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Highlights

- a hazmat routing and scheduling problem for a general transportation network is addressed;
- a multiple hazmat classes when incident probabilities are unknown or inaccurate are investigated;
- a multi-demon formulation is proposed to model the problem;
- the proposed formulation is transformed into other forms which are proved to be equivalent;
- a solution procedure, numerical examples, properties, a case study and insights are presented.

ACCEPTED MANUSCRIPT

Link-Based Multi-Class Hazmat Routing-Scheduling Problem: A Multiple Demon Approach

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ABSTRACT

This paper addresses a hazmat routing and scheduling problem for a general transportation network with multiple hazmat classes when incident probabilities are unknown or inaccurate. A multi-demon formulation is proposed for this purpose. This formulation is link-based (i.e., the decision variables are link flows) and can be transformed into other forms so that a wide range of solution methods can be used to obtain solutions. This paper also proposes a solution strategy to obtain route flow solutions without relying on exhaustive route enumeration and route generation heuristics. Examples are set up to illustrate the problem properties, the method of obtaining route flows from link flows, and the computational efficiency of the solution strategy. Moreover, a case study is used to illustrate our methodology for real-life hazmat shipment problems. From this case study, we obtain four key insights. First, to have the safest shipment of one type of hazmat, different trucks carrying the same type of hazmat need to take different routes and links. Second, in case of multiple-hazmat transportation, it is recommended to use different routes and links for the shipment of different hazmat types. This may increase travel time but can result in safer shipment. Third, if the degree of connectivity in a transportation network is high, the shipment company may have multiple solutions. Fourth, the hazmat flows on critical links (whose removal would make the network disconnected) must be distributed or scheduled over different periods to have safer shipment.

Keywords: transportation; vehicle routing; non-cooperative game; hazardous materials; scheduling.

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1. INTRODUCTION

According to US Department of Transportation (DOT), a hazardous material (or hazmat in short) is defined as any substance or material capable of causing harm to people, property, and the environment. Hazmats are classified into 9 classes according to their physical, chemical, and nuclear properties (Keller and Associates, 2001). They are transported daily in many countries because the demand and supply locations are always different. The shipments of hazmats can be substantial. In some countries such as the USA, the volume and weight of hazmat shipments even increase over time. In 1998, 800,000 domestic daily shipments of hazmats were estimated to be transported in the USA whereas in 2009, the estimate increased to almost 1 million (US DOT, 2014).

Given substantial shipments of hazmats, the related accidents do happen. Moreover, the accidents can occur anywhere along the trips, but these accidents only correspond to a small proportion of traffic accidents. The annual number of transportation accidents in the USA was about 6 million in 2008 (US DOT, 2008) in contrast to the approximately 20,340 hazmat transportation incidents in the same year (US DOT, 2009). According to the recent report of PHMSA (2014), between 2009 and 2013, the number of hazmat incidents increased by 3.8 percent. The number of hazmat incidents in a country is still miniscule compared to the number of road accidents currently. To get some ideas regarding the number of hazmat incidents in the US, interested readers may refer to (<http://www.phmsa.dot.gov/hazmat/library/data-stats/incidents>). However, the total number of injuries and fatalities from each hazmat accident is drastically higher than that from a normal accident. Moreover, the release of these materials during transportation can be extremely undesirable as this can cause environmental pollution in addition to economic damage, injuries, and fatalities (Smith, 2009). Meanwhile, many transportation companies in a country are in charge of hazmat shipments. These transportation companies need to consider safety and environmental issues and legal limitations to choose the best routes for their fleets but the regulations and constraints do not often apply to many non-hazmat trips with possible accidents. This is probably why the shipment of these hazardous materials has drawn considerable attention over the last few decades.

The traditional approach to modeling the routing and/or scheduling decisions assume that incident probabilities are known (e.g., Meng et al., 2005). The alternative approach is that these probabilities are unknown. To deal with this assumption, non-cooperative game theory was often used in the literature (e.g., Bell, 2000, 2003, 2004; Bell and Cassir, 2002; Cassir et al., 2003; Szeto et al., 2006; Laporte et al., 2010; Qiao et al., 2014). This theory was also used when attack probabilities in the defender-attacker framework were assumed to be known (e.g., Dadkar et al., 2010a,b; Reilly et al., 2012) or it was assumed that there was some information on link incident probabilities (e.g., Schmöcker, 2010). Here, non-cooperative games are those, in which “players are unable to make enforceable contracts outside of those specifically modeled in the game. Hence, it is not defined as games in which players do not cooperate, but as games in which any cooperation must be self-enforcing”. (Shor, 2005).

This paper addresses the problem of routing and scheduling hazardous materials in a general transportation network with multiple origin-destination (OD) pairs, multiple classes of hazmats, and unknown link incident probabilities: *Multiple dispatchers are responsible for sending out their vehicles to transport various classes of hazmats in a network with multiple OD pairs and have both route and departure time choices on a given day. Moreover, during the journey, the dispatchers can decide their hazmat vehicles to stop at some locations and their stop duration before continuing the journey. However, the probability of an incident to occur for each combination of route choice, departure time choice, intermediate stopping location choice, and duration choice is unknown. If an incident occurs, the impact of the incident depends on the type and volume of hazmat involved.* We consider

multiple hazmat vehicles, in which each individual vehicle may encounter an incident. This does not mean that the incident must be between two or more than two hazmat vehicles. Any incident in which a hazmat vehicle is involved is related to this research. This research also looks at the problem from the company's perspective while observing the country-wide restrictions and approved routes.

The problem is considered to be a non-cooperative game between multiple dispatchers and multiple demons on a space-time expanded network. A demon is an imaginary evil entity that intentionally attacks a link to cause explosion or an incident on the link when a hazmat vehicle is on the link. Each demon has enough knowledge on all links, leading to the most number of fatalities and injuries when a particular link is selected. Each demon must cause an incident on one and only one link. Each demon aims at seeking its link selection strategy to maximize the impacts of the incident. The game is non-cooperative between dispatchers and demons because the dispatchers and the demons make decisions independently. We assume that the shipment between an OD pair is responsible by just one private company, and a company cannot handle the shipment between more than one OD pair. Therefore, the game among dispatchers is also non-cooperative. However, this game can be easily extended to consider cooperation between dispatchers, which will be mentioned in the conclusion.

The problem is formulated by both route- and link-based approaches. The route-based approach develops the formulation with route flows as decision variables whereas the link-based approach develops the formulation with link flows as decision variables. The equivalence of the route- and link-based problems, in terms of the maximum expected payoff to each demon, is proved. Both problems are formulated as a mixed system of equations and inequalities. The link-based problem is also reformulated into a variational inequality problem (VIP), a nonlinear complementary problem (NCP), an unconstrained minimization problem (UMP), and a fixed point problem (FPP) to allow a wider range of solution methods developed for VIPs, NCPs, UMPs, and FPPs to solve the proposed link-based problem.

Unlike solving the route-based problem, solving the link-based VIP, NCP, UMP, FPP, and mixed system of equations and inequalities do not require exhaustive route enumeration or route generation heuristics. However, the solutions to these formulations are link flows and link selection probabilities, which cannot tell the decision makers (or dispatchers) how to randomly select routes, departure times, intermediate stopping locations, and the corresponding stopping durations. This paper proposes a solution strategy, which is to firstly solve one of the link-based formulations by existing solution methods and then deduce route flows from link flows by our proposed route flow extraction algorithm. The route flow extraction algorithm is proved to be convergent. An example is given to illustrate the algorithm. Numerical examples are also provided to illustrate the problem properties. Problem insights and computational performance of the solution strategy are presented. Finally, a case study of Singapore is used to illustrate our proposed methodology for real-life hazmat shipment problems. The contribution of this paper includes the following: (i) This paper proposes link-based models to determine the routes and schedules of hazmat shipment under the situation of unknown incident probabilities, (ii) it introduces a solution strategy to obtain solutions on exhaustive route enumeration and route generation heuristics, and (iii) it presents the problem properties and problem insights.

The remainder of this paper is organized as follows: Section 2 reviews the literature of the subject. Section 3 presents the models and discusses their properties. Section 4 depicts the proposed solution strategy. Section 5 presents a numerical study. Section 6 focuses on algorithm complexity and computational results. Section 7 highlights the practical aspects of the formulated problem using a case study. Section 8 concludes the paper and

provides some future research directions.

2. LITERATURE REVIEW

Several streams of research are related to our work. Therefore, the literature is organized in terms of these streams as follows:

Hazmat routing and scheduling with known incident probabilities: To mitigate the level of the risk involved in hazmat transportation, a lot of research was done in the past. Comprehensive review papers on this research area can be found in List et al. (1991), Erkut and Verter (1995), Erkut and Verter (1998), and Verter and Kara (2008). As appropriate hazmat routing and scheduling decisions can reduce the level of the risk involved, most previous hazmat shipment studies focus on the planning of (1) routes (e.g., Batta and Chiu, 1988; Gopalan et al., 1990; Jin et al., 1996; Chang et al., 2005; Akgün et al., 2007; Carotenuto et al., 2007; Kang et al., 2014), (2) schedules (e.g., Cox and Turnquist, 1986), and (3) both routes and schedules simultaneously (e.g., Zografos and Androustopoulos, 2004; Meng et al., 2005). These studies assumed that link incident probabilities were known. For the low-probability events like incidents involving hazardous materials, these probabilities are usually unknown, because these events are rare and there is often insufficient data to estimate these probabilities (Bell, 2006). Over the time that it would take to accumulate adequate data to estimate the probabilities, circumstances may have changed (say, accident black spots may have been treated), making the calculated probabilities obsolete (Bell, 2006). Moreover, most dispatchers, when dealing with high-consequence events, exhibit risk aversion (Bell, 2006). This leads to one line of research given in the next subsection.

Hazmat transportation with unknown incident probabilities: To deal with unknown incident probabilities and risk aversion behaviors of dispatchers, the non-cooperative game approach was used in modeling hazmat routing (e.g., Bell, 2006, 2007). In particular, Bell (2006) proposed a minimax formulation to determine the safest set of routes and the safest share of traffic among these routes for hazmat shipment. This formulation has a game theory interpretation and can be considered a non-cooperative, zero-sum game between a dispatcher seeking the set of routes that minimize the expected population affected and a demon seeking to maximize the expected population affected by causing an incident on one link. Bell (2007) further considered the travel cost in the minimax formulation. Bell (2006, 2007) only considered route planning. In fact, incorporating scheduling decisions for hazmat shipment can further reduce the level of the risk involved (Nozick et al., 1997). Szeto (2013) further considered scheduling decisions. However, Bell (2006, 2007) and Szeto (2013) considered each origin-destination (OD) separately. In reality, there is interaction of hazmat shipment between OD pairs. Two or more hazmat shipments of the same class or different classes can use the same road section and have an incident at the same time. The impact of the incident can affect more people around the incident location compared with the incident due to only single class of hazmats because of the reaction between different classes of hazmats or a higher volume of hazmats involved. It is therefore important to model multiple OD pairs and multiple classes of hazmats. In this paper, we potentially “allow” several hazmat shipments of the same class or different classes using the same road section and having an incident simultaneously. However, this does not mean that several hazmat shipments must use the same road section. On the contrary, usually the model chooses different routes for different hazmat classes to avoid having large flows and consequently large possible accidents, injuries, and fatalities. In practice, the approved hazmat routes (inputs of our model and also shipping companies) in various countries are always the

same for different classes of hazmat shipments. However, for any reason, if a specific hazmat shipment cannot use a link, we can implement this constraint to our model by setting the flow on the forbidden link equal to zero. Of course, this can reduce our solution search space, which is a positive point for models that contain integer variables (because it usually reduces computational efforts).

Time-dependent hazmat routing and scheduling: Another line of research is time-dependent hazmat routing and scheduling, in which link travel times are time-varying. In this context, Haghani and Chen (2003) assumed that travel times over links could vary by time of day; they considered risks on routes, risks at nodes, and travel times and mathematically formulated the problem. In our research, we also consider that travel times can vary by time of day but our focus is more on reducing the number of affected people in case of emergency rather than explicitly minimizing travel time. Meanwhile, spreading risks in both time and space for time-dependent networks was suggested by Bersani et al. (2010). Toumazis (2012) and Toumazis and Kwon (2013) used the concept of conditional value-at-risk (CVaR) for mitigating hazmat transportation risks in a time-dependent network and tested the idea on the road network of Buffalo's, NY. Androutsopoulos and Zografos (2010) addressed a hazmat routing-scheduling problem, in which the two criteria, cost and risk, are time-dependent. Androutsopoulos and Zografos (2012) also considered dynamic travel times in a city network for their hazmat routing and scheduling problem and formulated it as a bi-objective problem. Similarly, we also consider that hazmat incident risk changes over time. Unlike the abovementioned research studies, we do not exploit a bi-criteria method to include both criteria. On the contrary, similar to the concept of lexicographic method, we apply travel time (not travel cost) and risk sequentially. To be more specific, we *implicitly* consider travel time to create the transportation network; after that we inject the element of time/scheduling to the network to spread potential hazmat explosion risk over time. Although we are also interested in shortest travel distance/time, the most important criterion in our hazmat routing problem is to use the safest set of routes. Therefore, instead of considering the only shortest route between any OD pair, we are interested in considering several (i.e., more than one) routes that are short/fast enough to allow us split the hazmat incident risk among them.

