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# Toll Policies for Mitigating Hazardous Materials Transport Risk

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**Abstract.** In this paper, we propose toll-setting as an alternative policy tool to regulate the use of roads for dangerous goods shipments. We propose a mathematical formulation as well as a solution method for the hazardous materials tool problem. Based on a comparative analysis of proposed mathematical models, we show that toll policies can be more effective than the popular network design policies that identify road segments to be closed for vehicles carrying hazardous materials. We present a summary of computation experiments on a problem instance from Western Ontario Canada.

**Keywords.** Hazardous materials transportation, toll-setting, network design, bilevel programming.

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## Introduction

An increasing amount of hazardous materials (*hazmats*) are shipped by road, rail, waterways and air. Explosives, gases, flammable liquids, poisonous and infectious substances and radioactive materials are among the hazmats that are transported in large volumes. These shipments are indispensable to our modern way of life, although they can be harmful to the people and the environment in the event that they are released from their container as a result of an accident. Due to the inherent transport risks, the transportation of hazmats is regulated under the Federal Hazardous Materials Transportation Act (which was amended by the Patriot Act in 2001) in the U.S. and under the Federal Transportation of Dangerous Goods Act in Canada.

The policies that are available to government agencies for hazmat transport risk management can be categorized into two main groups with respect to their underlying philosophy: *proactive* and *reactive*. The latter group of policies aims at confining the undesirable consequences of a hazmat incident *after* the occurrence of the accident. The development of emergency response plans -that involve the establishment of a network of responder teams specializing on different hazmat types- is the most popular example of reactive policies. Clearly, the consequences of an accident can be mitigated by better coordination of responder teams and faster response times to the incident sites. In contrast, the proactive risk mitigation policies aim at reducing the likelihood and consequences of hazmat incidents *a priori*. The establishment of inspection centers for hazmat trucks is a common example in this category.

Our focus is on the proactive policies regulating the use of road segments by hazmat carriers. In North America and Europe, government agencies do not have the authority to *dictate routes* to hazmat carriers for moving their shipments. These agencies mitigate hazmat transport risks by imposing (permanent or time-based) curfews on the use of the *road segments* under their jurisdiction. The closure of certain road segments to hazmat vehicles is a policy that is being used (or considered) in many large cities, such as Washington DC, Montréal, and Paris. In their seminal paper, Kara and Verter (2004) formulated the problem of identifying the road segments to be closed to hazmat shipments as a *network design* problem (ND). In their ND formulation, a regulator chooses the road segments to be closed for hazmat transportation so as to minimize population exposure (i.e., the total number of people within a threshold distance from the road segments that are utilized by hazmat vehicles), while taking into account the carriers' route choices based on transport cost. This problem involves two levels of decisions, which cannot be solved sequentially. There are usually more than one path left available for some carriers even after the design decisions are made (all carriers use the same road network and the closed arcs are the same for all shipments of the same type of hazmat). If the design decisions were solely made based on the objective of the regulator (i.e., without keeping in mind the carriers' objective), then it is probable that the total risk associated to the carriers' route choices made subsequently would be much higher than the risk anticipated by the regulator. One such example is provided in Erkut et al. (2007). Hence, this problem is considered as a bilevel problem. For a recent survey on bilevel programming, see, e.g., Colson et al. (2005) or Dempe (2005).

In this paper, we propose an alternative policy tool to regulate the use of roads for hazmat

transport, i.e., the use of tolls to deter the hazmat carriers from using certain road segments, which we refer as *toll-setting* policies (TS). This policy, also modeled as a bilevel problem, entails imposing tolls on certain road segments so as to channel the shipments on less populated roads. Although TS has been studied for regular freight transportation, to the best of our knowledge, this is the first paper that proposes TS as an effective means to mitigate hazmat transport risk. We are also unaware of the use of this policy tool by regulators around the globe. Nonetheless, our findings indicate that TS has significant potential as a policy tool since it is more flexible and effective than the popular ND policies for mitigating transport risk.

