓		✓		✓

This observation is fundamental for the approach we present in the next section. In preliminary experiments, we observe that balancing the outflow from the producer on cycle periods yields lower costs for the dynamic purchasing decision in general. For example, overlapping deliveries in the same period (i.e., Monday in the alternative solution) result in larger variances of the net outflow from the producer, resulting in more purchasing costs from the external supplier. In the next section, we introduce a generic approach using ideas from parameterized cost function approximations that balances the transportation delivery schedules of multiple clusters and thus decrease the total expected cycle cost in the SCIRP.

5. Parameterized Cost Function Approximation Approach

The joint optimization problem is highly non-linear. The outcome of the tactical-level decision ($\mathbf{x}$, the transportation delivery schedule) determines the state, action, and transition space of the MDP underlying the operational-level dynamic purchasing decisions. However, for a fixed transportation delivery schedule we can easily obtain the optimal dynamic purchasing decisions by solving the underlying MDP to optimality via value iteration. In this section, to handle the high complexity of the problem and improve upon solutions that ignore the relationship between the dynamic purchasing decision and the transportation delivery schedule, we introduce a parameterized cost function approximation (CFA) approach. Our approach is based on iteratively solving a parameterized mixed-integer programming model to obtain a transportation delivery schedule and subsequently solving an MDP for the dynamic purchasing decision.

Overall, this approach has various benefits. Firstly, by decomposing the approach into a MIP and an MDP part, we can rely on commercial MIP solvers and value iteration, easing the computational burden of our approach. Secondly, by parameterizing the set partitioning model, we can steer the transportation delivery schedules so that the expected cost of the combined tactical and operation-level decisions is reduced.

The remainder of this section is structured as follows. Firstly, we will explain the idea behind our approach and present the modified set-partitioning model. Secondly, we discuss how we efficiently enumerate customer clusters to populate the modified set-partitioning model. Thirdly, we detail how we numerically solve the MDP that is associated with the dynamic purchasing decision. Finally, we introduce an efficient algorithm to search through the parameter space of our CFA approach by iterative solving the modified set partitioning problem and MDP effectively.

5.1. Modified Set-Partitioning Model

The modified set-partitioning model is subject to two parameters, $\eta_1 \geq 0$ and $\eta_2 \geq 0$, that modify the objective function by introducing a cost that depends on the combination of selected clusters and their transportation delivery schedules. The modified objective function consists of three parts. First, we minimize the expected cyclic tactical-level costs $\sum_{r\in\mathscr{R}} c_r x_r$, similar as in the set-partitioning model (7)-(9). Secondly, we introduce decision variables M_{1t} and M_{2t} and scale them with the parameters η_1 and η_2 and add this to the objective function, i.e., $\frac{\eta_1}{T}\sum_{t\in\mathscr{T}} M_{1t} + \frac{\eta_2}{T}\sum_{t\in\mathscr{T}} M_{2t}$. The decision variables penalize features of the combined selection of clusters for the transportation delivery schedule (i.e., the tactical-level decision). In our case, we select these features as the deviations between cycle periods in terms of the mean and the variance of the demand of the selected clusters (see Constraints (20) and (21)). The modified set-partitioning model is given by:

$$\min \sum_{r\in\mathscr{R}} c_r x_r + \frac{\eta_1}{T}\sum_{t\in\mathscr{T}} M_{1t} + \frac{\eta_2}{T}\sum_{t\in\mathscr{T}} M_{2t} \tag{18}$$

$$\text{s.t} \sum_{r\in\mathscr{R}} \beta_r^i x_r = 1 \qquad \forall i \in \mathscr{N}, \tag{19}$$

$$-M_{1t} \le \frac{\sum_{t\in\mathscr{T}}\sum_{r\in\mathscr{R}} \Delta_r^t x_r}{T} - \sum_{r\in\mathscr{R}} \Delta_r^t x_r \le M_{1t} \qquad \forall t \in \mathscr{T}, \tag{20}$$

$$-M_{2t} \le \frac{\sum_{t\in\mathscr{T}}\sum_{r\in\mathscr{R}} \Lambda_r^t x_r}{T} - \sum_{r\in\mathscr{R}} \Lambda_r^t x_r \le M_{2t} \qquad \forall t \in \mathscr{T}, \tag{21}$$

$$x_r \in \{0,1\} \qquad \forall r \in \mathscr{R}, \tag{22}$$

$$M_{1t}, M_{2t} \ge 0 \qquad \forall t \in \mathscr{T}. \tag{23}$$

In Constraint (20), Δ_r^t is the mean demand generated by the customers in cluster r at period t, and $(\sum_{t\in\mathscr{T}}\sum_{r\in\mathscr{R}} \Delta_r^t x_r)/T$ is the average demand per period over the cycle. This constraint is defined for each cycle period, and we set the deviation from the mean demand equal to M_{1t} for each period. Similarly, Constraint (21) aims to minimize the deviation per period of the variance of the customer demand generated by the customer clusters. Here, Λ_r^t is the variance of the demand of cluster r on period t, and M_{2t} is set equal to the deviation from the average demand variance per period t.

In our SCIRP, the modified set-partitioning model creates a balance in the demand that the producer faces, which might lead to lower costs of buying or selling hydrogen in the dynamic purchasing decision. The decision maker can select higher values for η_1 and η_2 and the model automatically creates replenishment schemes that balance the demand over the periods in the cycle. Our experiments indeed confirm that increasing η_1 and η_2 increases the costs associated with the tactical level while it decreases the costs of purchasing from the external supplier in general.

Finally, we like to stress our presented approach is fairly general. The characteristics we select for the SCIRP (demand and variance variability) do not depend on any demand distribution. Of course, without a known demand distribution creating tactical-level decisions on its own becomes much more complex. Nevertheless, assuming a method exists to derive tactical-level decisions, our modeling strategy provides a simple but elegant way to connect this to the quality of operational-level decisions. This even surpasses the applications we study in this paper.

5.2. Populating the Set-Partitioning Model

The modified set-partitioning model requires as input the customer clusters, their costs, and associated decisions such as the base-stock policy and delivery periods. In this section, we provide an algorithm that recursively finds all the feasible customer clusters that are candidates to be selected in an optimal solution. Let $\mathscr{R}$ be the set of customer groups. Each customer group $r \in \mathscr{R}$ is defined by i) a set of customers, ii) the shortest vehicle route among the customers in r, iii) the base-stock policy S_r^{it} to meet the predefined service-level α for each customer $i \in \mathscr{N}_r$, and iv) the delivery periods in the cycle.

The algorithm works as follows. First, we compute all the base-stock levels required for covering demand n periods ahead, $I_{in}^{-1}(\alpha)$. Next, we enumerate all potential customer clusters assuming that we deliver them at each period, i.e., a full transportation delivery schedule. Customers are recursively added to clusters until Constraint (4) is violated. For each feasible customer cluster assuming a full transportation delivery schedule, the algorithm then checks the feasibility of all transportation delivery schedules and calculates the relevant parameters including costs and the penalized features in the modified set-partitioning model. The pseudocode of the algorithm is given in Algorithm 1.

Algorithm 1 Precompute the set $\mathscr{R}$.