Security considerations in hazmat routing and scheduling: Huang et al. (2003) believed that routing hazmat vehicles should not only ensure the safety of travellers but also consider the risk of the hazmat being used as a mass destruction weapon. They evaluated the risk of hazmat transportation by integrating geographic information systems (GIS) and the analytic hierarchy process (AHP) to determine the weights of various criteria of the alternative routes. Huang et al. (2004) used a set of evaluation criteria in hazmat routing with the special focus on criteria related to security. Both of these methods were tested on a case study in Singapore. DeLorenzo et al. (2005) described a real-life project related to the benefits of wireless communications systems with GPS technology in enhancing the safety, security, and efficiency of hazmat transportation. Security and safety in hazmat routing is not only limited to road transportation mode. For example, Gordon and Young (2015) focused on hazmat trains to address the rules regulating the movement and handling of hazmats and explore the security of how the train hazmat routing information can be safeguarded while ensuring that first responders and affected communities have what is needed to address the risks and be able to effectively respond to incidents. In our research, we also consider a risk-averse strategy with the special focus on spreading risks in both space and time. Unlike Huang et al. (2003) who used a multi-attribute technique, we exploit a non-cooperative game theoretic approach. Moreover, Huang et al. (2004) used a meta-heuristic technique to solve their problem while we analytically model and solve our

problem.

Demon, covert attacks, and hazmat transportation: In this research, our game theoretic approach is based on imaginary demons playing the role of attackers. In game theory, there is a big difference between games between intelligent opponents and games against nature. The latter does not exclude win-win solutions but the former excludes these solutions. Imaginary demons in our game theoretic approach are responsible for implementing covert attacks, which is based on the worst-case situation in high-consequence-low-probability events in case of lack of sufficient historical data. In the literature, few scholars exploit such concept to connect hazmat and covert attacks. For instance, Yates (2008) introduced mathematical models based on the hypercube spatial queuing model for locating sensors within a large geographic region to detect covert attacks using hazmat vehicles; the models were tested on a case study within the region of Los Angeles County, California. Yates et al. (2011) considered two aspects in the protection of infrastructures from covert attacks: i) the optimal location of sensors to detect vehicles posing potential threats and ii) the sizing of the interception team and the placement of these resources on the network. Yates and Casas (2012) investigated how GIS can assist in a critical infrastructure protection problem. They considered a region, in which an attacker plans to attack multiple targets; the model helps the defender analyse the resource allocation strategy in the network. Yates et al. (2012) examined this resource allocation problem in an urban environment using a bi-level mixed integer and hypercube queuing model. In our paper, some imaginary demons may be considered to be those exploding the hazmat consignments or causing accidents; the number of demons is considered a known input. The more risk averse the model user is, the more number of demons are used in modeling. The model is developed based on a zero-sum game to exclude win-win situations.

Acyclic networks in hazmat routing: The hazmat routing scheduling problem in this research is based on acyclic networks. The requirement of acyclic network may seem restrictive. In the literature, many scholars including Klein (1991), Nozick et al. (1997), Meng et al. (2005), Bell (2006), and Szeto (2013) explicitly considered acyclic networks to model and solve such problems. While considering acyclic networks is one of our basic assumptions, our solution procedure proposed in the later part of this paper (which is used to deduce route flows from link flows) is not started with an acyclic network but we convert it to acyclic using a conversion that was originally designed for the connectivity test in the graph theory context. This conversion implicitly and partially applies the shortest travel distance criterion not allowing a hazmat vehicle to travel on a cycle going back to a node that has already been visited. To sum up, we can use a cyclic digraph as an input to the solution procedure but convert it to an acyclic network.

3. FORMULATIONS

In the section, we first define the concept of Space-Time Expanded Network (STEN) that helps us to formulate the study problem as a mixed system of equations and inequalities using route- and link-based approaches. We then prove the equivalent between route- and link-based problem, followed by the reformulation of the link-based mixed system of equations and inequalities into a VIP, an NCP, a UMP, and a FPP, and the discussion on their problem properties. The notations for the formulations are given in Table A in the appendix.

3.1. Space-Time Expanded Network Representation

Consider a connected base network $G = [N, A]$ with multiple OD pairs, where N is the set of nodes and A is the

set of directed links. The links represent road segments whereas the nodes represent intersections, the origins, or the destinations of hazmat shipments. These links and nodes may only be opened for certain time periods due to transportation policies. Based on this network, a space-time expanded network (STEN) $G' = [N', A']$ is constructed to capture T departure time choices as well as waiting choices of the problem, where N' and A' are respectively the set of nodes and directed links of the STEN. The STEN comprises n_o dummy origins, n_d dummy destinations, $(n_o + n_d)T$ dummy links, and T connected subgraphs G^t . Each connected subgraph represents the transportation network for any shipment of hazmats departing at a particular time t with each *travel link* in a subgraph corresponding to one link in the base network at that time. If the base network modeled does not change over time, each subgraph is the same as each other. Except G^T , each subgraph G^t is connected to G^{t+1} through *waiting links*, each of which represents a share of traffic for hazmat shipment waiting/stopping at a particular node for one period. Each origin r^t (destination s^t) in subgraph G^t is connected from (to) the corresponding dummy origin r^t (destination s^t) by one dummy link. The dummy links are used for modeling departure time choice. The special case is that the STEN has only subgraph (i.e., $T = 1$) with one origin and destination, which represents the pure routing problem with single OD pair as discussed in Bell (2006). In this case, the two dummy links can be removed.

The expanded network in this paper differs from the classical space-time network like the one in Yang and Meng (1998) as follows:

1. Travel links in this paper are horizontal whereas they are inclined in the classical space-time expanded network, because unlike the classical space-time expanded network, travel time is not explicitly considered in our network. In the later sections, using the concept of minimum spanning tree, we consider travel time in the expanded network prior to solving the hazmat routing-scheduling problem. However, we can easily modify the expanded network to incorporate travel time by assuming all travel links having the same travel time and by adding more nodes and travel links in the resulting network.
2. There is no queuing link in the expanded network. Waiting links can be considered to be queuing links but we do not use queuing theory techniques because the number of shipments/trucks dispatched by the shipment company compared with all other types of vehicles on a road transportation network is very small. Additionally, the problem is solved at the tactical level but queue length can be considered an operational issue.

An example of a base network with two OD pairs is given in Figure 1. The corresponding STEN considering two departure time choices (one for the daytime, one for the night time) is given in Figure 2, where the solid, dashed, and dash-dotted arrows represent travel, dummy, and waiting links, respectively. For the ease of reference, a^t is used to denote a link in the STEN. If a is not greater than the number of links in the base network $|A|$, $a^t \in A'$ is a travel link and corresponds to link a in the base network. If a is greater than the sum of the numbers of travel and waiting links, then $a^t \in A'$ is a dummy link. Otherwise, $a^t \in A'$ is a waiting link.

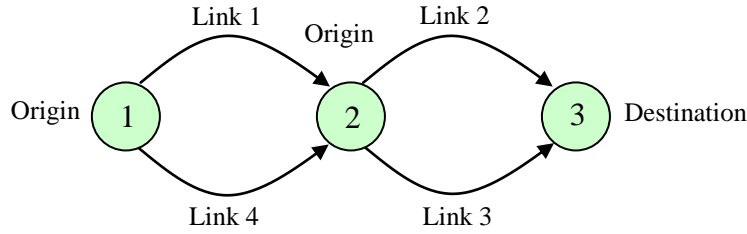


Figure 1. The base network.

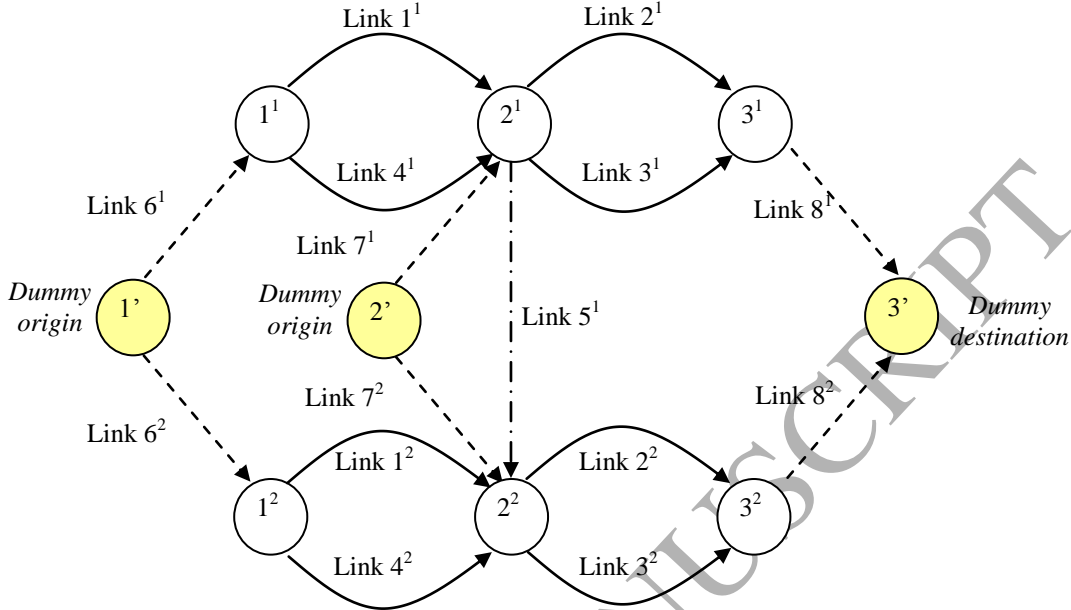


Figure 2. The time-expanded replica of the base network.

3.2. Route-based Formulation

The proposed integrated routing and scheduling problem involves three definitions: loss, expected loss, and total expected loss. *Loss (expected loss)* is defined as the number (expected number) of people affected in the event of accidents. *Expected loss* can be defined on the link, route, and network levels. The expected loss on a link (route) is the expected number of people affected in the events of accidents on that link (route). The sum of the expected loss on all links or routes gives the *total expected loss*. With these definitions, the proposed problem can be modeled as a non-cooperative game with two sub-problems, namely demon and dispatcher subproblems.

3.2.1. The Demon Subproblem

This subproblem has M demons. The number of demons M is a proxy of how risk averse a decision maker (e.g., a transport planner or a traffic manager) is. A more risk-averse decision maker can set a larger number of demons. Each demon is an imaginary evil entity that intentionally attacks a link to cause explosion on the link when a hazmat vehicle is on the link. Each demon has enough knowledge on all links, leading to the most number of fatalities and injuries when a particular link is selected. Each demon must cause an incident on one and only one link in the STEN. Two or more demons can cause incidents on the same link in the STEN. Therefore, each demon has $|A'|$ choices, and $|A'|^M$ link selection combinations or scenarios are possible. Each demon aims at seeking its link selection strategy to maximize its *expected pay-off* which numerically equals *total expected loss*. The expected payoff P can be mathematically formulated as follows:

$$P = \sum_{a'} \sum_k u_k c_{a'k}(\mathbf{v}), \quad (1)$$

where u_k is the probability of scenario k .

The scenario probability u_k is determined by the link selection strategy. Let $p_{l'_m}$ be the probability of demon m to cause an incident on link $l'_m \in A'$, and let $(l'_1, \dots, l'_m, \dots, l'_M)$ be the scenario where each demon m ($m=1, \dots, M$) causes an incident on a particular link $l'_m \in A'$. By assuming that all demons select their links independently, the probability of scenario $k = (l'_1, \dots, l'_m, \dots, l'_M)$ in (1) can be expressed in terms of $p_{l'_m}$ as

$$u_k = \prod_{m=1}^M p_{l'_m}. \quad (2)$$

In (1), $c_{a^t k}(\mathbf{v})$ is the loss of link $a^t \in A'$ in scenario k if the hazmat vehicle departs in time period t . The loss $c_{a^t k}(\mathbf{v})$ is a function of $\mathbf{v} = [v_{a^t}^q]$, where $v_{a^t}^q$ is the flow of class- q hazmats on link $a^t \in A'$, because the impact to the people highly depends on the flow magnitude and class of hazmats passing through $a^t \in A'$. The loss $c_{a^t k}(\mathbf{v})$ also depends on departure time period t as the human activity pattern is time-dependent. The loss is defined as

$$c_{a^t k}(\mathbf{v}) = c_{a^t, (l'_1, \dots, l'_m, \dots, l'_M)}(\mathbf{v}) = \begin{cases} 0 & a^t \neq l'_i, i=1, \dots, M, \\ c_{a^t}(\mathbf{v}) & \text{otherwise,} \end{cases} \quad (3)$$

where $c_{a^t}(\mathbf{v})$ is the worst case loss on link a^t if incidents occur on this link. The worst case loss $c_{a^t}(\mathbf{v})$ is the population inside a circle of a given impact radius, centered at any point on link $a \in A$, and the impact radius depends on hazmat class and its volume. Note that if $a^t \in A'$ is a dummy link, we have $c_{a^t}(\mathbf{v}) = c_{a^t k}(\mathbf{v}) = 0$ by definition because no population is around the link. If $a^t \in A'$ is a waiting link, the worst case loss $c_{a^t}(\mathbf{v})$ is the time average loss at node $a - |A| \in N$ between periods t and $t+1$ in scenario k . The population density of a node may be different from period t to $t+1$. That is why we consider the time average loss at the node between periods t and $t+1$. The time average concept should also be applied to a travel link when the change in population density is relatively large over the time spent on that link. We can set the damage equal to zero if the vehicle is waiting in a safe location where it is sufficiently far away from residential areas. Alternatively, without loss of generality, we can consider the loss on the waiting link as the maximum loss at the node between periods t and $t+1$.