Since dangerous goods constitute an integral part of industrialized societies, the economic viability of the hazmat transport sector cannot be ignored while attempting to reduce the public and environmental risk. On the other hand, the carriers must take into account the risks as well as the costs associated with their routing decisions in order to both minimize their insurance costs (Verter and Erkut (1997)) and manage their public image. Therefore, in this paper, we first extend the work of Kara and Verter (2004) to incorporate the cost *and* risk (i.e., population exposure) considerations at both the regulator and the carrier levels. Based on this extended framework, we also present some improvements on the ND solution methodology which permit to solve much larger instances than those reported in Kara and Verter (2004). Yet, our main contribution is the proposed methodology for implementing the TS policy for hazmat transportation. To this end, we present a mathematical formulation for the bilevel hazmat TS problem and show that this model can also be posed as a single-level MIP formulation. Perhaps more importantly, we show that not only TS can be more effective than ND in reducing hazmat transport risk, it can also be much easier to solve. As a matter of fact, when the objective of the government is to minimize risk only (i.e, when costs are only included at the carrier level), we show that the toll problem is not a true bilevel problem and that it can be solved very efficiently by inverse optimization. Finally, since the effectiveness of the hazmat transport policies devised by a government agency depends on the extent of buy-in received from the hazmat carriers during the consultation process (Verter and Kara (2007)), we elaborate the use of our methodology on a restricted set of road segments considered for setting tolls in order to produce solutions that are more acceptable to the carriers.

The remainder of the paper is organized as follows. An overview of the relevant literature that highlights the contributions of this paper is provided in the next section. Section 2 presents the mathematical formulations for the network design and the toll problems in the context of hazmat transportation. In this section, we also provide an example showing that these two models are not equivalent. Section 3 shows how the toll problem can be used by a regulator to obtain minimum risk solutions very efficiently. Our solution methodology is outlined in Section 4, which is followed by a summary of our computational experiments in Section 5. Our experiments are based on the problem instance in Western Ontario, Canada, studied by Kara and Verter (2004).

# 1 Overview of the Literature

In this section, we provide a selective overview of the two streams of research that are most relevant for our work, i.e., hazmat ND models and TS applications in transportation. Although hazmat logistics is a mature field of research (see the comprehensive and recent review by Erkut et al. (2007)), the regulation of the use of road segments has attracted the attention of researchers fairly recently. We know of four papers focusing on the hazmat ND problem. Also, we are not aware of any work on the hazmat TS problem discussed in this paper. Nonetheless, the literature contains numerous applications of TS to road pricing and regular freight transportation, which we will review at the end of this section.

As mentioned in the previous section, Kara and Verter (2004) were the first to propose a bilevel programming formulation for the hazmat ND problem. The outer-level problem chooses road segments to close for hazmat transportation so that the total number of people exposed to dangerous goods is minimized, taking into account that the inner-level problem route all O-D shipments so that the carriers' costs are minimized. Using complementary slackness conditions, the authors reformulate the problem as a single-level MIP that is solved using CPLEX. The problem is modeled as an optimistic bilevel problem, i.e., it is assumed that the carriers would take the lower risk path in case of equal cost, which is a reasonable assumption. Kara and Verter (2004) present an application of the proposed methodology in Western Ontario, Canada (the case also used for the computational experiments reported in this paper). Their results show that significant reductions in population exposure can be achieved through government intervention on the use of road segments by hazmat vehicles. However, their method cannot solve large-scale instances in a reasonable amount of computation time.

Erkut and Gzara (2007) also formulate the network design problem as a bilevel problem, but instead of solving the complete problem, they propose a heuristic algorithm that iterates between the outer-level and the inner-level problems (that are both pure network flow problems). As a result, they improve the computational performance of the solution methodology, but obtain sub-optimal solutions. The authors also generalize the model to a bi-objective model by including the traveling cost in the regulator's objective function (outer-level).