Input: Demand distributions and instance parameters.
Output: The set $\mathscr{R}$ with corresponding parameters c_r, β_r^i, Δ_r^t, and Λ_r^t.

Compute $I_{in}^{-1}(\alpha)$ for all $i \in \mathscr{N}$ and $n \in \mathscr{T}$.
While computing I_{in}, store $\Theta_i := \max\{n | I_{in} \leq U\}$ for all $i \in \mathscr{N}$.
Recursively find all possible partitioning of customers, $\mathscr{K}$, in which a full transportation delivery schedule is possible without violating Constraint (4).
While computing $\mathscr{K}$, store UB^k as the longest time in between two consecutive deliveries without violating Constraint (4) for partition $k \in \mathscr{K}$.
for each partition $k \in \mathscr{K}$ **do**
  for each 2^{T-1} transportation delivery schedules **do**
    if the longest replenishment of the schedule $\leq \min\{UB^k, \min_{i \in N^k} \Theta_i\}$ **then**
      Add a cluster in $\mathscr{R}$ by computing c_r, β_r^i, Δ_r^t, and Λ_r^t for all $i \in \mathscr{N}$ and $t \in \mathscr{T}$.
    end if
  end for
end for

5.3. Obtaining Optimal Dynamic Purchasing Decisions

We solve the modified set partitioning model subject to the enumerated cluster set $\mathscr{R}$ given parameters (η_1, η_2). The tactical-level decision, $\mathbf{x}$, is then input for the MDP that describes the dynamic purchasing decisions. We use value iteration (see, e.g., Puterman 2014), where we discretize the continuous sets of inventory in at least 100 levels. As the value iteration algorithm provides ϵ-optimality, we conducted preliminary experiments and set $\epsilon = 0.1$ to get the right balance between computational efficiency and the quality of the solution. That is, the obtained solutions will not significantly improve for smaller values of ϵ. After we obtain the ϵ-optimal solutions, the obtained policy is simulated over 30 million periods to derive all the relevant cost components.

5.4. Line Search on the Parameterized CFA

Our final approach for solving the SCIRP iterates between solving the modified set-partitioning model with given (η_1, η_2) and evaluating the associated optimal dynamic purchasing decisions. In this section, we provide an efficient search algorithm in the (η_1, η_2) space to find the values of (η_1, η_2) that results in the joint solution of minimum cost. We make use of the observation in preliminary experiments that the total cost function is typically unimodal in η_1 and η_2. Using this idea, we propose a line search on the parameterized CFA where we iteratively update either η_1 or η_2 in each iteration. The algorithm, which we call Line Search, is provided in Algorithm 2.

Algorithm 2 Line Search.

Input: Initial values of $(\eta_1, \eta_2) = (\epsilon, \epsilon)$, increment value of ζ, an upper bound of UB, and the set $\mathscr{R}$ with corresponding parameters c_r, β_r^i, Δ_r^t, and Λ_r^t.

Output: The minimum found cost of $z = \sum_{r \in \mathscr{R}} c_r x_r + C(\pi^*(\mathbf{x}))$.

Initialize $z = \infty$, $\psi = 0$, and $i = 0$.
while $i \neq 2$ and $(\eta_1, \eta_2) \neq (UB, UB)$ **do**
  Solve the modified set-partitioning model with c_r, β_r^i, Δ_r^t, Λ_r^t, and (η_1, η_2) to record x'_r and $\sum_{r \in \mathscr{R}} c_r x'_r$.
  Solve MDP with the corresponding tactical routing solution, x'_r, to derive the optimal policies.
  Simulate the optimal MDP policy to derive $C(\pi^*(\mathbf{x}'))$ and record $z' = \sum_{r \in \mathscr{R}} c_r x'_r + C(\pi^*(\mathbf{x}'))$.
  if $z' \leq z$ **then**
    Update $z := z'$.
    if $\max(\eta_1, \eta_2) < UB$ **then**
      Update $\eta_1 := \eta_1 + \psi\zeta$, and $\eta_2 := \eta_2 + (1 - \psi)\zeta$.
    else
      Update $\psi := 1 - \psi$ and $i := i + 1$.
    end if
  else
    Update $\eta_1 := \eta_1 - \psi\zeta$, and $\eta_2 := \eta_2 - (1 - \psi)\zeta$.
    Update $\psi := 1 - \psi$ and $i := i + 1$.
  end if
end while

The algorithm starts by initializing $(\eta_1, \eta_2) = (\epsilon, \epsilon)$, with an arbitrarily small positive value to activate the CFA approach, and then iteratively updates either η_1 or η_2. We first incrementally increase the parameter η_1 until the expected cycle cost is non-increasing, or until the predetermined upper bound of η_1 is reached. The algorithm, then, fixes η_1 and incrementally increases η_2 until the same stopping criteria are met. On each selected pair of parameters, three operations are executed. These three operations define a feasible solution for the corresponding pair of parameters, yielding an expected cycle cost of the feasible solution. First, the MIP model of parameterized CFA is solved. Second, the corresponding MDP upon the tactical-level solution is solved. Thirdly, the optimal policy of MDP is simulated to derive the costs of the MDP policy. Among the solutions that are obtained during the process, the one with the minimum expected cycle cost is selected as the best solution.

6. Computational Experiments

This section evaluates our Line Search method in terms of solution quality and computation time. The experiments are performed using an Intel Core i7-10750H CPU (2.6 GHz) with 16GB of RAM. The algorithms are implemented in C++20 in combination with Gurobi 9.1.1. We first describe the base system of our test instances in Section 6.1. Next, our approach is compared to a step-by-step solution in Section 6.2; where the transportation delivery schedules are obtained assuming infinite supply, thus ignoring the impact and cost of the dynamic purchasing decisions similar to the extant literature. Afterward, we compare our Line Search method with a full parameter grid search on medium-sized instances in Section 6.3.

6.1. Base System

We consider a base system given in Table 4. In each instance, 15 customers are randomly allocated into a region of $[0,10] \times [0,10]$. For each customer, we assign the mean demand in the range of $[100,400]$ kg per period, where the mean supply equals the total mean demand. The standard deviation of customer demands is randomized in the range of $[0.025, 0.05]$ times the mean demand. For the producer, the standard deviation equals 0.15 times the mean supply.

Table 4 **Parameter set of the base system.**

W	w	e	Q	h	α	γ	U	C	K_1	K_2	c_1	c_2
100	20	10	1000	0.05	0.95	0.9	1000	4500	3000	15000	25	2

6.2. Comparison of Our Approach with the Step-By-Step Solution

In previous research, the SCIRP is studied while assuming an infinite supply. To compare our Line Search method with the literature, we solve our benchmark instances also by a step-by-step solution. This ignores the relation between the tactical and operational-level decisions, and thus solely optimizes the static, inventory-routing decisions. The resulting solution is simply evaluated in the associated MDP to obtain the cost of the optimal dynamic purchasing decision.