By substituting (2) into (1), the payoff to each demon can then be written as follows:

$$P = \sum_{a^t} \sum_k u_k c_{a^t k}(\mathbf{v}) = \sum_k u_k \sum_{a^t} c_{a^t k}(\mathbf{v}) = \sum_{l'_1} \dots \sum_{l'_M} \left(\prod_{b=1}^M p_{l'_b} \right) \sum_{a^t} c_{a^t, (l'_1, \dots, l'_m, \dots, l'_M)}(\mathbf{v}).$$

Based on the above condition, we can derive the derivative $\frac{dP}{dp_{l'_m}}$ and let it be $\theta_{l'_m}$. Then,

$$\theta_{l'_m} = \sum_{l'_1=1}^n \dots \sum_{l'_b=1, b \neq m}^n \dots \sum_{l'_M=1}^n \left\{ \left(\prod_{b=1, b \neq m}^M p_{l'_b} \right) \left[\sum_{a^t} c_{a^t, (l'_1, \dots, l'_m, \dots, l'_M)}(\mathbf{v}) \right] \right\}, \quad (4)$$

which can be interpreted as the expected payoff to demon m when demon m causes an incident on link $l'_m \in A'$.

Let also

$$\pi^m = \max_{l'_m} \theta_{l'_m} \quad (5)$$

be the maximum expected payoff to demon m . The first-order Karush–Kuhn–Tucker (KKT) conditions of the

non-cooperative, link selection strategy game for the demon subproblem can then be written as the following nonlinear complementarity conditions:

$$p_{l'_m} \left\{ \pi^m - \theta_{l'_m} \right\} = 0, m = 1, \dots, M, l'_m = 1, \dots, |A'|, \quad (6)$$

$$\pi^m - \theta_{l'_m} \geq 0, m = 1, \dots, M, l'_m = 1, \dots, |A'|, \text{ and} \quad (7)$$

$$p_{l'_m} \geq 0, m = 1, \dots, M, l'_m = 1, \dots, |A'|. \quad (8)$$

According to (8), the link selection probability $p_{l'_m}$ can be positive or zero, depending on whether demon m causes an incident on a particular link $l'_m \in A'$. If demon m causes an incident on a particular link l'_m with some probability ($p_{l'_m} > 0$), then the term inside the braces in (6) must be zero and the maximum expected pay-off π^m to that demon must be equal to the expected payoff $\theta_{l'_m}$. If demon m does not cause an incident on link l'_m ($p_{l'_m} = 0$), then according to (7), the expected payoff to that demon must be not be greater than π^m .

The worst case loss $c_{a'}(\mathbf{v})$ is proposed to have the following form:

$$c_{a'}(\mathbf{v}) = \sum_q \beta_{a'}^q (v_{a'}^q)^{\alpha_{a'}^q}, \quad (9)$$

where $\alpha_{a'}^q > 0$ and $\beta_{a'}^q > 0$ are parameters associated with $v_{a'}^q$ in the loss function. When $a' \in A'$ is not used, the loss is zero. Moreover, the larger the value of $v_{a'}^q$, the greater the loss. Then, based on (1) and (3), condition (4) can be simplified as $\theta_{l'_m} = c_{l'_m}(\mathbf{v}) + \sum_{a' \neq l'_m} q_{a', -m} c_{a'}(\mathbf{v})$, where $q_{a', -m} = 1 - \prod_{i=1, i \neq m}^M (1 - p_{l'_i})$ is the probability of a' selected by at least one demon excluding demon m .

By the definition that each demon must cause an incident on one and only one link in the STEN, the link selection probability $p_{l'_m}$ must satisfy

$$\sum_{l'_m} p_{l'_m} - 1 = 0, m = 1, \dots, M. \quad (10)$$

3.2.2. The Dispatcher Subproblem

The dispatcher problem can be viewed as a non-cooperative game between n dispatchers in which each dispatcher is responsible for sending vehicles to transport one class of hazmats between an OD pair. Each dispatcher aims to select a route selection strategy in the STEN (which incorporates departure time choice, waiting time, and location choice in addition to route choice) to minimize his or her expected loss. The expected loss to each dispatcher can be expressed as

$$\eta_j^{rs_q} = \sum_{a'} \delta_{a'j} \sum_k u_k c_{a'k}(\mathbf{v}), \quad rs_q = 1, \dots, n, \forall j \in P^{rs_q}, \quad (11)$$

where $\eta_j^{rs_q}$ is the expected loss to dispatcher rs_q who selects route j . The notation P^{rs_q} is the route set for the flow of class- q hazmats between r' and s' in the STEN and is also the route set of dispatcher rs_q . The parameter $\delta_{a'j}$ is the link-route incidence indicator for the STEN. It equals 1 when link $a' \in A'$ is on route j between OD pair rs in the STEN and zero otherwise. Equation (11) states that the expected loss on a route is the sum of the

expected losses of each link on that route, $\sum_k u_k c_{a^t k}(\mathbf{v})$. Again, we assume no extra loss is induced if more than one incident occurs on the same link. Then, based on (3), we get $\sum_k u_k c_{a^t k}(\mathbf{v}) = q_{a^t} c_{a^t}(\mathbf{v})$, where

$q_{a^t} = 1 - \prod_{m=1}^M (1 - p_{t^m})$ is the probability of a^t selected by at least one demon.

Let $h_j^{rs_q}$ be the flow of class- q hazmats on route $j \in P^{rs_q}$, and

$$\phi^{rs_q} = \min_j \eta_j^{rs_q} \quad (12)$$

be the minimum expected loss between OD pair rs for class- q hazmats, which is also the minimum expected loss to dispatcher rs_q . The necessary and sufficient conditions of the non-cooperative route selection strategy game for the dispatcher subproblem can then be formulated as

$$h_j^{rs_q} \{ \eta_j^{rs_q} - \phi^{rs_q} \} = 0, rs_q = 1, \dots, n, \forall j \in P^{rs_q}, \quad (13)$$

$$\eta_j^{rs_q} - \phi^{rs_q} \geq 0, rs_q = 1, \dots, n, \forall j \in P^{rs_q}, \text{ and} \quad (14)$$

$$h_j^{rs_q} \geq 0, rs_q = 1, \dots, n, \forall j \in P^{rs_q}. \quad (15)$$

These conditions imply that if dispatcher rs_q selects j for shipment, the expected loss to the dispatcher must equal its minimum expected loss, and not be greater than the expected loss when the dispatcher selects any other routes.

In conditions (13)-(15), the route flow $h_j^{rs_q}$ must satisfy the following flow conservation condition:

$$\sum_j h_j^{rs_q} = d^{rs_q}, \forall rs_q, \quad (16)$$

where d^{rs_q} is the demand for transporting class- q hazmats between OD pair rs . In addition, the route flow $h_j^{rs_q}$ relates to the flows of class- q hazmats on link a^t by

$$v_{a^t}^{rs_q} = \left(\sum_j \delta_{a^t j} h_j^{rs_q} \right), \forall rs_q, a^t, \text{ and} \quad (17)$$

$$v_{a^t}^q = \sum_{rs} v_{a^t}^{rs_q}, \forall q, a^t, \quad (18)$$

where $v_{a^t}^{rs_q}$ denotes the flows on link a^t due to dispatcher rs_q .

3.2.3. The Proposed Integrated Routing and Scheduling Problem

The proposed integrated routing and scheduling problem is to find $[p_{t^m}]$ and $[h_j^{rs_q}]$ to simultaneously satisfy (1)-(18). This route-based problem has two properties as stated below:

Proposition 1: *All the demons must have the same maximum expected payoff for any solution to the problem (1)-(18).*

Proposition 2: *If the allowable route sets for all classes of hazmat shipment between the same OD pair are the same, the lowest expected loss routes for these classes are the same and the corresponding dispatchers receive the same expected loss.*

Their proofs are given in the Appendix. \square

3.3. Basic Link-Based Formulation

The route selection probabilities obtained from the route-based formulation can also give useful information to dispatchers such as how to choose routes, departure times, intermediate stopping locations, and the stopping duration to transport hazmats. However, the route-based formulation explicitly requires a complete route set for each dispatcher in the dispatcher subproblem. This requirement is not attractive for large networks because it requires either 1) exhaustive and time-consuming route enumeration to generate a complete route set during solution process in order to ensure convergence but the route set can be very large even for a medium network or 2) a column generation heuristic to determine a smaller route set to solve the route-based problem but the convergence is not guaranteed. Therefore, the dispatcher problem is reformulated via the link-based approach.

We reformulate equations (16)-(17) as

$$\sum_{a' \in O(z^t)} v_{a'}^{rs_q} - \sum_{b' \in I(z^t)} v_{b'}^{rs_q} - Q_{z^t}^{rs_q} = 0, \forall rs_q, z^t, \quad (19)$$

where $Q_{z^t}^{rs_q} = \begin{cases} -d^{rs_q}, & \text{if } z^t = s', \\ 0, & \text{otherwise,} \end{cases}$ the notation $O(z^t)$ denotes the set of outbound links emanating from node

$z^t \in N'$; the notation $I(z^t)$ denotes the set of inbound links feeding into node z^t . Note that the flow conservation equations at dummy origins are not required as they are redundant.

We also let

$$\phi_{a'}^{r'q} = \sum_k c_{a'k}(\mathbf{v}) u_k - [\phi^{r'y,q} - \phi^{r'x,q}], \forall a' = (x, y) \in A'_{r'q}, \forall r' \in N', \forall q, \quad (20)$$

where $x \in N'$ and $y \in N'$ are the entry and exit nodes of link $a' \in A'$, respectively, and $A'_{r'q}$ is the link set for class- q hazmats from dummy origin r' . The notation $\phi^{r'y,q}$ represents the lowest expected loss for class- q hazmat flow from r' to y and $\phi^{rs,q} = \phi^{rs_q}$. The first term in (20) is the expected loss in the event of incidents on link a' and the square bracket term is the lowest expected loss for class- q hazmat flow from r' through x to y . The variable $\phi_{a'}^{r'q}$ can then be interpreted as the difference between the expected loss on link a' (directly connecting x and y) and the minimal expected loss for class- q hazmat flow from r' through x to y .

With (20), we can express the dispatcher choice conditions as follows:

$$v_{a'}^{rs_q} \phi_{a'}^{r'q} = 0, \forall rs_q, q, r', a', \quad (21)$$

$$\phi_{a'}^{r'q} \geq 0, \forall r', q, a', \text{ and} \quad (22)$$

$$v_{a'}^{rs_q} \geq 0, \forall rs_q, a'. \quad (23)$$

Conditions (21)-(23) mean that when link a' is used by class- q hazmat flow from r' , link a' must be on the minimal expected loss route from r' to the exit node of link a' . These conditions are equivalent to conditions (13)-(15) as stated below.

Proposition 3: *The link-based dispatcher choice conditions (21)-(23) are equivalent to the route-based dispatcher choice conditions (13)-(15) in terms of the maximum expected payoff to each demon.*

Proof: See the Appendix. \square

The proposed link-based integrated routing and scheduling problem is to determine $\left[p_{l'_m} \right]$ and $\left[v_{a'}^{rs_q} \right]$ to simultaneously satisfy conditions (1)-(10), (18)-(23) that form a *mixed system of equations and inequalities*. This link-based problem is equivalent to the route-based problem (1)-(18):

Proposition 4: The basic link-based problem (1)-(10), (18)-(23) is equivalent to the route-based problem (1)-(18).

Proof: See the Appendix. \square

3.4. Alternative Link-Based Formulations and Solution Properties

The link-based problem (1)-(10), (18)-(23) is reformulated into a nonlinear complementarity problem (NCP), an unconstrained minimization problem (UMP), a variational inequality problem (VIP), and a fixed point problem (FPP) to allow examining the properties of the proposed problem (1)-(18) and solving the link-based problem (1)-(10), (18)-(23) via existing efficient solution methods for NCPs, UMPs, VIPs, and FPPs. In all these reformulations, both $\phi^{r'z,q}$ and π^m are treated as additional decision variables, but in the basic formulation (1)-(10), (18)-(23), both $\phi^{r'z,q}$ and π^m are functions of decision variables $\left[p_{l'_m} \right]$ and $\left[v_{a'}^{rs_q} \right]$.

3.4.1. Nonlinear Complementarity Problem Formulation

The link-based problem can be reformulated as an NCP to determine a solution \mathbf{y}^* such that

$$\mathbf{y}^* \geq \mathbf{0}, \mathbf{H}(\mathbf{y}^*) \geq \mathbf{0}, \text{ and } \mathbf{y}^{*T} \cdot \mathbf{H}(\mathbf{y}^*) = 0, \quad (24)$$

where \mathbf{y} and $\mathbf{H}(\mathbf{y})$ are defined by

$$\mathbf{y} = \begin{bmatrix} v_{a'}^{rs_q}, \forall rs_q, a' \\ p_{l'_m}, \forall m, l'_m \\ \hat{\phi}^{rs_q z}, \forall rs_q, z / r' \\ \pi^m, \forall m \end{bmatrix}, \mathbf{H}(\mathbf{y}) = \begin{bmatrix} \psi_{a'}^{rs_q}, \forall rs_q, a' \\ \pi^m - \theta_{l'_m}, \forall m, l'_m \\ \sum_{a' \in \mathcal{O}(z')} v_{a'}^{rs_q} - \sum_{b' \in \mathcal{I}(z')} v_{b'}^{rs_q} - Q_{z'}^{rs_q}, \forall rs_q, z' / r' \\ \sum_{l'_m} p_{l'_m} - 1, \forall m \end{bmatrix}, \quad (25)$$

$$\hat{\phi}^{rs_q z} = \phi^{r'z,q}, \forall rs_q, \forall z \in N', \text{ and} \quad (26)$$

$$\psi_{a'}^{rs_q} = \phi_{a'}^{r',q}, \forall rs_q, a', \quad (27)$$

where $\theta_{l'_m}$ and $\phi_{a'}^{r',q}$ are defined by (4) and (20), respectively.