The results are given in Table 5. Upon the base case, we vary the number of customers between 10, 15, and 20, the cycle length between 7 and 10, the vehicle capacities between 800 and 1000, and demand uncertainty levels between 'L' and 'H'. A demand uncertainty of L is the base case, while for H we randomize the customer demands in the range $[0.02, 0.1]$ times the mean demand. For each scenario, 20 instances are generated and solved, where $\#_{\text{rep}}$ is the number of solutions that are solved within the set memory limit. $\Delta(\%)$ is the increase in cost of the step-by-step solution compared to our approach. For both our approach and step-by-step, the average values of the objective function values and the solution times are reported. For our Line Search approach, we also report the average number of iterations found on the search algorithm ($\#_{\text{iter}}$), where the solution times of Line Search are given as the average of each iteration of the algorithm.

Table 5 Performance of the Line Search compared to the step-by-step solution.

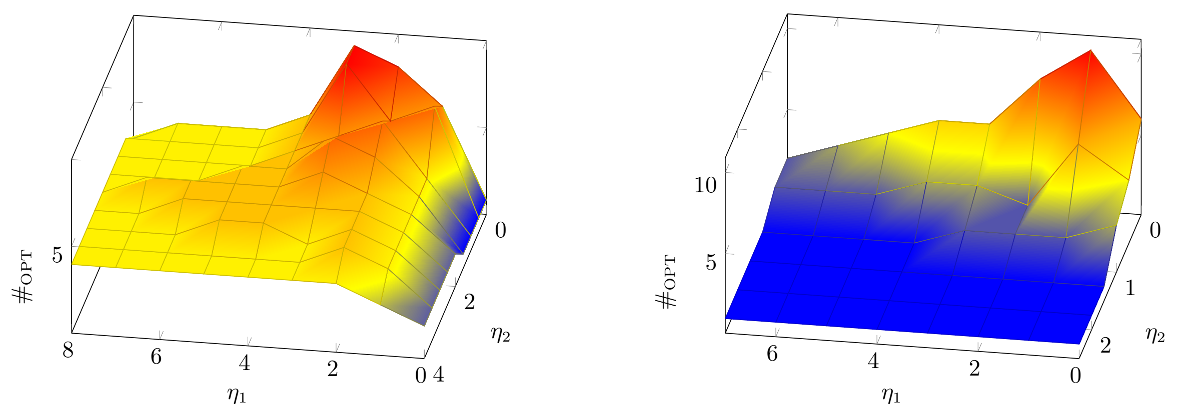
					$\Delta(\%)$		Step-By-Step				Line Search				
N	T	Unc.	Q	$\#_{\text{rep}}$	avg.	max	obj_{MIP}	obj_{MDP}	time_{MIP}	time_{MDP}	obj_{MIP}	obj_{MDP}	time_{MIP}	time_{MDP}	$\#_{\text{iter}}$
10	7	L	800	20	11.0	48.3	10218	7642	0.03	0.14	10338	5809	9.5	0.15	11.3
			1000	20	15.5	62.6	8657	8184	0.05	0.13	8776	5870	7.0	0.15	9.7
		H	800	20	8.0	27.9	11216	7907	0.03	0.12	11315	6404	3.1	0.13	8.7
			1000	20	8.8	44.3	9446	7966	0.03	0.13	9582	6496	7.2	0.14	8.8
	10	L	800	19	17.4	51.2	9932	8716	0.17	0.16	10054	5889	25.7	0.22	11.5
			1000	19	32.6	191.5	8155	10423	0.35	0.14	8302	5805	84.9	0.22	15.5
		H	800	18	18.5	72.6	11327	10059	0.14	0.15	11443	6671	23.6	0.19	10.7
			1000	16	19.5	82.2	9388	9761	0.26	0.15	9547	6543	85.8	0.20	10.0
15	7	L	800	20	2.6	10.5	14942	8619	0.04	0.20	15049	7914	5.2	0.19	10.1
			1000	20	4.6	12.7	12520	9103	0.09	0.19	12655	8023	19.1	0.19	10.0
		H	800	20	2.0	8.2	16574	9110	0.05	0.18	16656	8530	5.4	0.17	8.2
			1000	20	5.2	19.4	14010	9712	0.09	0.18	14107	8539	24.7	0.18	7.9
	10	L	800	19	6.7	18.5	15096	9692	0.44	0.24	15164	8020	119.3	0.26	11.5
			1000	18	12.3	40.6	12190	10604	1.11	0.21	12305	8055	115.6	0.25	11.6
		H	800	16	5.3	12.2	16656	10057	0.32	0.25	16723	8656	109.2	0.24	10.7
			1000	14	8.0	39.5	13601	10238	0.94	0.24	13725	8422	50.9	0.25	9.1
20	7	L	800	20	1.1	4.2	19354	10246	0.11	0.21	19468	9822	38.3	0.19	9.5
			1000	19	3.0	10.2	16251	10802	0.25	0.18	16311	10003	80.8	0.18	8.1
		H	800	20	0.9	4.3	21406	10728	0.10	0.20	21480	10361	28.0	0.18	8.5
			1000	20	2.1	5.6	17861	11057	0.20	0.21	17963	10356	98.7	0.19	7.3
	10	L	800	16	4.7	15.1	19302	11847	0.99	0.28	19360	10384	644.5	0.27	12.8

In all solutions, we observe a sharp decrease in the cost of the dynamic purchasing decision at the expense of only a slight increase in transportation delivery schedule costs when using Line Search compared to the step-by-step solution. As expected, the Line Search solutions are strictly better than the step-by-step solution. The average differences range between 32.6% and 0.9%, while the maximum difference is 191.5%. This represents a 191.5% increase in costs when using the step-by-step solution compared to our approach. Comparing the average and the maximum cost difference between Line Search and the step-by-step solution ($\Delta(\%)$) for an increasing number of customers, we see the differences reduce. However, the Line Search appears to be very robust compared to the step-by-step solution, indicated by the significant maximum differences for the largest instances. Furthermore, we observe that the solution time of the MDP does not depend on the number of customers, whereas the MIP does, because we use the same number of discretized state values in its formulation. The solution time of MIP is strongly correlated to the selected values of η_1 and η_2, which is explained further in Section 6.3.

6.3. Comparison of Our Approach with Grid Search

In this section, we test the solution quality of Line Search by comparing it with a grid search on the (η_1, η_2) space. For the grid search, we let $\eta_1 \in \{0, 0.0001, 1, 2, 3, 4, 5, 6, 7, 8\}$ and $\eta_2 \in \{0, 0.0001, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4\}$, except for the high demand uncertainty systems. For this or when $N = 20$, we let $\eta_1 \in \{0, 0.0001, 1, 2, 3, 4, 5, 6, 7\}$ and $\eta_2 \in \{0, 0.0001, 0.5, 1.0, 1.5, 2.0, 2.5\}$. We add a low value of 0.0001 to these sets in order to test how activation of our approach with an epsilon value affects the solution quality.

We observe that the gap between our approach and the best found in the grid search is 0.07% on average for the instances in Section 6.2, while 88% of the time Line Search finds the best objective function value in the grid. In Figure 4, we plot how many times the best solution is on a particular parameter pair in the grid, including all alternative solutions.