Proposition 5: The NCP (24)-(27) is equivalent to the link-based problem (1)-(10), (18)-(23).

The proof is given in the Appendix. The above proposition implies that solving the NCP (24)-(27) is equivalent to solving the link-based problem (1)-(10), (18)-(23). Hence, the existing solution methods for NCPs can be used for obtaining solutions to the link-based problem.

3.4.2. Unconstrained Minimization Problem Formulation

The NCP (24)-(27) can also be transformed to a UMP:

$$\min_{\mathbf{y}} G(\mathbf{y}) = \frac{1}{2} \sum_i \left[\sqrt{(y_i^2 + H_i(\mathbf{y})^2)} - (y_i + H_i(\mathbf{y})) \right]^2, \quad (28)$$

where y_i and $H_i(\mathbf{y})$ are respectively the i -th element of \mathbf{y} and $\mathbf{H}(\mathbf{y})$ defined by conditions (25)-(27). The properties of the UMP are stated in Propositions 6-8.

Proposition 6: The global minimum of the UMP (25)-(28) is zero.

Proof: The sum of squares must be non-negative so the minimum objective value is zero. \square

Proposition 7: The UMP (25)-(28) is equivalent to the NCP (24)-(27) and hence the link-based problem (1)-(10), (18)-(23).

Proof: See the Appendix. \square

Proposition 8: If $c_{a'k}(\mathbf{v})$ is smooth, then the UMP (25)-(28) is smooth.

Proof: If $c_{a'k}(\mathbf{v})$ is smooth, then $G(\mathbf{y})$ is smooth because the sum of smooth functions is smooth. \square

The implication of the above propositions is that if $c_{a'k}(\mathbf{v})$ is smooth, derivative-based methods can be used for solving the optimization problem (25)-(28) and hence the link-based problem (1)-(10), (18)-(23). Furthermore, if a local optimization method is used, we need to ensure whether the objective value is zero. If not, another initial solution should be used until a zero objective value is achieved.

3.4.3. Variational Inequality Problem Formulation

The NCP (24)-(27) is equivalent to the following VIP. Find \mathbf{y}^* such that

$$(\mathbf{y} - \mathbf{y}^*)^T \mathbf{H}(\mathbf{y}^*) \geq 0, \quad \forall \mathbf{y} \in R_+^\omega, \quad (29)$$

where \mathbf{y} and $\mathbf{H}(\mathbf{y})$ are defined by conditions (25)-(27); $\omega = (n + M)|A| + n|N'| - n_o + M$.

Proposition 9: The VIP (25)-(27), (29) is equivalent to the NCP (24)-(27) and the link-based problem (1)-(10), (18)-(23).

Proof: This follows directly from Proposition 1.4 in Nagurney (1999) and Proposition 5. \square

Proposition 10: A solution exists to the VIP (25)-(27), (29) and the link-based problem (1)-(10), (18)-(23).

Proof: See the Appendix. \square

The above two propositions imply that a solution exists to the proposed route-based problem (1)-(18) and the NCP (24)-(27). The solution is a Nash equilibrium one. Because the mapping function $\mathbf{H}(\mathbf{y})$ is not strictly monotone in general, solution uniqueness is not guaranteed.

3.4.4 Fixed Point Formulation

The VIP (25)-(27), (29) can be rewritten as following fixed point problem (FPP): Find \mathbf{y}^* such that

$$\mathbf{y}^* = \mathbf{Y}(\mathbf{y}^*), \quad (30)$$

where $\mathbf{Y}(\mathbf{y})$ represents a general vector function.

Proposition 11: If $\mathbf{Y}(\mathbf{y}) = \mathbf{P}_{R_+^\omega}(\mathbf{f} - \kappa \mathbf{H}(\mathbf{y}))$, where the projection operator $\mathbf{P}_{R_+^\omega}(\mathbf{y}) = \arg \min_{\mathbf{z} \in R_+^\omega} \|\mathbf{y} - \mathbf{z}\|$, $\kappa > 0$, then the FPP (30) and the VIP (25)-(27), (29) have the same set of solutions.

Proof: This follows directly from Proposition 1.3 in Nagurney (1999) and Proposition 9. \square

4. SOLUTION APPROACHES TO LINK-BASED FORMULATIONS

This paper proposes to firstly solve one of the link-based formulations by existing solution methods and then

deduce route flows from link flows by our proposed route flow extraction algorithm. This leads to two approaches:

- 1) One method is to solve one of the alternative link-based formulations in section 3.4 to firstly obtain $\left[v_{a^t}^{rs,q*} \right]$, $\left[P_{l_m^*} \right]$, $\left[\phi^{r'z,q} \right]$, and $\left[\pi^m \right]$ by existing solution methods and then deduce route flows $\left[h_j^{rs,q*} \right]$ from link flows $\left[v_{a^t}^{rs,q*} \right]$ by the route-flow extraction algorithm.
- 2) Another method is to directly solve the basic link-based mixed system of equations and inequalities to obtain $\left[v_{a^t}^{rs,q*} \right]$ and $\left[P_{l_m^*} \right]$ by a nonlinear optimization algorithm with an embedded recursive dynamic algorithm for calculating $\phi^{r'y,q}$, and then deduce route flows $\left[h_j^{rs,q*} \right]$ from link flows $\left[v_{a^t}^{rs,q*} \right]$ by the route-flow extraction algorithm.

Both solution approaches are very attractive especially when the final route set selected by each dispatcher is very small compared with its complete route set. Note that in the NCP and other alternative formulations, the minimal expected loss $\hat{\phi}^{rs,qz}$ is treated as a decision variable and is not obtained from the recursive dynamic algorithm; in the basic link-based mixed system of equations and inequalities, the minimal expected loss $\hat{\phi}^{rs,qz}$ is a function of $\left[v_{a^t}^{rs,q*} \right]$ and $\left[P_{l_m^*} \right]$, and is obtained from the recursive dynamic algorithm.

4.1. Route-Flow Extraction Algorithm

The route-flow extraction algorithm can be used in any *acyclic* STENs. The method first decomposes the problem of the determination of route flows by OD pair and hazmat class. For each class in each OD pair, the method first finds out a route comprising the links with non-zero link flows $v_{a^t}^{rs,q}$ in the STEN, and set the route flow to be equal to the minimum of all link flows $v_{a^t}^{rs,q}$ of the links on this route. The algorithm then updates all link flows $v_{a^t}^{rs,q}$ on this route by deducting the route flow from each of these link flows, records the order of links to be visited, and deduces the departure time. Based on the updated link flows $v_{a^t}^{rs,q}$, this algorithm seeks another positive flow route for class- q hazmats between the subject OD pair in the STEN. This procedure is repeated until all $v_{a^t}^{rs,q}$ on the dummy links are zero.

The detailed algorithmic procedure is as follows:

- Step 0: Select an OD pair and a hazmat class.
- Step 1: Set $j = 0$ and $v_{a^t}^{rs} = v_{a^t}^{rs*}, \forall a^t$.
- Step 2: If $v_{a^t}^{rs,q}$ on all dummy links emanating from r' equal zero, go to Step 9.
- Step 3: Set the current node to be r' .
- Step 4: Set $j = j + 1$, $h_j^{rs,q} = d^{rs,q}$, and the list R_j containing the links composing the current route j to be empty.
- Step 5: If the current node is s' , set $v_{a^t}^{rs,q} = v_{a^t}^{rs,q} - h_j^{rs,q}, \forall a^t \in R_j$ and go to Step 2.
- Step 6: Select any link $a^t \in A'$ emanating out from the current node with a non-zero link flow $v_{a^t}^{rs,q}$. Put link a^t at the end of the list R_j .

Step 7: If $v_{a^t}^{r's_q} < h_j^{r's_q}$, set $h_j^{r's_q} = v_{a^t}^{r's_q}$.

Step 8: Set the current node to be the exit node of link a^t . Go to Step 5.

Step 9: Repeat Steps 0-8 until all classes of hazmats for all OD pairs are selected.

In Steps 4 and 6 of the developed algorithm, the link selection rule determines the final used route set for a given class of hazmats' route flows between the subject OD pair. If the link selection rule is random, for each execution, the procedure can generate different used route sets and also different route flows from the same set of initial link flows. However, if the selection rule is deterministic and according to a specific principle, there is a one-to-one relationship between the given link flows and the resultant route flows. The selection rule can be based on the largest link flows, the alphabetical order of links, or a combination of them.

The time complexity is $O(nT|N'|)$, where $O(|N'|)$ is the time complexity of one route building iteration. One route-building iteration is defined by Steps 5-8, the steps for building a route from dummy origin r' to dummy destination s' . During a route-building iteration, the following two cases cannot be happened: 1) At an intermediate node, no link is available for selection, and 2) the same node is visited more than one. As vertex conservation is ensured throughout the algorithm (by Step 5 and the initial link flows), once a link except the dummy link connected to s' is selected, at least one link with non-zero flow is available for selection during a route-building iteration. Moreover, acyclic graphs rule out the case of visiting a node more than once within one iteration. Hence, a route must be able to be built within each route-building iteration.

According to time complexity $O(nT|N'|)$, it is clear that more time periods in the time span (i.e., larger T value), more nodes in the STEN, and more number of dispatchers lead to longer computation time.

4.2. Recursive dynamic algorithm

One of the issues in solving the mixed system of equations and inequalities is the calculation of $\phi^{r'y,q}$ whose value is a function of $[p_{i_m}^{r'q}]$ and $[v_{a^t}^{r's_q}]$. To tackle this issue, we suggest exploiting the concept of *dynamic programming* using the following recursive equations:

$$\mathbf{Initiation:} \quad \phi^{r'y,q} = 0 \quad (r', y) \in A'_{r'q}, \forall r' \in N', \forall q. \quad (31)$$

This is for the arcs directly outgoing from r' (the only dummy origin). Naturally, the lowest expected losses for the arcs coming out of the dummy origin (which are actually dummy links) is zero. Then, the following recursive equations can be utilized:

$$\mathbf{Recursive equation:} \quad \phi^{r'y,q} = \underset{x}{\text{Min}} \{ \phi^{r'x,q} + \sum_k c_{a^t_k}(\mathbf{v}) u_k \}; \forall a^t = (x, y) \in A'_{r'q}, \forall r' \in N', \forall q \quad (32)$$

It is similar to Dijkstra's Algorithm and takes $O(|N'|^2)$ time. The equations (31)-(32) will be used in section 6.1 to solve our real-life case problem.

5. NUMERICAL STUDY

To illustrate the route-flow extraction algorithm and properties of the problem, numerical studies are carried out. In these studies, the network adopted is the one described in section 2 (see Figure 2). Four classes of hazmat flows are considered: Class-1 and -2 hazmat flows between OD pair (1,3), and Class-1 and -3 hazmat flows between OD pair (2,3). They are allowed to use any link with the following exceptions: Class-3 hazmat flow is not allowed to pass through link 2 whereas class- 1 and -2 hazmat flows are not allowed to pass through link 3. The parameters adopted

in these studies are as follows:

(a) Demands: $d^{13_1} = d^{13_2} = 100$ vph; $d^{23_1} = d^{23_2} = 50$ vph.

(b) Loss functions: $\alpha_{a'}^q = 1, \forall a', q$, $\alpha_{a'}^q > 0$; $\beta_1^q = 10$, $\beta_2^q = 5, \forall q$; $\beta_2^q = 25$, $\beta_2^q = 25, q = 1, 2$; $\beta_3^q = 100$, $\beta_3^q = 100, q = 3$; $\beta_4^q = 10, \beta_4^q = 12, \forall q$; $\beta_5^q = 20, \forall q$; $\beta_a^q = \beta_{a'}^q = 0, \forall q, a = 6, 7, 8$.

Three cases are examined: $M = 1$, $M = 2$, and $M = 3$. The problem in each case assumes that no extra loss is induced if more than one incident occurs on the same link. Each problem is written in an unconstrained optimization problem format and was solved by SOLVER. SOLVER stopped when the objective value $G(\mathbf{y})$ was very close to zero.

Tables 1-3 show the results for all the three cases. One can easily verify that for each case, the result satisfies flow conservation at each node, the first-order optimality conditions for the demon and dispatcher subproblems, and the definitional constraint for link selection probabilities. For example, in Table 1, the sum of class-1 flows on links 6^1 and 6^2 equals the demand of 100 vph. In Table 2, we can see that when the demon selects a link to cause an incident with some probability, the corresponding payoff must be the largest. Moreover, the selected link must have a non-zero expected loss as shown in Table 1, which equals the difference between the lowest expected losses at the entry and exit nodes of that link. For instance, the lowest expected loss at the entry and exit nodes of link 2^1 are, respectively, 0 and 1562.5 according to Table 3. Their difference equals the expected loss on link 2^1 as shown in Table 1. Furthermore, from Table 2, we can see that the sum of link selection probabilities of a demon equals one. In addition, according to Table 2, even though we allow two or more demons selecting the same link for causing incidents on it, in the solution, such case will not happen, because the loss associated with a link due to multiple attacks by different demons is set to be the same as the loss due to single attack by one demon.

Table 1. Loss, expected loss, and flow on each link.