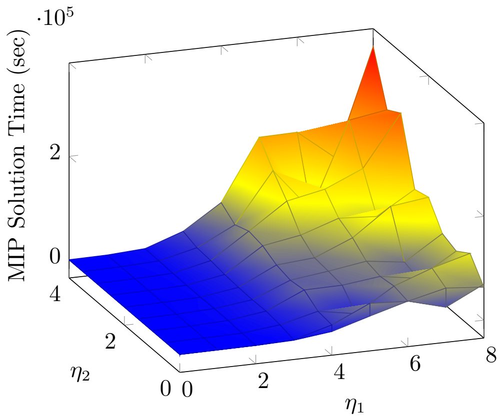
(a) $N = 15$, $T = 7$, Unc $= L$, $Q = 1000$.
(b) $N = 20$, $T = 7$, Unc $= H$, $Q = 800$.

Figure 4 Number of best solutions on each pair of η values.

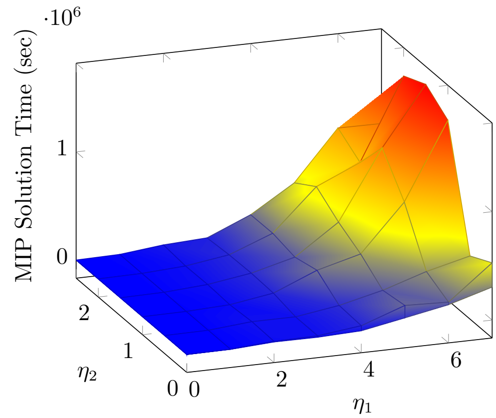
The solution time of the Line Search is highly dependent on the value of η_1 and η_2. In Figure 5, we provide the average times on each parameter pair for two of our instances. We observe that with an increased value of parameters, the solution time is increased sharply. This also results in a higher chance of breaking the memory limit set for the experiments.

7. Case Study in the Northern Netherlands

This case is based on the green hydrogen transportation in the Northern Netherlands region during the transition towards a green hydrogen based economy as a part of the project *Hydrogen Energy Applications in Valley Environments for Northern Netherlands* (HEAVENN 2022). We apply our approach at two different supply locations considering expert-reviewed growth scenarios. Experts



(a) $N = 15$, $T = 7$, $Q = 1000$ (avg. of 3).



(b) $N = 20$, $T = 7$, $Q = 800$ (avg. of 6).

Figure 5 Average MIP solution time (in seconds) of 3 instances on each pair of η values.

envision that growth in the region affects the number of customers, the level of supply and demand uncertainty, and the associated costs of hydrogen production and distribution (New Energy Coalition 2020). This case study analyses the effect of these changes on hydrogen distribution in the Northern Netherlands.

We use the parameter sets given in Table 6. These parameters are selected based on multiple resources. For the transportation costs (W per replenishment and w per distance), the capacities (Q, U, and C per kg), and the risks of holding green hydrogen (h per kg), we decide on the parameters according to the expert reviews and the stakeholders in HEAVENN. The capacities are planned to be expanded for each location over time. Although it is expected that similar vehicles will be used in the long run, the vehicle capacity will increase over years due to technological advancements resulting in more pressured tanks. For the service level probabilities (α and γ) and the emergency shipment cost (e per kg), we refer to Sonntag, Schrotenboer, and Kiesmüller (2022) and set them as $\alpha = 0.95$, $\gamma = 0.9$, and $e = 5$. For the buy and sell prices of hydrogen per kg ($c1$ and $c2$ per kg), we refer to the expert discussion with partners (such as Shell, Engie, GasUnie, and Green Planet) conducted within the HEAVENN program. The current hydrogen price varies between €10 to €25 per kg. In the long run, the targeted price of hydrogen is about €2 per kg, which is a competitive price to its carbon-based alternatives. We incur a difference in the buy and the sell prices which motivates the utilization of the producer's own supply. For the fixed ordering cost $K1$ and emergent purchase $K2$, we consider the future projections of the region and assume that the more hydrogen is available, the less fixed cost is imposed on each purchase.

The stakeholders in HEAVENN foresee two major producers in the following years in the Northern Netherlands region; one in Emmen, and one in Eemshaven. Emmen is planned as a producer location supplying hydrogen to the nearby industry park and the refueling stations. In the longer term, a global supply chain of hydrogen is envisioned where imports and exports of hydrogen

Table 6 Parameters for the case study.

Case	W	w	e	Q	h	α	γ	U	C	K_1	K_2	c_1	c_2
Emmen	100	1	5	400	0.05	0.95	0.9	200	500	1000	1000	10.0	2
Eemshaven 1	100	1	5	700	0.05	0.95	0.9	800	4000	750	750	7.5	2
Eemshaven 2	100	1	5	1100	0.04	0.95	0.9	1500	8000	200	200	3.5	2

become prominent bringing forward the role of seaports. In that respect, Eemshaven is being considered for taking the lead on supplying hydrogen (New Energy Coalition 2020). Thus, we analyze these two regions in our case study. The customer locations are selected from the existing and potential hydrogen refueling stations (HRS) in the region. The list of locations, and corresponding mean and standard deviation values are given in Table 10 in Appendix B. The mean and variances of supply and demand are derived from the short- and mid-term projections within HEAVENN (Scholten 2021, Smid 2021, Hagedoorn 2021).

In the following, we solve three base cases in total, one for supply in Emmen (in Section 7.1) and two for supply in Eemshaven (in Section 7.2). For these base cases, the expected supply per day is set equal to the expected total demand per day. We further relax this assumption in Section 7.3, where the impacts of uncertainty levels are also considered.

7.1. Supply from Emmen

Our results show a total weekly estimated cost of €8582 for the Emmen case. The total cost for delivering and inventory holding is found to be €2.45 per kg. This includes a transportation cost of €1.15 per kg. This seems too high once we consider the target long run selling price of €2 per kg, but it is reasonable with the current selling prices of €10 to €25 per kg. We expect the cost to decrease sharply within the maturation of the economy making the target price attainable, which is also validated by our case studies. The costs associated due to interaction with the external supplier (i.e. purchasing costs) is €1.22 per shipped kg. Due to the high supply and demand uncertainty under low volumes of the early transition states, we observe a high reliance on the external hydrogen market. The vehicle routes are shown in Figure 7.

These routes are implemented with the transportation delivery schedule given in Table 7. We notice a relatively big cluster 1 (including major demand locations such as Groningen), where the vehicle capacity is only enough to deliver these customers on each day of the week. If a day is skipped, the targeted service level of vehicle utilization would not be met. Moreover, Groningen and Leeuwarden have relatively restricted inventory capacities (i.e., a high ratio of μ_i/U), which leads to delivering these customers as frequently as possible, in order to have $\alpha = 95\%$ chance of service level for customer inventory. For the remaining clusters, the model groups two or three customers into one cluster and delivers them as seldom as possible to achieve the targeted service level. This

Figure 6 The routing of case of Emmen in the suggested policy.

is cost-efficient due to the relatively high transportation cost compared to the inventory holding costs. Finally, we observe that the emergency shipment is almost never used, only 0.003% of the total hydrogen is expected to be delivered by additional vehicles. Overall, we see the transportation and the purchasing costs incur 96% of the total costs in this case with the remaining amount barring the costs for inventory holding and emergency shipment.

Table 7 The weekly transportation delivery schedule of Emmen case.