Link	Loss for all three cases	Expected loss			Flow for all three classes				
		$M=1$	$M=2$	$M=3$	Class 1 OD (1,3)	Class 3 OD (2,3)	Class 2 OD (1,3)	Class 1 OD (2,3)	
Travel or waiting links	1^1	500	0	0	0	25		25	
	2^1	3125	1562.5	3125	3125	50		50	25
	3^1	2500	0	0	1250		25		
	4^1	500	0	0	0	25		25	
	5^1	0	0	0	0	0	0	0	0
	1^2	250	0	0	0	25		25	
	2^2	3125	1562.5	3125	3125	50		50	25
	3^2	2500	0	0	1250		25		
	4^2	600	0	0	0	25		25	
	Dummy links	6^1	0	0	0	0	50		50
7^1		0	0	0	0		25		25
8^1		0	0	0	0	50	25	50	25
6^2		0	0	0	0	50		50	
7^2		0	0	0	0		25		25
8^2		0	0	0	0	50	25	50	25

Table 2. Link selection probability and payoff.

Link	$M=1$		$M=2$				$M=3$					
	Selection prob.	Payoff	Selection prob.		Payoff		Selection prob.			Payoff		
			Demon 1	Demon 2	Demon 1	Demon 2	Demon 1	Demon 2	Demon 3	Demon 1	Demon 2	Demon 3
1^1	0	0	0	0	3625	3625	0	0	0	6125	6125	6750
2^1	0.5	1562.5	1	0	6250	3125	1	0	0	8750	5625	6250
3^1	0	0	0	0	5625	5625	0	0	0.5	6875	6875	8750
4^1	0	0	0	0	3875	3875	0	0	0	6125	6125	6750
5^1	0	0	0	0	3625	3625	0	0	0	5625	5625	6250
1^2	0	0	0	0	3250	3250	0	0	0	6125	6125	6750
2^2	0.5	1562.5	0	1	3125	6250	0	1	0	5625	8750	6250
3^2	0	0	0	0	5625	5625	0	0	0.5	6875	6875	8750
4^2	0	0	0	0	3725	3725	0	0	0	6225	6225	6850
	max	1562.5		max	6250	6250		max	8750	8750	8750	

Table 3. Lowest expected costs from dummy origins to nodes.

	Node	$M=1$			$M=2$			$M=3$		
		Class 1	Class 2	Class 3	Class 1	Class 2	Class 3	Class 1	Class 2	Class 3
OD pair (1,3)	1 ¹	0	0		0	0		0	0	
	2 ¹	0	0		0	0		0	0	
	3 ¹	1562.5	1562.5		3125	3125		3125	3125	
	1 ²	0	0		0	0		0	0	
	2 ²	0	0		0	0		0	0	
	3 ²	1562.5	1562.5		3125	3125		3125	3125	
	3 ³	1562.5	1562.5		3125	3125		3125	3125	
OD pair (2,3)	2 ¹	0		0	0		0	0		0
	3 ¹	0		1562.5	0		3125	1250		3125
	2 ²	0		0	0		0	0		0
	3 ²	0		1562.5	0		3125	1250		3125
	3 ³	0		1562.5	0		3125	1250		3125

Expected losses on dummy links are zero (see Table 1) as the loss is assumed to be zero on each of these links. These links must not be selected by demons as selecting these links would not increase their payoffs. When the number of demons is greater than 1, the maximum payoff to each demon is the same as shown in Table 2, which agrees with Proposition 1. The number of links selected by demons is non-decreasing with the number of demons adding to the network as reflected in Table 2. When M equals 1 or 2, the number of links selected is two. When $M=3$, the number of links selected is four. The reason is also follows. According to the base network, link 2 is the only route to destination 3 for flows from node 1, and is used by most classes of hazmats (or by class-1 and -3). Therefore, links 2¹ and 2² must be selected when $M=1$. When one more demon is introduced (i.e., $M=2$), both links are selected with certainty so as to maximize the payoff to each of the two demons and therefore the number of link selected remains unchanged. When another demon is introduced (i.e., $M=3$), links 3¹ and 3² are also selected as the impact of an accident on these links to people is very large according to the loss parameters $\beta_{3^1}^q$ and $\beta_{3^2}^q$.

Although the number of links selected can remain unchanged after introducing one more demon, the expected payoff must be increased. Indeed, from Table 2, we can observe that the maximum expected payoff increases with the number of demons involved. This is expected as more incidents can be occurred in the network. This raises the question of how many demons should be introduced to the network. The number of demons is actually a proxy of the maximum number of simultaneous incidents associated with hazmat shipment in the network. A more risk-averse decision maker can use a larger number of demons. Without a deep analysis to this question, we suggest using a maximum historical number. According to Incident Reports Database Search of PHMSA (Office of Hazardous Materials Safety) (<https://hazmatonline.phmsa.dot.gov/IncidentReportsSearch/IncrSearch.aspx>), it is not very likely to have more than two hazmat incidents simultaneously. Therefore, considering a maximum of two demons is sufficient for the purposes of planning the worst case situation.

Table 3 also illustrates the effect of route sets on the lowest expected loss. According to Table 3, for OD pair (2,3), the lowest expected costs for class-1 and -3 hazmats from dummy node 2' to node 3¹ are different. This is because links 3¹ and 3² are not allowed to be used by class-1 and -3 hazmats. Should one of the two classes were allowed to use these links, the lowest expected cost for class-1 (class-3) hazmats would increase (decrease) but the lowest expected costs of the two classes from dummy node 2' to node 3¹ would be the same. The same argument applies at node 3² and dummy node 3'.

The solutions given in Tables 1-3 are not the only solutions to the link-based problem. Solutions to the problem are not unique in terms of link selection probabilities, link flows, and maximum expected payoffs. For simplicity, we consider $M=2$. The two demons exchange their selections but the link flows follow those in Table 1. The new maximum expected payoff for each demon is still 6250. Alternatively, we can obtain the same maximum expected

payoff under the link selection probabilities described by Table 2 if the flows on links 1^2 and 6^2 are all reduced by one unit and the flows on links 1^1 , 5^1 , and 6^1 all increase by one unit. This is because those links are the low impact links and must not be selected by demons, leading to zero expected losses on these links before and after flow adjustment. The third example for $M = 2$ is that both demons 1 and 2 selects both links 2^1 and 2^2 with equal probability but the link flows follow the ones in Table 1. In this situation, the maximum payoff is reduced to 4687.5. This suboptimal result is due to the lack of coordination between the two demons, and may not be useful for risk-averse decision makers who strongly believe that the attackers are cooperative. These decision makers normally consider the worst-case situation to make the most risk-averse decision. To avoid suboptimal results, one should try more different initial solutions to obtain different solutions and pick the solution with the largest payoff. Alternatively, one can develop a bi-level model which aims at finding the most risk-averse solution or maximizing the payoff to each demon or attacker. This is left to future research.

To generate route flows, the developed route-flow extraction algorithm together with the alphabetical-order link-selection rule are adopted. This algorithm was written in Fortran and used to generate routes for class-1 hazmats between OD pair (1,3) when $M = 3$. This sub-problem has 11 links (i.e., 11 link flow variables) and 8 nodes, and could be solved in less than 0.001 second by a Laptop with Window 7 Professional, 8.00 GB RAM, and an Intel(R) Core(TM) i7 2640M-M CPU@ 2.80 GHz. The procedure is illustrated in Figure 3. The thickened arrows represent the route considered in each iteration. The number next to each link is the corresponding link flows. As we can see, for each iteration, one route is built. The route flow is the minimum of all link flows on this route. The link flows are updated by subtracting the route flow from them. Consequently, in the following iteration, at least one link is removed from consideration. In this example, four iterations are required and four routes are generated. The results are summarized in Table 4.

According to Table 4, one can see that the route flows satisfy the optimality conditions (13)-(15). Moreover, one link on each route is selected by a demon (Its link number is in bold face). If these links were removed, the subgraph for class-1 hazmats would be disconnected. These imply that the links selected by demons form a cut set for at least one type of hazmats transported between one OD pair, in which a cut set is a set of links whose deletion would be sufficient to disconnect the origin from the destination in a strongly connected network.

In fact, more than one link on a route can be selected by demons. For example, if $\beta_{3^1}^q = \beta_{3^2}^q = \beta_{4^2}^q, \forall q$ were reduced to 10, two links would be selected by demons on each route. At least one link on each route is selected in Table 4 because in this example, there is no route with $\beta_{d^q}^q$ of all links on this route to be zero. If there were such a route, all dispatchers would select that route because there would be no people affected in the event of an incident along that route.

The travel links on different routes can correspond to the same set of links in the base network. For instance, the travel links on routes 1 and 3 correspond to links 1 and 2 in the base network. However, the links selected by a demon on these routes can be different (Szeto, 2013). This can occur because the number of people affected along these routes depends on time of day, which is related to departure time. This implies that the potential location of an incident on a route depends on departure time.

Minimum link flow = 25 vph

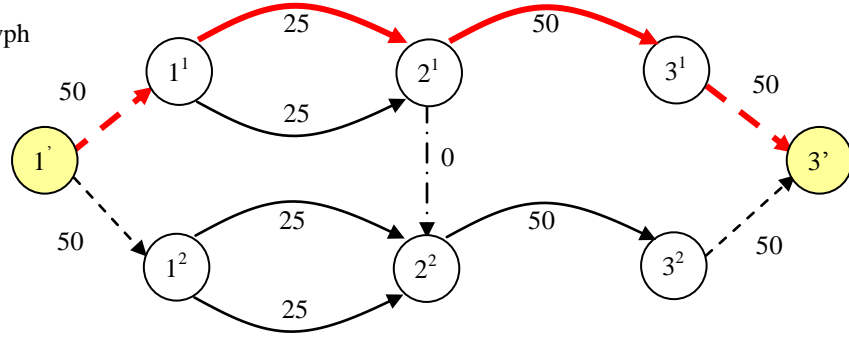


Figure 3a. Route 1

Minimum link flow = 25 vph

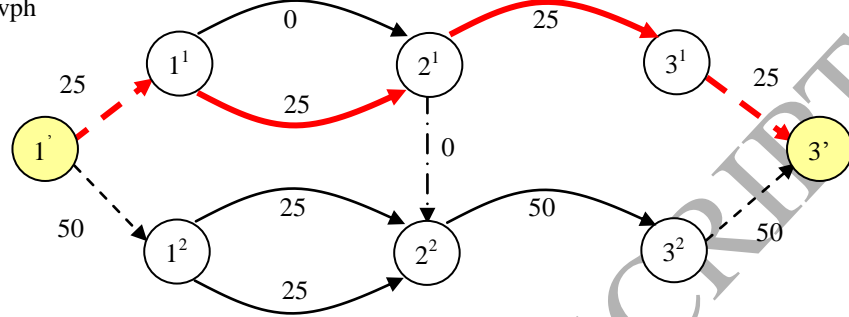


Figure 3b. Route 2

Minimum link flow = 25 vph

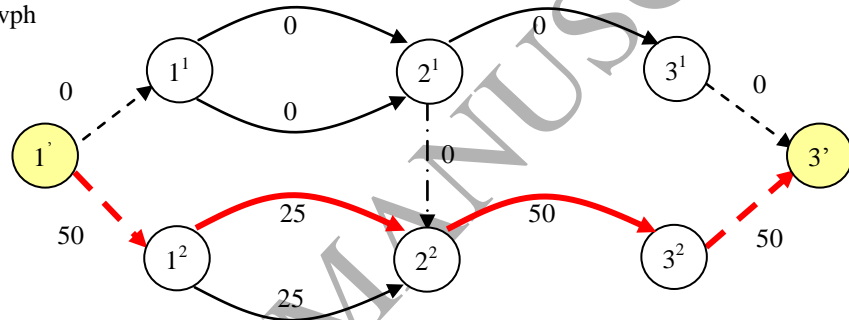


Figure 3c. Route 3

Minimum link flow = 25 vph

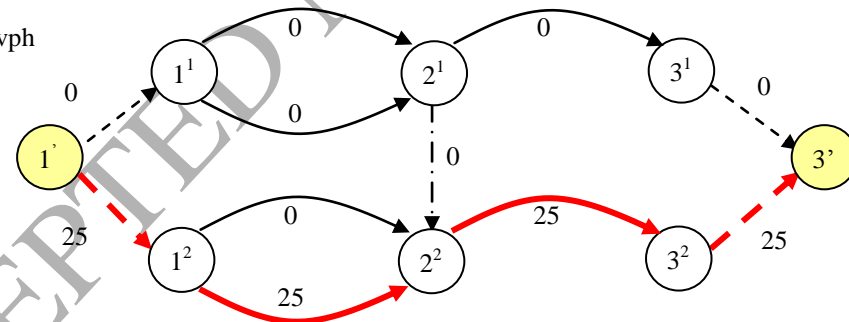


Figure 3d. Route 4

Figure 3. Illustration of the procedure of finding routes and their route flows for class-1 hazmats between OD pair (1,3).

Table 4. Routes, their flows, and their optimality conditions when $M = 3$.

Route j	Link sequence	$h_j^{13_1}$	$\eta_j^{13_1}$	ϕ^{13_1}	$h_j^{13_1} \{ \eta_j^{13_1} - \phi^{13_1} \}$
1	$6^1, 1^1, 2^1, 8^1$	25	3125	3125	0.00
2	$6^1, 4^1, 2^1, 8^1$	25	3125	3125	0.00
3	$6^2, 1^2, 2^2, 8^2$	25	3125	3125	0.00
4	$6^2, 4^2, 2^2, 8^2$	25	3125	3125	0.00

6. COMPUTATIONAL RESULTS AND INSIGHTS

In this section, we actually solved the mixed system of equations and inequalities (1)-(10), (18)-(23) rather than NCP (24). Solving this mixed system of equations and inequalities requires the recursive-dynamic algorithm (31)-(32) to obtain the minimal expected loss $\phi^{r^y, q}$ whose is a function of $[p_{t_m}^r]$ and $[v_{a'}^{rs, q}]$. The main objective of

this section is to present the insights of the studied problem. The computational speed of the solution method used and the specification of the original link-based model (1)-(10), (18)-(23) are also discussed.