Cluster	Mo	Tu	We	Th	Fr	Sa	Su
1	✓	✓	✓	✓	✓	✓	✓
2			✓			✓	
3		✓		✓			✓
4	✓				✓		

7.2. Supply from Eemshaven

In the mid- and long-term for the region, Eemshaven is foreseen to be the major supplier in the Northern Netherlands. Additionally, a growth is expected in terms of number of locations and volumes of hydrogen per location compared to the short-term future, while the uncertainties decrease with a maturing hydrogen economy. We take these into account and create the instance set shown in Table 10 in Appendix B. The suggested weekly transportation delivery schedules are provided in Table 8a and the delivery routing is given in Figure 7a.

Since transportation costs are the major cost element of the system, we observe that the number of customers in a group increases within a higher density of customer locations in the area. Once the farthest customer from the supplier is delivered, it is more cost-efficient to deliver to other

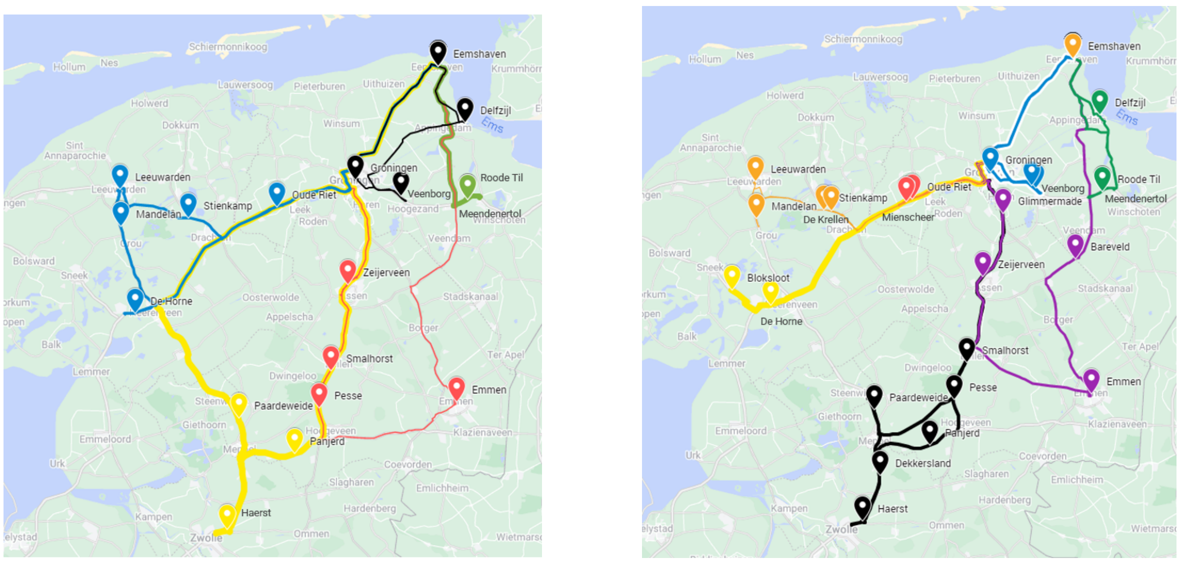
Table 8 The weekly transportation delivery schedules of Eemshaven cases.

(a) Eemshaven 1.

Cluster	Mo	Tu	We	Th	Fr	Sa	Su
1		✓		✓		✓	✓
2	✓		✓		✓		
3	✓	✓	✓	✓	✓	✓	✓
4	✓	✓	✓	✓	✓	✓	✓
5	✓	✓	✓	✓	✓	✓	✓

(b) Eemshaven 2.

Cluster	Mo	Tu	We	Th	Fr	Sa	Su
1	✓		✓			✓	
2		✓			✓		✓
3	✓	✓	✓	✓	✓	✓	✓
4	✓	✓	✓	✓	✓	✓	✓
5	✓	✓	✓	✓	✓	✓	✓
6	✓		✓	✓		✓	
7	✓	✓	✓	✓	✓	✓	✓



(a) Eemshaven 1. (b) Eemshaven 2.

Figure 7 The routing on Eemshaven cases in the suggested policy.

customers that are close to the farthest customer. This leads to more frequent deliveries in order to attain the vehicle capacity service level for the groups with many customers. Finally, this also minimizes the effects of customer uncertainties since combined groups have less uncertainty in total. In this case, the total weekly expected cost is €11814. The transportation cost per kg is €0.54. Note that this is less than half of the Emmen case due to the increased vehicle capacity and higher number of customers in the region which results in less traveling in between consecutive deliveries. The purchasing cost per shipped kg is €0.16, which is only 14% of the Emmen case. This is because, with frequent deliveries and more customers on a route, the dynamic purchasing problem can provide policies with much lower costs due to reduced variances between week days. The percentage of emergency shipments to the customers is 0.27% and therefore the system is mostly run on its own vehicle fleet.

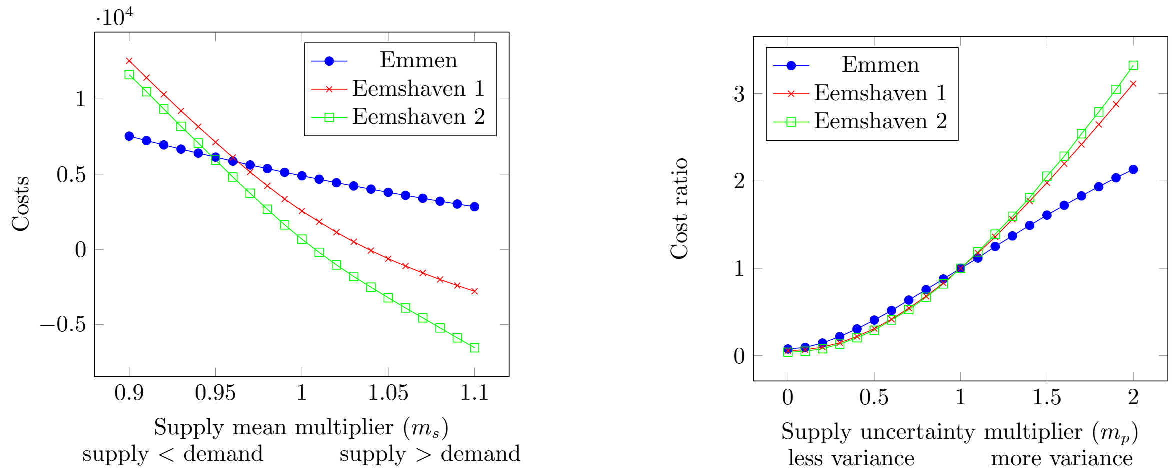
***Eemshaven** 2:* Since the region is expected to become a major hub port in the long run, we study an additional scenario with mature hydrogen economy settings. In this scenario, the producer is expected to replenish a total of 24 customers. The mean levels for supply and demand are further increased. Similar to the first Eemshaven case (i.e. Eemshaven 1), we assume a reduced uncertainty on both supply and demand in the mature stage (i.e. Eemshaven 2), for example, the variance of daily demand of candidate HRS does not change from Eemshaven 1 to Eemshaven 2 while the mean value increases (see Table 10 in Appendix B). The solution has an expected cost of €12877 per week. The routes are shown in Figure 7b, and the transportation delivery schedule is provided in Table 8b.