6.1. Specification for the Link-based Mixed System of Equations and Inequalities

Among our formulations, we chose to solve the link-based mixed system of equations and inequalities (1)-(10), (18)-(23) for realistic applications because it does not have any objective function and a feasible solution to the system can be found in a very short time. The following is the size specification of the STEN: number of travel arcs = $T \times |A|$; number of waiting links = $(T-1) \times |N|$; number of dummy links = $(n_o + n_d) \times T$; total number of arcs $|A'| = (T \times |A|) + ((T-1) \times |N|) + ((n_o + n_d) \times T)$, and the number of nodes in the STEN $|N'| = (T \times |N|) + n_o + n_d$. The number of decision variables in the problem equals the sum of the following:

- The number of continuous variables $v_{a'}^{rsq} : n \times |A'|$
- The number of continuous variables $p_{l'_m} : M \times |A'|$

From the above, it is clear that more time periods in the time span considered leads to a larger problem and more decision variables as there are more arcs in the STEN.

6.2. Test Instances and Computational Speed

To illustrate the computational efficiency of the solution strategy, various tested instances with different problem sizes and parameter values were created and solved. For the test problem size in the literature of hazmat routing and scheduling, Erkut and Alp (2007) solved their problems up to 138 nodes and 368 arcs. Our problem sizes were up to 180 nodes and 500 arcs. Different parameter values were set: $M = 1, 2, 3$; $T = 1, 2, 3, 4, 5$; $n_o = 1, 2, 3$; $n_d = 1, 2, 3$; $Q = 1, 2, 3$; $n = 27$. To avoid scaling problems, we decided not to choose large numbers as parameter values in the test instances. We used random integer numbers between 1 and 10 for the loss of each waiting link. For any size (i.e., any combination of the numbers of nodes and links, the number of demons, etc.), five test problems were run.

To ensure that all demons did not attack to the same link (to give the worst-case situation), we added a set of quadratic conditions for any combination of two demons (whenever the number of demons is equal to or more than two) to the models. For example, for two demon cases, we added such a set of conditions: $p_{l'_1} \times p_{l'_2} = 0$. The model was run on the latest version of professional LINGO optimization software (LINGO 15.00, unlimited version) which can solve mixed integer nonlinear models and mixed system of equations and inequalities. The used computer was a Laptop with Window 7 Professional, 4.00 GB RAM, and an Intel(R) Core(TM) i5 3210-M CPU@ 2.50 GHz.

If we used only one starting point in the “Global solver” option of LINGO and also one strategy among all nonlinear solver strategies, for most of the test instances, the model was solved in less than a minute. In the worst case where a wider area of solutions was searched, it took no more than 207 seconds. Because the link-based model is highly nonlinear for large, realistic problems in general and the functions involved in the system may not be convex, all nonlinear solver strategies such as successive linear programming (SLP) direction, steepest edge, etc. in LINGO were checked. For models with alternative solutions (i.e., multiple solutions), we used the “Multi-start” option in the “Global solver” option of LINGO to search for more than one solution. When using this option with less than 10 different initial solutions, we could normally find at least one solution; otherwise, the local search

procedure might not be able to find a solution. The run time linearly increases with either the number of starting points in the “Global solver” or the number of nonlinear solver strategies. For example, if we use 10 starting points and two nonlinear solve strategies, then the run time will be $10 \times 2 = 20$ times longer. Pay attention that these problems may have more than one solution with the same payoff and changing the starting points and strategies may help us find alternative solutions.

6.3. Observations and Insights

Based on the test instances in the previous section, we have the following observations and insights.

- In order to have the safest shipment of one type of hazmat, different trucks carrying the same type of hazmat need to take different routes and links. This can spread the risks.
- In case of multiple hazmat transportation, it is recommended to use different routes and links for different hazmat types to avoid having large route and link flows and consequently a high chance of accidents, injuries, and fatalities. Of course, this may increase travel time but can result in safer shipment.
- There is no need to split a long time horizon (e.g., day) to many smaller periods. The number of periods required depends on the number of major changes in population density over the time horizon. For example, in urban areas, the time horizon can be divided into three periods: morning peak hours, off-peak hours, and evening peak hours. Splitting the day to more periods will not introduce us safer routes but will increase computational efforts drastically.
- Computational time is highly dependent on the number of demons because the more number of demons generate more number of link attack scenarios.
- If the degree of connectivity in the transportation network is high (i.e., any node is accessible from other nodes through many routes), the shipment company may have multiple solutions.
- Hazmat shipments must pass through the critical links whose removal would make the network disconnected. In this case, the flows on the critical links must be distributed or scheduled over different periods to have safer shipment. Therefore, during each period, each carrier needs to wait before using each of the critical links until the next period unless the previously scheduled carrier passes through it.

7. CASE STUDY

To illustrate our methodology for solving a practical hazmat routing and scheduling problem, we present a Singapore case study. The details are given in sections 7.1-7.3.

7.1. Methodology and Practical Aspects

Figure 4 illustrates our proposed methodology. It shows how our proposed models (e.g., NCP and VIP models) and solution methodology are linked to public policy decision making. The methodology is applicable to urban areas where hazmat trucks always avoid passing through congested residential areas. Before we apply the models, we need to observe regulations and use only approved routes. However, the proposed methodology does not have any specific restriction in applications.

7.2. Network and Demand Setting

For the ease of illustration, in this case study, we consider two hazmat classes which correspond to two groups of hazmats regulated by Singapore Civil Defense Force (SCDF) (SCDF, 2011), namely:

- Petroleum (which can further be divided into three subclasses with respect to flash points) and
- Flammable materials listed in the Second Schedule of the Fire Safety (Petroleum & Flammable Materials) Regulations 2005, which can be further divided into 238 types (SCDF, 2011).

Singapore 3-PL companies responsible for hazmat shipment must apply for a transportation license specifying the route, the schedule, and the type of hazmat. The route should be consistent with the approved routes given by Astrata Group in 2011¹. We consider the base network similar to the one in Meng et al. (2005). However, because we aim to investigate a hazmat shipment problem with more than one OD pair, we consider two OD pairs instead of one. Moreover, both classes of hazmats are transported between each of the two OD pairs.

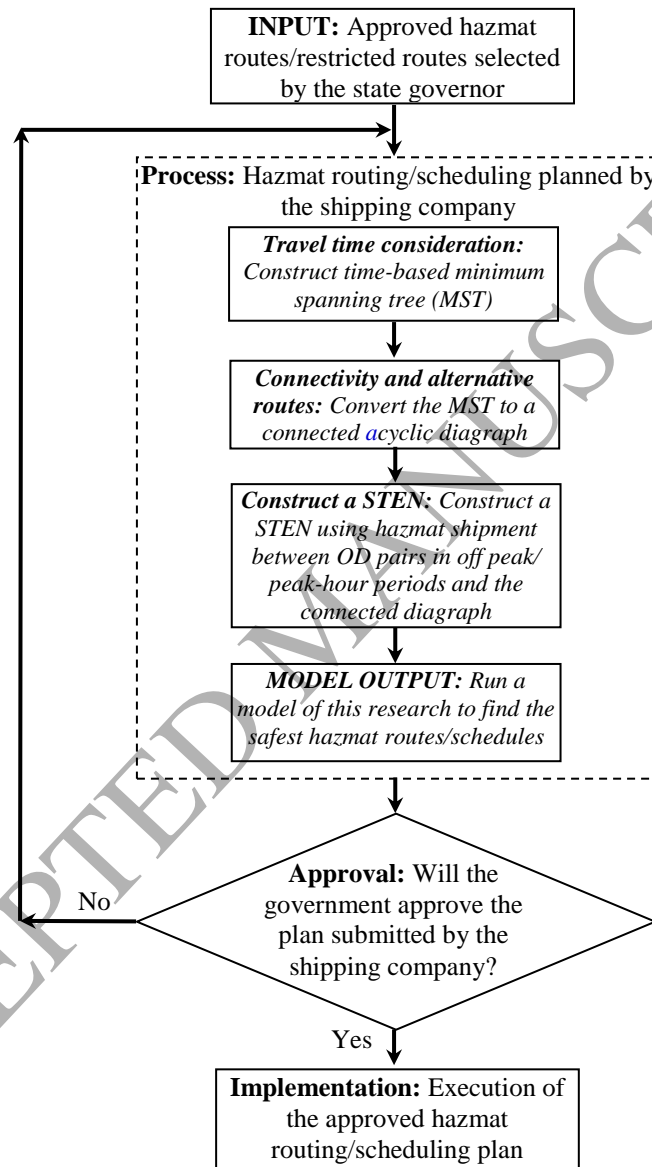


Figure 4. Hazmat routing-scheduling decision making procedure involving the shipment organization and the governor.

To illustrate the time-varying nature of the population, we consider two periods with different populations around the roads. The approved daily transportation time horizon in accordance to various government agencies in Singapore (especially SCDF) is 07:00-19:00 daily. We thus consider two representative one-hour periods: 7:00-8:00 and 9:00-10:00. Since in Singapore, working time span is 8:30-18:00, it is reasonable to assume that during the first period, the majority of residents stay at home. For the second period, we need to know about the number of

¹ At the moment, these routes may have been changed by Astrata Group, which is an organization in charge of the Hazardous Transport Vehicle Tracking System (HTVTS) for the Singapore Civil Defense Force (SCDF).

employees from their home to work in other districts. To estimate this number, we solved a trip distribution problem using the well-known gravity model assigning higher weights to areas which are closer to central business districts (CBD)². The number of employees, green areas, and the type of buildings in residential areas were embedded in our calculation. The gravity model calculations were coded and run using MATLAB. The distance function between district λ , located in (X_λ, Y_λ) , and district μ , located in (X_μ, Y_μ) , is assumed to be the Minkowski distance of order b , which is defined as follows (Uster and Love, 2003):

$$D_{\lambda\mu} = (|X_\lambda - X_\mu|^b + |Y_\lambda - Y_\mu|^b)^{\frac{1}{b}} \quad (33)$$

The most popular values for b are $b = 1$, 2 , and $b = \infty$. For rectilinear distance, $b = 1$, which is suitable to be applied to internal transportation in production facilities. For Euclidean distance, $b = 2$, which is appropriate to be applied to sea and air transportation and transportation in desert, during which there are not many physical obstacles. For urban areas, the aisle distance measure is more realistic but it cannot be measured based on the coordinates of origin and destination (Drezner & Wesolowsky, 2001). In urban areas, we mostly face the shipment situations where the travel distances can sometimes be best represented by Euclidean distance ($b=2$) and sometimes be best represented rectilinear distance ($b=1$). Therefore, in this research, we assume $b=1.5$ for our case problem, which is in an urban city.

Since we intend to test our algorithm on an acyclic network, we converted the road network to an acyclic network with one-way links only. To have a reasonable network and consider shortest travel distance in addition to population exposure, we used the Dijkstra algorithm. Through this shortest route algorithm and setting node 1 as an origin, we found a directed spanning tree³ covering all 22 nodes and changed the existing 21 edges to 21 directed links. We identified the direction for the rest of the links (which are not in the directed tree) randomly. The resulted network can be transformed to the STEN (see Figure 5) with two OD pairs, namely, OD pairs (1,21) and (3,22). In Figure 5, for the ease of illustration and clarity, we have not drawn waiting links due to having many arcs in the resultant network; these links are directed from a node on the left side of the network to its corresponding node on the right side. In summary, the STEN considers two periods, and has 48 nodes (including 44 normal nodes, 2 dummy origins, and 2 dummy destinations), 92 links (including 58 travel links, 24 waiting links, and 8 links connecting to dummy origins/destinations to the network). We set demands between OD pairs as $d^{1,21} = 100$; $d^{1,21_2} = 150$; $d^{3,22} = 130$; $d^{3,22_2} = 170$.

For class-1 hazmats, we consider the lowest flash point. Therefore, we set its evacuation distance equal to 1600 meters (Verter and Kara, 2008). For class-2 hazmats, the impact zone is assumed to be 800 meters in all directions (Meng et al., 2005). In other words, total population exposed for class-1 hazmats is four times bigger than that for class-2 hazmats. Table 5 shows the data extracted from Singapore hazmat routes and the loss associated with each hazmat type for each district. For all waiting links, we used an arbitrary number (here 90000) as the loss. In fact, this number can be interpreted as the time average between losses at a particular location. Using the same loss for all waiting links allow us to reduce the direct impacts of waiting links on shifting traffic from the first period to the second period and this helps us to better analyze the results.

² According to Papacostas and Prevedouros (2001), the most important factor in determining the population of a district especially in working hours is the distance from the CBD (so-called city center in Singapore).

³ This was actually done by DFS (depth-first-search) algorithm, which has several applications. One of its applications is testing connectivity of a graph by labelling nodes (by numbers) and marking edges. This numbering can also help us to convert a connected graph to a strongly connected digraph (Balakrishnan and Ranganathan, 2000).

7.3. Analysis, Results, and Discussion

To solve the case study problem, we used the link-based model with the same software and hardware mentioned in section 6, the “Multi-start” option, and different nonlinear strategies for one and two demons (i.e., $M = 1, 2$). For $M = 1$ and $M = 2$, the solver found at least one solution in 1209.65 and 2685.36 seconds, respectively. The elapsed times are quite reasonable for such an operational/tactical decision problem. For $M = 1$, the demon attacks link $(17^2, 22^2)$ with a probability of one. The answer is rational because $(17, 22)$ is a critical link⁴ in the original graph (not in the STEN) and it is chosen by two out of four dispatchers heading to destination 22 and the demon gets some certain payoff by attacking this link.

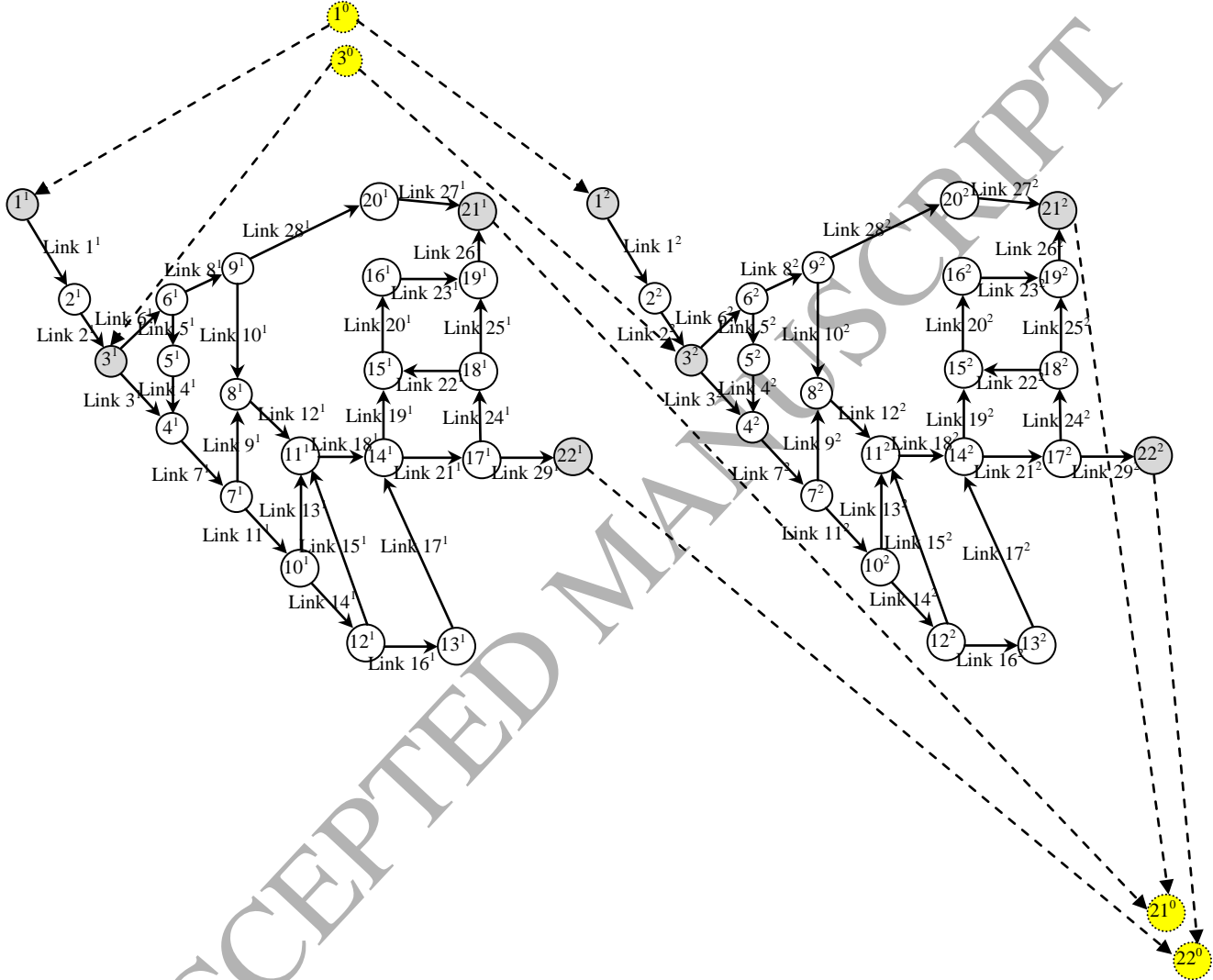


Figure 5. The time-expanded replica of the case network.

When setting $M = 2$, the demons' overall payoff gets higher. In this case, there are multiple solutions. Again, one of the demons attacks link $(17^2, 22^2)$ with a probability of one but the other can have more than one choice. For example, one solution for demon 2 is to attack link $(9^2, 20^2)$ with a probability of one; alternatively, demon 2 can also attack link $(20^2, 21^2)$ with a probability of one. Rarely is a link being attacked with a probability 1. In the case study problem, there are a few critical links including link $(17^2, 22^2)$. When a critical link is definitely chosen by all dispatchers and is in a populated area, there must be a payoff to a demon if the link is targeted, and therefore it must be attacked by the demon. Because one demon has already attacked the critical link $(17^2, 22^2)$, the other demon attacks other links to maximize the payoff. However, both demons get an equal payoff, which confirms

⁴ A critical link (so-called “bridge” in graph theory content) is a link that if removed, the graph would be disconnected.

proposition 1, but the four dispatchers choose different routes and have different minimum expected losses. For dispatchers, the flows split in both periods but the flow is higher in the second period because in all of the links, loss in the first period is higher than that in the second. We need to pay attention that in the loss calculation, we used the concept of CBD but in fact the three CBDs in Singapore are not next to the approved hazmat routes. This is reasonable because the CBD is the most congested area of city and it attracts much trip generated by other districts during working hours.

Table 5. Population forecasting for the case network during two periods of a day.

Link	Related district	Loss (1600m) (T=1)	Loss (800m) (T=1)	Loss (1600m) (T=2)	Loss (800m) (T=2)
1,2	Yishun	255356	63839	218677	54669
2,3	Woodlands	232486	58121	202406	50601
3,4	Choa Chu Kang	332067	83016	286594	71648
5,4	Choa Chu Kang	332067	83016	286594	71648
6,5	Choa Chu Kang	332067	83016	286594	71648
3,6	Bukit Panjang	293875	73468	250378	62594
4,7	Choa Chu Kang	332067	83016	286594	71648
6,9	Bukit Batok	175371	43842	148058	37014
7,8	Jurong West	327198	81799	282633	70658
9,8	Jurong East	262765	65691	220082	55020
7,10	Choa Chu Kang	332067	83016	286594	71648
8,11	Jurong West	327198	81799	282633	70658
10,11	Jurong West	327198	81799	282633	70658
10,12	Jurong West	327198	81799	282633	70658
12,11	Jurong West	327198	81799	282633	70658
12,13	Jurong West	327198	81799	282633	70658
13,14	Jurong West	327198	81799	282633	70658
11,14	Jurong East	262765	65691	220082	55020
14,15	Jurong East	262765	65691	220082	55020
15,16	Jurong East	262765	65691	220082	55020
14,17	Jurong East	262765	65691	220082	55020
18,15	Jurong East	262765	65691	220082	55020
16,19	Clementi	236098	59024	190232	47558
17,18	Hougang	173130	43282	143685	35921
18,19	Hougang	173130	43282	143685	35921
19,21	Clementi	236098	59024	190232	47558
20,21	Clementi	236098	59024	190232	47558
9,20	Clementi	236098	59024	190232	47558
17,22	Clementi	236098	59024	190232	47558

8. CONCLUSIONS

This paper studies the integrated routing and scheduling hazmat problem over space-time expanded networks with multiple OD flows, multiple classes of hazmats, and unknown link incident probabilities. Various multiple-demon models for the problem are proposed. Their equivalence is proved. A solution strategy is proposed to solve the problem without exhaustive route enumeration and route generation heuristics and is demonstrated by a simple example. Numerical examples are also provided to illustrate and discuss the solution method for converting link flows to route flows, and the problem properties, including the effect of the number of demons on the total expected loss and the number of links selected by demons, the effect of the non-cooperative behavior of the demons on the total expected loss, the effect of route sets on the lowest expected loss, and the existence of multiple link flows, link selection probabilities, and maximum expected payoffs. The computational efficiency of the solution strategy is also demonstrated and problem insights are discussed. A Singapore case study is presented to illustrate our methodology for solving a practical hazmat routing and scheduling problem.

Like all research activities, there are limitations and assumptions in our research that can lead us toward future research directions. First, the input road network in our problem is formed by unidirectional (one way) links but in reality, the network is formed by a combination of one-way and two-way links. Of course, it is very likely that

solutions are mainly based on one-way links but the input can also be two-way. The proposed methodology will be extended to handle two-way links in the future. Second, using the concept of minimum spanning tree, we consider travel time in the network prior to solving the hazmat routing-scheduling problem. This hierarchical decision is practical but from the perspective of optimization, it is not as good as concurrent decision making. Moreover, using models in which travel time and hazmat routing-scheduling decision are being considered simultaneously may reduce loss for shipping companies. Given that cost saving is not the first objective compared to hazmat risks, we may use bi-level programming or multi-objective decision making techniques like the lexicographic one to extend our methodology to handle travel time in the future research. Third, while probabilistic concepts are exploited in this research in great detail, the main parameters in the research are deterministic. Considering uncertainty in parameters and also using relevant techniques such as robust optimization can be another future research direction. Fourth, the number of demons used can be set as the mean or maximum historical number of hazmat incidents occurred simultaneously. Which is a better choice? Should we consider other factors simultaneously? These questions lead to one future research direction. Fifth, several OD pairs can belong to a certain private company or a regional authority in reality. For this case, we can consider the “company” or “regional authority” as a player in the dispatcher subproblem who can make the routing decisions of all trucks between those OD pairs in the STEN; we can define the expected loss to the player based on the total expected loss of those OD pairs (i.e., sum of expected loss of all paths on these OD pairs) to cater the cooperation between OD pairs, and define the KKT condition based on the marginal cost concept as in classic system optimum traffic assignment. Our framework can be easily extended to cater this case. This can be left to future studies. Finally, when it comes to applications, there is an analogy between the concept of our demon approach and terrorist attack; the demon approach can be used in dealing with man-made disasters. Manmade disasters can be divided into human errors (like in our hazmat problem) and terrorist attacks that are being done intentionally using human intelligence. In fact, in dealing with terrorist attacks, we need to focus on system resiliency based on the worst-case situation. An extension of our demon approach to terrorist attacks can be another interesting research on network routing and scheduling.

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APPENDIX

Table A. The notation used throughout the paper.

<i>Sets and indices</i>	
A :	Set of directed links in the base network G
N :	Set of nodes in the base network G
A' :	Set of directed links in the STEN G'
N' :	Set of nodes in the STEN G'
$A'_{r,q}$:	Set of links for class- q hazmats departing from dummy origin r'
$O(z^t)$:	Set of outbound links emanating from node $z^t \in N'$
$I(z^t)$:	Set of inbound links feeding into node $z^t \in N'$
$G = [N, A]$:	A connected base network with multiple OD pairs
$G' = [N', A']$:	A STEN
$P^{rs,q}$:	The route set for the flow of class- q hazmats between r' and s' in the STEN (i.e., the route set of dispatcher rs_q)
a :	Index for a link in the base network
x, y :	Indices for nodes in the STEN
t :	Index for a particular departure time
$a^t = (x, y)$:	A link in the STEN ($a^t \in A'$)
q :	Index for a hazmat class
m :	Index for a demon ($m = 1, \dots, M$)
l'_m :	Index for a link in the STEN, on which demon m causes an accident ($l'_m = 1, \dots, A' $)
$k = (l'_1, \dots, l'_m, \dots, l'_M)$:	Index for a scenario formed by combination of links chosen by demons; each of the demons m ($m = 1, \dots, M$) causes an incident on link $l'_m \in A'$
r' :	Dummy origin
s' :	Dummy destination
r :	Index for an origin (O) in the STEN
s :	Index for a destination (D) in the STEN
rs_q :	Index for the dispatcher who is responsible for sending out his/her vehicles to transport class- q hazmats between OD pair rs
j :	Index for a route selected by a dispatcher
r^t :	Origin of the subgraph G^t
s^t :	Destination of the subgraph G^t
<i>Parameters</i>	
M :	Number of demons
n :	Number of dispatchers
n_o :	Number of dummy origins in the STEN
n_d :	Number of dummy destinations in the STEN
T :	Number of departure time choices
Q :	Number of hazmat classes
$\alpha_{a^t}^q, \beta_{a^t}^q$:	Loss function parameters associated with hazmat q on link a^t
$d^{rs,q}$:	Demand for transporting class- q hazmats between OD pair rs
<i>Variables</i>	
u_k :	Occurrence probability of scenario k
$v_{a^t}^q$:	The flow of class- q hazmats on link $a^t \in A'$
$\mathbf{v} = [v_{a^t}^q]$:	Vector of hazmat flows
$v_{a^t}^{rs,q}$:	Flow on link a^t due to dispatcher rs_q
$P_{l'_m}$:	The probability of demon m to cause an incident on link $l'_m \in A'$
π^m :	The maximum expected payoff to demon m
$\phi^{rs,q}$:	The minimum expected loss between OD pair rs for class- q hazmats
$\phi^{r^t, y, q}$:	The lowest expected loss for class- q hazmat flow from r' to y and $\phi^{rs,q} = \phi^{rs,q}$
$q_{a^t, -m}$:	The probability of link a^t selected by at least one demon excluding demon m
$\eta_j^{rs,q}$:	The expected loss to dispatcher rs_q who selects route j
$h_j^{rs,q}$:	The flow of class- q hazmats on route $j \in P^{rs,q}$
P :	The expected payoff to each demon
$c_{a^t, k}(\mathbf{v})$:	The loss of link $a^t \in A'$ in scenario k if the hazmat vehicle departs in time period t
$\theta_{l'_m}$:	The expected payoff to demon m when demon m causes an incident on link $l'_m \in A'$
$c_{a^t}(\mathbf{v})$:	The worst case loss on link a^t if incidents occur on this link

Proof of proposition 1: From equation (1), we can observe that all the demons receive the same expected payoff for any given solution. Therefore, their maximum expected payoffs, which are the expected payoff evaluated at Nash equilibrium, must be the same. \square

Proof of proposition 2: According to condition (11), the expected loss on a route is the sum of the expected losses on all links on that route, but the expected loss on a link is the same for all dispatchers choosing that link. This implies that the expected loss on a route is the same for all of the dispatchers choosing that route, which further implies that they select the same route and have the same expected loss. \square

Proof of proposition 3: The proof is made by the following six steps:

Step 1: (13) \Rightarrow (21).