In the results, we observe a similar structure to the Eemshaven 1 case, where more and more local customers are grouped in a cluster. It is cost-efficient to have larger groups that are delivered once every day. The transportation cost per kg is €0.33. Even though this is the lowest compared to all cases, it is still the main cost element of the system. The purchasing cost per shipped kg is decreased to €0.02. In all problem instances, with less uncertainty and more capacities, the daily purchasing problem yields relatively less costs. Therefore, in a mature hydrogen market where the uncertainties are quite low, we suggest that decision makers first optimize the tactical level operations regarding the supply of hydrogen, and then make the necessary postponements in individual transportation delivery schedules of clusters to further optimize their daily purchasing problem of distributing the hydrogen to end users as a second goal.

7.3. Impacts

Impact of supply quantity: For the base cases of Emmen, Eemshaven 1, and 2, we assume that the mean daily supply equals the mean total daily demand. However, for example, due to uncertainty in how the green hydrogen economy will emerge in society or the disruptions in supply chains, we may observe cases where this equality does not hold. In order to find the effects of the possible imbalances, we analyze all three cases by increasing and decreasing the supply amounts. Let μ_p and σ_p be the mean and the standard deviation of daily supply, respectively. For m_s in $\{0.90, 0.91, 0.92, \ldots, 1.09, 1.10\}$, we analyze varying levels of supply by setting the mean equal to $m_s\mu_p$ and standard deviation equal to $m_s\sigma_p$. In Figure 8a, we give the percentage change for the purchasing costs for each multiplier.

In all three cases, we observe a decrease in costs with an increase in supply. This is because increasing supply decreases the need for buying hydrogen from the external supplier, and moreover increases profits by selling the hydrogen to the external supplier. The effects of the multiplier are higher in Eemshaven cases compared to the Emmen case, possibly due to the higher supply/demand quantities which result in more purchases within, say, 1% change in m_s. While this is an advantage for the Eemshaven cases when $m_s > 1$, it results in a sharp increase in costs if the supply is disrupted ($m_s < 1$). Thus, the more the ratio of supply/demand is decreased, the more we recommend to the



(a) Purchasing costs of each case.

(b) Percentage of purchasing costs of each case.

Figure 8 Effects of the supply distribution.

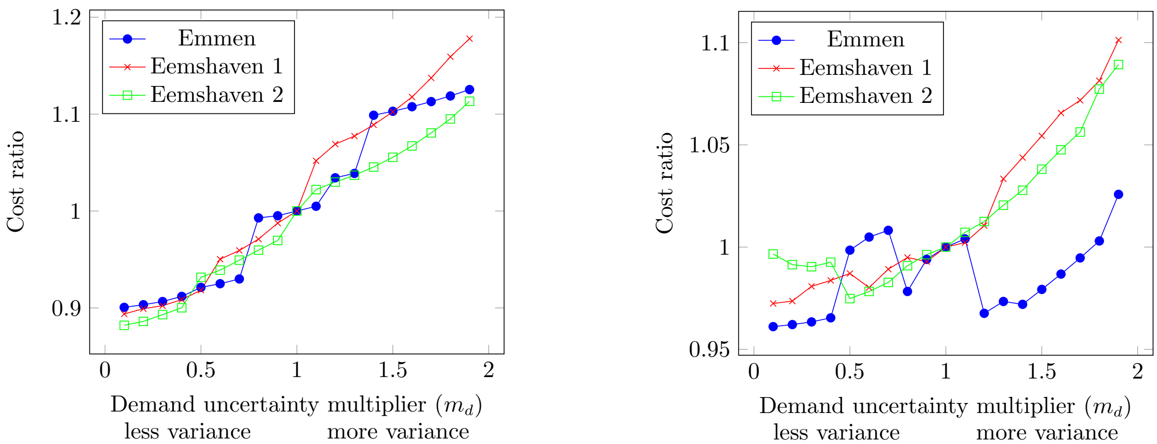
decision makers to focus on their daily purchasing problem. This recommendation gains importance within the maturation of the hydrogen economy due to the higher supply and demand quantities.

Impact of supply uncertainty: In our cases, we assume some level of uncertainty in both supply and demand. While this is decided within the expert discussions, we may observe a higher or a lower level of uncertainty in the future. To see how the system performs under different uncertainties, we test various supply uncertainty levels. For $m_p \in \{0, 0.1, \ldots, 1.9, 2\}$, we analyze varying levels of supply uncertainty by setting the standard deviation equal to $m_p\sigma_p$. The weekly expected purchasing costs are provided in Figure 8b.

We observe almost a parabolic increase in purchasing costs within the increase in supply variance in Figure 8b. The purchasing costs are converging almost to zero in all cases when m_p is converging to zero. Even though the system still has uncertainty in demand with $m_p = 0$, the daily purchasing problem handles that uncertainty with almost no purchase from the external supplier. This shows that, as one of our key contributions in this paper, supply uncertainty is a major factor affecting the dynamic purchasing costs, and is crucial to consider.

Impact of demand uncertainty: As we did with supply uncertainty, we further study the effects of demand uncertainty. For m_d in $\{0.1, 0.2, \ldots, 1.8, 1.9\}$, we analyze varying levels of demand uncertainty by setting the standard deviation of the customer demand i, σ_i, equal to $m_d\sigma_i$ for all customers. For each multiplier, the tactical-level costs and the purchasing costs are shown in Figures 9a and 9b, respectively. In both figures, the costs are given relative to the base cases, where a cost ratio of 1 represents the same cost as the base case.

Unlike the previous analysis, we observe that in Figures 9a and 9b, the change in costs is not following a smooth function. In the subparts where the costs are smoothly increasing, for example from $m_d = 1.4$ to $m_d = 1.8$ in Emmen case, we observe no change in the solution structure; the



(a) Tactical-level costs (transportation + inventory holding + emergency shipment).

(b) Purchasing costs of each case.

Figure 9 Comparison of tactical-level and purchasing costs to the base case over demand uncertainty multiplier (m_d).

routing and the transportation delivery schedule. The costs are gradually increasing due to higher safety stocks and higher chances of emergency shipment. However, the same does not apply from $m_d = 0.7$ to $m_d = 0.8$ in Emmen case, where a different solution is selected with a different route and associated daily purchasing problem. This is either because the solution of $m_d = 0.7$ is less efficient with increased uncertainty levels, or because this solution is no longer feasible due to service target levels. Additionally, the more customers we have in a region, the more combinations of feasible clusters exist. Thus, the bumpiness in costs decreases towards a mature market, due to higher possibilities for distribution. Overall, especially in the early transition stages, we recommend decision makers to update their system solutions even with a tiny change in uncertainties in customer demand.

8. Conclusions

In this study, we present a novel solution framework for jointly addressing tactical-level and operational-level decision making in the context of green-hydrogen logistics. We consider a stochastic cyclic inventory routing problem that generalizes several existing problems in the context of inventory routing. The particular innovation is the consideration of supply uncertainty, due to uncertain hydrogen production from renewable sources, in combination with cyclic transportation delivery schedules that impose deliveries at fixed periods.

Our approach combines two models: a Mixed Integer Programming (MIP) model that solves tactical-level decisions to generate a transportation delivery schedule for hydrogen, and a Markov decision process (MDP) model that optimizes operational-level decisions for buying and selling hydrogen on the market to ensure the feasibility of the transportation delivery schedule. We propose a parameterized cost function approximation approach for the tactical-level MIP model to anticipate the cost of operational-level dynamic decisions. Our approach includes an efficient search algorithm that iteratively solves MIPs and MDPs to find the optimal parameters for the modified MIP model. This allows us to effectively balance tactical and operational considerations to maximize the overall efficiency of green-hydrogen logistics operations.

We show that our approach provides high-quality solutions on a stylized benchmark set. First, our approach outperforms an algorithm that takes a classic two-stage approach in which first the transportation delivery schedules are created (i.e., the tactical-level decision), and afterward, the dynamic purchasing decisions are made (i.e., the operational-level decisions). In addition, our efficient search over the parameter space, as required for the cost function approximation, shows excellent performance in comparison to a grid search over the parameter space.

Furthermore, as a part of the project *Hydrogen Energy Applications in Valley Environments for Northern Netherlands* (HEAVENN 2022), we show the results of a case study to give insights into efficient green hydrogen distribution. We solve three expert-reviewed base scenarios. Furthermore, we analyze the impact of various problem elements upon these base scenarios and it appears that supply uncertainty is a key factor for operational-level decisions and should be anticipated while designing transportation delivery schedules on a tactical level.

The opportunities for future research are numerous. Some of these require no fundamental change in the model and approach, such as consideration of a heterogeneous vehicle fleet, enabling the use of multiple vehicles per replenishment, and nonstationary customer demand and producer supply. Furthermore, the problem may be dealt with in a dynamic setting, enabling daily reoptimization of vehicle routes. This latter element would also require predicting future hydrogen production based on weather forecasts, which we deem a very interesting avenue for further research.

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References

Abe JO, Popoola A, Ajenifuja E, Popoola O, 2019 *Hydrogen energy, economy and storage: Review and recommendation. International Journal of Hydrogen Energy* 44(29):15072–15086.

Adelman D, 2004 *A price-directed approach to stochastic inventory/routing. Operations Research* 52(4):499–514.

Adulyasak Y, Cordeau JF, Jans R, 2014 *Optimization-based adaptive large neighborhood search for the production routing problem. Transportation Science* 48(1):20–45.

Adulyasak Y, Cordeau JF, Jans R, 2015a *Benders decomposition for production routing under demand uncertainty. Operations Research* 63(4):851–867.

Adulyasak Y, Cordeau JF, Jans R, 2015b *The production routing problem: A review of formulations and solution algorithms. Computers & Operations Research* 55:141–152.

Almaraz SDL, Azzaro-Pantel C, Montastruc L, Domenech S, 2014 *Hydrogen supply chain optimization for deployment scenarios in the Midi-Pyrénées region, France. International Journal of Hydrogen Energy* 39(23):11831–11845.

Alvarez A, Cordeau JF, Jans R, Munari P, Morabito R, 2021 *Inventory routing under stochastic supply and demand. Omega* 102:102304.

Anvari M, Lohmann G, Wächter M, Milan P, Lorenz E, Heinemann D, Tabar MRR, Peinke J, 2016 *Short term fluctuations of wind and solar power systems. New Journal of Physics* 18(6):063027.

Ball M, Wietschel M, 2009 *The future of hydrogen – opportunities and challenges. International Journal of Hydrogen Energy* 34(2):615–627.

Bertazzi L, Bosco A, Guerriero F, Lagana D, 2013 *A stochastic inventory routing problem with stock-out. Transportation Research Part C: Emerging Technologies* 27:89–107.

Bertazzi L, Laganà D, Ohlmann JW, Paradiso R, 2020 *An exact approach for cyclic inbound inventory routing in a level production system. European Journal of Operational Research* 283(3):915–928.

Coelho LC, Cordeau JF, Laporte G, 2014a *Heuristics for dynamic and stochastic inventory-routing. Computers & Operations Research* 52:55–67.

Coelho LC, Cordeau JF, Laporte G, 2014b *Thirty years of inventory routing. Transportation Science* 48(1):1–19.

Crama Y, Rezaei M, Savelsbergh M, Woensel TV, 2018 *Stochastic inventory routing for perishable products. Transportation Science* 52(3):526–546.

Diabat A, Archetti C, Najy W, 2021 *The fixed-partition policy inventory routing problem. Transportation Science* 55(2):353–370.

Drücke J, Borsche M, James P, Kaspar F, Pfeifroth U, Ahrens B, Trentmann J, 2021 *Climatological analysis of solar and wind energy in Germany using the Grosswetterlagen classification. Renewable Energy* 164:1254–1266.

European Union, 2012 *Energy: Roadmap 2050* (Publications Office of the European Union), URL `http://dx.doi.org/10.2833/10759`.

Gaur V, Fisher ML, 2004 *A periodic inventory routing problem at a supermarket chain. Operations Research* 52(6):813–822.

Hagedoorn F, 2021 *Infrastructure development for green hydrogen use in railway transport – a case study in the Northern Netherlands*. Master's thesis, Rijksuniversiteit Groningen, the Netherlands.

HEAVENN, 2022 *Hydrogen energy applications in valley environments for Northern Netherlands*. URL `https://heavenn.org`.

Kleywegt AJ, Nori VS, Savelsbergh MW, 2002 *The stochastic inventory routing problem with direct deliveries. Transportation Science* 36(1):94–118.

Kleywegt AJ, Nori VS, Savelsbergh MW, 2004 *Dynamic programming approximations for a stochastic inventory routing problem. Transportation Science* 38(1):42–70.

Liu C, Li F, Ma LP, Cheng HM, 2010 *Advanced materials for energy storage. Advanced Materials* 22(8):E28–E62.

Malicki S, Minner S, 2021 *Cyclic inventory routing with dynamic safety stocks under recurring non-stationary interdependent demands. Computers & Operations Research* 131:105247.

Michel S, Vanderbeck F, 2012 *A column-generation based tactical planning method for inventory routing. Operations Research* 60(2):382–397.

Mulder J, van Jaarsveld W, Dekker R, 2019 *Simultaneous optimization of speed and buffer times with an application to liner shipping. Transportation Science* 53(2):365–382.

Neves-Moreira F, Almada-Lobo B, Cordeau JF, Guimarães L, Jans R, 2019 *Solving a large multi-product production-routing problem with delivery time windows. Omega* 86:154–172.

New Energy Coalition, 2020 *The Northern Netherlands hydrogen investment plan 2020: Expanding the Northern Netherlands hydrogen valley*. Technical report, URL `https://www.newenergycoalition.org/custom/uploads/2020/10/investment-plan-hydrogen-northern-netherlands-2020-min.pdf`.

Oliveira AM, Beswick RR, Yan Y, 2021 *A green hydrogen economy for a renewable energy society. Current Opinion in Chemical Engineering* 33:100701.

Powell WB, Ghadimi S, 2022 *The parametric cost function approximation: A new approach for multistage stochastic programming. arXiv preprint arXiv:2201.00258* .