Without loss of generality (W.L.O.G.), let $J = (r' = z_1 - z_2 - \dots - z_l = s') \in P^{rs_q}$ be the minimum expected loss path for dispatcher rs_q where $z_i \in N', i=1, \dots, l$ is the node on path J and $h_j^{rs_q} > 0$. Condition (13) implies that for every $i=2, 3, \dots, l-1$, subpath $J_1 = (r' = z_1 - z_2 - \dots - z_i)$ is the minimum expected loss path from r' to z_i for dispatcher rs_q . This subpath optimality condition can be proved by contradiction. Suppose J is the minimum expected loss path from r' to s' for dispatcher rs_q but subpath J_1 is not the minimum expected loss path from r' to intermediate node z_i for dispatcher rs_q . This implies that there is a lower expected loss path J_2 from r' to intermediate node z_i compared with J_1 . As a result, there is a lower expected loss path formed by J_2 and subpath $z_i - z_{i+1} - \dots - z_l = s'$ connecting r' and s' , contradicting the assumption. Therefore, we conclude that subpath J_1 is the minimal expected loss path from r' to z_i for dispatcher rs_q . The expected loss on J_1 is

$$\phi^{r'i,q} = \sum_{b=1}^{i-1} \sum_k c_{(z_b, z_{b+1})k}(\mathbf{v}) u_k. \quad (\text{A1})$$

Similarly, the minimal expected loss from r' to z_{i+1} is

$$\phi^{r',i+1,q} = \sum_{b=1}^i \sum_k c_{(z_b, z_{b+1})k}(\mathbf{v}) u_k. \quad (\text{A2})$$

Condition (A2) minus (A1) gives $\phi^{r',i+1,q} - \phi^{r'i,q} = \sum_k c_{(z_i, z_{i+1})k}(\mathbf{v}) u_k$ and

$$\sum_k c_{(z_i, z_{i+1})k}(\mathbf{v}) u_k - (\phi^{r',i+1,q} - \phi^{r'i,q}) = 0. \quad (\text{A3})$$

As $h_j^{rs_q} > 0$, the flow on each link of this path must be greater zero (i.e., $v_{a'}^{rs_q} > 0$), which must occur with

condition (A3) simultaneously. We therefore have $v_{a'}^{rs_q} \left(\sum_k c_{(z_i, z_{i+1})k}(\mathbf{v}) u_k - (\phi^{r',i+1,q} - \phi^{r'i,q}) \right) = 0$. Since the above

proof can apply to any arbitrarily minimum expected loss path for any dispatcher, we conclude (13) \Rightarrow (21).

Step 2: (14) \Rightarrow (22).

Consider $a^i = (z_i, z_{i'})$, the minimum expected loss route for dispatcher rs_q ,

$J = (r' = z_1 - z_2 - \dots - z_i - \dots - z_{i'} - \dots - z_l = s') \in P^{rs_q}$ and path $J_3 = (r' = z_1 - z_2 - \dots - z_i - z_{i'} - \dots - z_l = s')$

via a^i . By definition, the expected losses on these routes are

$$\eta_j^{rs,q} = \phi^{rs,q} = \left[\sum_{b=1}^{i-1} \sum_k c_{(z_b, z_{b+1})k}(\mathbf{v}) u_k + \sum_k c_{a^t k}(\mathbf{v}) u_k + \sum_{b=i}^l \sum_k c_{(z_b, z_{b+1})k}(\mathbf{v}) u_k \right] \text{ and } \eta_{j_3}^{rs,q} = \sum_{b=1}^l \sum_k c_{(z_b, z_{b+1})k}(\mathbf{v}) u_k .$$

From (14), we have $\sum_k c_{a^t k}(\mathbf{v}) u_k - \sum_{b=i}^{i'-1} \sum_k c_{(z_b, z_{b+1})k}(\mathbf{v}) u_k \geq 0$. The second term on the left hand side equals

$$\phi^{r'i',q} - \phi^{r'i,q} \text{ according to (A1). Therefore, we have } \sum_k c_{a^t k}(\mathbf{v}) u_k - (\phi^{r'i',q} - \phi^{r'i,q}) \geq 0, a^t = (i, i'). \text{ By applying}$$

this analysis to other links in the network, we have (14) \Rightarrow (22).

Step 3: (15) \Rightarrow (23).

Since $\delta_{a^t j} \geq 0, \forall a^t$, we have $h_j^{rs,q} \geq 0, \forall rs_q, j \Rightarrow \left(\sum_j \delta_{a^t j} h_j^{rs,q} \right) \geq 0, \forall rs_q, a^t$. As the left hand side of the second

inequality equals $v_{a^t}^{rs,q}$, we can conclude (15) \Rightarrow (23).

Step 4: (21) \Rightarrow (13).

Consider a path $j = (r' = z_1 - z_2 - \dots - z_{i'} - \dots - z_i - \dots - z_l = s') \in P^{rs_q}$ in which all links a^t on this path carry class- q hazmat flow (i.e., $v_{a^t}^{rs,q} > 0$). Conditions (20) and (21) require

$$\sum_k c_{(z_i, z_{i+1})k}(\mathbf{v}) u_k - [\phi^{r'z_{i+1},q} - \phi^{r'z_i,q}] = 0, \forall (z_i, z_{i+1}), i = 1, \dots, l-1. \text{ By rearranging this equation, we get}$$

$$\phi^{r'z_{i+1},q} = \sum_k c_{(z_i, z_{i+1})k}(\mathbf{v}) u_k + \phi^{r'z_i,q}. \text{ This recursive relationship implies } \phi^{r's',q} = \sum_{i=1}^{l-1} \sum_k c_{(z_i, z_{i+1})k}(\mathbf{v}) u_k + \phi^{r'r',q}, \text{ where}$$

the first term is the expected loss on path j and the second term equals zero by definition. We can conclude that (21) implies the expected loss of a used path j for dispatcher rs_q to be equal to the minimal expected loss to that dispatcher. As this analysis can be repeated for other used paths, we get (21) \Rightarrow (13).

Step 5: (22) \Rightarrow (14).

W.L.O.G., consider a path $j = (r' = z_1 - z_2 - \dots - z_{i'} - \dots - z_i - \dots - z_l = s') \in P^{rs_q}$. By applying (22) to all links on this path and adding all the corresponding inequalities together, we have

$$\sum_k c_{(z_i, z_{i+1})k}(\mathbf{v}) u_k - [\phi^{r'z_{i+1},q} - \phi^{r'z_i,q}] \geq 0, \forall a = (z_i, z_{i+1}), i = 1, \dots, l-1 \text{ and hence } \eta_j^{rs,q} - \phi^{rs,q} \geq 0. \text{ By repeating the}$$

same analysis to other paths, we can complete Step 5.

Step 6: (23) \Rightarrow (15).

Suppose (23) holds but $h_j^{rs,q} < 0$ for some paths j . Consider a link a^t that is only on one path. Since the flows on this path can be negative, the flow on a^t can be negative, contradicting the assumption. Hence, (23) \Rightarrow (15).

This completes the proof. \square

Proof of proposition 4: Conditions (1)-(10) and (18) are common to both problems. Moreover, equation (19) is the alternative formulation of the flow conservation conditions (16)-(17). Furthermore, according to Proposition 3, the link-based dispatcher choice conditions (21)-(23) are equivalent to the corresponding route-based conditions (13)-(15), where conditions (20) and (11)-(12) are respectively used to define conditions (21)-(22) and (13)-(14). Consequently, the link-based problem is equivalent to the route-based problem, in terms of the expected payoff to

each demon. \square

Proof of proposition 5: Conditions (6)-(8) and (21)-(23) are already rewritten in NCP format and (1)-(5), (9)-(10), (18), and (20) are definitions common to both the mixed system of equations and inequalities and NCP. Hence, we can just focus on (10) and (19) when proving the equivalency. If a solution satisfies the system (1)-(10), (18)-(23), it implies i) the minimal expected loss from r' to node $z' \in N'$, $\phi^{r'z,q} = \hat{\phi}^{rs_q z}$, and π^m must be positive by nature;

ii) conditions (10) and (19) hold; iii) the solution must also satisfy $\sum_{a' \in O(z')} v_{a'}^{rs_q} - \sum_{b' \in I(z')} v_{b'}^{rs_q} - Q_{z'}^{rs_q} \geq 0$ and

$\sum_{l'} p_{l'}^m - 1 \geq 0$, a relaxed condition of conditions (10) and (19). Conditions i) and ii) further imply that the solution

must satisfy $\hat{\phi}^{rs_q z} \left[\sum_{a' \in O(z')} v_{a'}^{rs_q} - \sum_{b' \in I(z')} v_{b'}^{rs_q} - Q_{z'}^{rs_q} \right] = 0, \forall rs_q, z' / r'$ and $\pi^m \left[\sum_{l'} p_{l'}^m - 1 \right] = 0, \forall m$. Therefore, the

solution to the mixed system is also a solution to the NCP (24)-(27). If a solution satisfies (24)-(27), it implies that (10) and (19) hold as π^m and $\phi^{r'z,q}$ are positive by nature. Therefore, the solution to the NCP is also a solution to the system.

Proof of proposition 7: According to Proposition 6, the first part of Proposition 7 is equivalent to $G(\mathbf{y}^*) = 0 \Leftrightarrow \mathbf{y}^* \geq \mathbf{0}, \mathbf{H}(\mathbf{y}^*) \geq \mathbf{0}$, and $\mathbf{y}^{*T} \cdot \mathbf{H}(\mathbf{y}^*) = 0$. That is, \mathbf{y}^* is a global minimum of the UMP if and only if \mathbf{y}^* is a solution of the NCP.

When $G(\mathbf{y}^*) = 0$, every square term and hence the square bracket term in objective function (28) must equal zero because of the sum of squares. By Fisher (1992), we have $\left[\sqrt{(y_i^{*2} + H_i(\mathbf{y}^*)^2)} - (y_i^* + H_i(\mathbf{y}^*)) \right] = 0 \Rightarrow y_i^* \geq 0, H_i(\mathbf{y}^*) \geq 0, y_i^* H_i(\mathbf{y}^*) = 0$ for each i . Hence, $G(\mathbf{y}^*) = 0 \Rightarrow \mathbf{y}^* \geq \mathbf{0}, \mathbf{H}(\mathbf{y}^*) \geq \mathbf{0}$, and $\mathbf{y}^{*T} \cdot \mathbf{H}(\mathbf{y}^*) = 0$.

Conversely, according to Nagurney (1999), when $y_i^* \geq 0, H_i(\mathbf{y}^*) \geq 0, y_i^* H_i(\mathbf{y}^*) = 0$, $\left[\sqrt{(y_i^{*2} + H_i(\mathbf{y}^*)^2)} - (y_i^* + H_i(\mathbf{y}^*)) \right] = 0$. Hence, $\frac{1}{2} \sum_i \left[\sqrt{(y_i^{*2} + H_i(\mathbf{y}^*)^2)} - (y_i^* + H_i(\mathbf{y}^*)) \right]^2 = G(\mathbf{y}^*) = 0$. The second part follows directly from Proposition 5. \square

Proof of proposition 10: The mapping function $\mathbf{H}(\mathbf{y})$ in inequality (29) is continuous with respect to \mathbf{y} under the assumption of $c_{a'k}(\mathbf{v})$ to be continuous since the algebraic operations of addition, subtraction, and multiplication of continuous functions yield continuous functions. Moreover, the solution set of this VIP can be reduced to a closed ball $B_r(\mathbf{0})$ centered at $\mathbf{0}$ with the radius $r = \max \left\{ 1, \sum_{a'} \sum_k c_{a'k}(\mathbf{v}'), \max_{rs_q} d^{rs_q} \right\}$, where

$$\mathbf{v}' = \left[\sum_{rs_q} d^{rs_q}, \forall a^t \right], \text{ because } p_{t_m} \leq 1, \pi^m \leq \sum_{a^t} \sum_k c_{a^t k}(\mathbf{v}'), \hat{\phi}^{rs_z, q} \leq \sum_{a^t} \sum_k c_{a^t k}(\mathbf{v}'), \text{ and } v_{a^t}^{rs_q} \leq \max_{rs_q} d^{rs_q}.$$

Therefore, by Theorems 1.4 and 1.5 in Nagurney (1999) and Proposition 9, the VIP and the link-based problem must have at least one solution. \square

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