Puterman ML, 2014 *Markov decision processes: discrete stochastic dynamic programming* (John Wiley & Sons).

Raa B, Aghezzaf EH, 2009 *A practical solution approach for the cyclic inventory routing problem. European Journal of Operational Research* 192(2):429–441.

Raa B, Aouam T, 2021 *Multi-vehicle stochastic cyclic inventory routing with guaranteed replenishments. International Journal of Production Economics* 234:108059.

Rau H, Budiman SD, Widyadana GA, 2018 *Optimization of the multi-objective green cyclical inventory routing problem using discrete multi-swarm PSO method. Transportation Research Part E: Logistics and Transportation Review* 120:51–75.

Safari A, Das N, Langhelle O, Roy J, Assadi M, 2019 *Natural gas: A transition fuel for sustainable energy system transformation? Energy Science & Engineering* 7(4):1075–1094.

Schenekemberg CM, Scarpin CT, Pecora Jr JE, Guimarães TA, Coelho LC, 2021 *The two-echelon production-routing problem. European Journal of Operational Research* 288(2):436–449.

Scholten H, 2021 *Structuring the hydrogen refuelling station network to accommodate fuel cell electric trucks.* Master's thesis, Rijksuniversiteit Groningen, the Netherlands.

Sgarbossa F, Arena S, Tang O, Peron M, 2022 *Renewable hydrogen supply chains: A planning matrix and an agenda for future research. International Journal of Production Economics* 108674.

Smid F, 2021 *Laying the foundation for a hydrogen refueling network for inland cargo ships in the Netherlands and Germany: A roadmap to 2050.* Master's thesis, Rijksuniversiteit Groningen, the Netherlands.

Sonntag DR, Schrotenboer AH, Kiesmüller GP, 2022 *Stochastic inventory routing with time-based shipment consolidation. European Journal of Operational Research* .

Staffell I, Scamman D, Abad AV, Balcombe P, Dodds PE, Ekins P, Shah N, Ward KR, 2019 *The role of hydrogen and fuel cells in the global energy system. Energy & Environmental Science* 12(2):463–491.

Vansteenwegen P, Mateo M, 2014 *An iterated local search algorithm for the single-vehicle cyclic inventory routing problem. European Journal of Operational Research* 237(3):802–813.

Welder L, Ryberg DS, Kotzur L, Grube T, Robinius M, Stolten D, 2018 *Spatio-temporal optimization of a future energy system for power-to-hydrogen applications in Germany. Energy* 158:1130–1149.

Woo Yb, Cho S, Kim J, Kim BS, 2016 *Optimization-based approach for strategic design and operation of a biomass-to-hydrogen supply chain. International Journal of Hydrogen Energy* 41(12):5405–5418.

Yu Y, Chu C, Chen H, Chu F, 2012 *Large scale stochastic inventory routing problems with split delivery and service level constraints. Annals of Operations Research* 197(1):135–158.

Appendix A: Overview of Notation Used

Table 9: Overview of notation used

Sets:	
$\mathcal{T}$	set of periods
$\mathscr{T}$	set of cycle periods
$\mathscr{N}$	set of customers
$\mathscr{N}^0$	set including all customers and the producer
$\mathscr{N}_r$	set of customers in cluster r
$\mathscr{R}$	set of clusters
$\mathcal{R}$	set of inventory levels
Indices:	
t	index for cycle periods
T	number of cycle periods
τ	index for periods
N	number of customers
i	index for nodes
r	index for clusters
ω	index for inventory levels
s_1, s_2	index for states
Parameters:	
θ_r^t	parameter that equals 1 if cluster r is delivered on period t, 0 otherwise
β_r^i	parameter that equals 1 if cluster r contains customer i, 0 otherwise
d_r	the vehicle route length of cluster r
S_r^{it}	the base-stock policy of customer i of cluster r on the replenishment of period t
$\vec{S}_r^i$	the set of the base-stock policies of customer i of cluster r
$IL_{it}^+\left(\vec{S}_r^i\right)$	stock on hand at the period t on customer i depending on the base-stock policy $\vec{S}_r^i$
$D_r^{it}\left(\vec{S}_r^i\right)$	random variable of shipped units to customer i on period t on the base-stock policy $\vec{S}_r^i$
Q	vehicle capacity
U	customer inventory capacity
α	target service-level
γ	target probability that the vehicle capacity is not exceeded
μ_i	mean of the supply/demand distribution of node i
σ_i	standard deviation of the supply/demand distribution of node i
I_{in}	the demand distribution of customer i for n consecutive periods
z_α	z-score of α
n_{tr}	the number of periods until the next replenishment for a delivery period t of cluster r
m_{tr}	the number of periods since the previous replenishment for a delivery period t of cluster r
D_0	the probability distribution of daily supply
D_t	the probability distribution of daily demand of deliveries of period t
Decision variables:	
x_r	binary decision variable that equals 1 if cluster r is in the solution, 0 otherwise
$\pi(\mathbf{x})$	the policy of dynamic purchasing problem, depending on tactical solution $\mathbf{x}$
Cost components:	
c_r^{T}	cyclic transportation cost of cluster r
c_r^{H}	expected cyclic holding cost of cluster r
c_r^{E}	expected cyclic emergency shipment cost of cluster r
c_r	expected cyclic tactical cost of cluster r
W	fixed transportation cost of a replenishment
w	variable transportation cost per distance

h	holding cost per unit per period
e	emergency shipment cost per unit
$v(s_1), y(s_2)$	future costs of states
c_1, c_2	variable buy/sell costs of the hydrogen
K_1, K_2	fixed costs of purchases from the outside market

Appendix B: Case Study Information

Table 10 **Mean and standard deviations of daily demand distributions (in kg) of the case study.**

		Emmen		Eems1		Eems2	
Node	Location	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
0	Emmen	500	250	-	-	-	-
0	Eemshaven	-	-	2195	658.5	4670	934
1	Groningen	100	20	350	52.5	600	60
2	Delfzijl	35	14	100	25	150	30
3	Leeuwarden	100	20	200	40	400	60
4	Emmen	65	16	250	50	450	67.5
5	Pesse	50	15	120	30	250	37.5
6	Meendenertol	30	12	75	22.5	120	24
7	Panjerd	30	12	100	30	150	30
8	Haerst	30	12	100	30	150	30
9	Paardeweide	30	12	100	30	150	30
10	Oude Riet	30	12	100	30	150	30
11	Roode Til	-	-	100	30	150	30
12	Veenborg	-	-	100	30	150	30
13	Smalhorst	-	-	100	30	150	30
14	Zeijerveen	-	-	100	30	150	30
15	Mandelân	-	-	100	30	150	30
16	De Horne	-	-	100	30	150	30
17	Stienkamp	-	-	100	30	150	30
18	Bloksloot	-	-	-	-	150	30
19	De Krellen	-	-	-	-	150	30
20	Mienscheer	-	-	-	-	150	30
21	Glimmermade	-	-	-	-	150	30
22	Dekkersland	-	-	-	-	150	30
23	Bareveld	-	-	-	-	150	30
24	Dikke Linde	-	-	-	-	150	30