Erkut and Alp (2007) formulate the minimum risk network design problem as a Steiner tree selection problem. By reducing the possibilities of the carriers to only one path for every O-D shipment, this methodology simplifies the bilevel problem to a single level problem. However, it can result in increased population exposure as well as higher travel costs for the carriers. To circumvent the latter weakness, the authors propose a greedy heuristic to add edges to the tree (corresponding to shortest paths) while keeping the risk increase to a minimum. They also include traveling costs to the risk in the objective function of the tree selection problem.

Finally, Verter and Kara (2007) introduced a single-level path-based formulation for the hazmat ND problem where only those paths that are acceptable to the carriers are included in the model. These paths are determined a priori for each O-D shipment and are ranked according to the carrier's preferences. Consequently, the optimal solution of the Verter and

Kara (2007) model determines not only the road segments to be closed to hazmat shipments by the regulator, but also the routes that would be used for each shipment on the resulting network. The proposed methodology is intended to facilitate the consultation between the regulator and the hazmat carriers during the policy design process.

Some other interesting work on the hazmat global routing problem can be found in the operations research literature. This planning problem belongs to a government agency whose mandate is to route the hazmat shipments within and through its jurisdiction. This problem is not modeled as a bilevel problem since it is used in a context where the regulator can decide on the routes used by the carriers. The objective of the regulator is to minimize the total risk for the population, but also to ensure equity in the spatial distribution of the risk. The most recent contributions include Marianov and Revelle (1998), Akgün et al. (2000), Dell’Olmo et al. (2005) and Carotenuto et al. (2007).

We now turn to an overview of the applications of TS in transportation. The congestion pricing problem usually considers a regulator setting tolls so as to minimize the total traveling time for the users (or maximize the social welfare), while an optimal solution to the users’ problem is an equilibrium where none of the users is interested in altering his path choice. When all road segments are subject to tolls, marginal cost pricing induces the optimal use of the network (Morrison (1986)). In that case, tolls can be seen as the difference between the social cost (contribution to total traveling time) and the perceived cost for the users. If there are more than one toll schemes inducing an optimal use of the road network, then one scheme optimizing a secondary objective such as minimizing the total tolls collected can be utilized (see, e.g., Bergendorff et al. (1997) or Larsson and Patriksson (1998)). In many situations, however, only second-best solutions are considered, i.e., solutions in which not every road segments can be tolled. For example, situations calling for second-best solutions occur when pricing is allowed on certain highways only, or in the presence of pay-lanes or a toll-cordon around a city. These problems are usually more realistic, but a lower social welfare is expected and they are also more difficult to solve. Instead of maximizing total welfare, owners of private roads might wish to maximize the profit related to the tolls set on the road segments. Among others, Viton (1995), Liu and McDonald (1999), Palma and Lindsey (2000) and Verhoef (2005)) studied second-best pricing. In such problems, the optimal location of the toll points can also be considered (see, e.g., Verhoef (2002)).

Labbé et al. (1998) introduced a general bilevel toll model where a regulator seeks to maximize the profits generated by tolls put on a subset of road segments taking into account that the users choose minimum cost paths with respect to the chosen tolls. These authors have shown that this problem, having bilinear objective functions at both levels, is strongly NP-hard, while primal-dual algorithms aimed at solving large-scale instances of regular freight transportation problems were derived by Brotcorne et al. (2000) and Brotcorne et al. (2001). Also in the context of a profit-maximizing firm, Lederer (1993), Bashyam (2000) and Brotcorne et al. (2007) consider the problem of jointly designing and pricing a network. Conflicting objectives between the leader and the follower are not present in the bilevel hazmat TS where the regulator may even want to minimize, in part, the revenues raised from tolls.

## 2 Mathematical Formulation

Let  $G = (N, A)$  be a road network where  $N$  is the node set and  $A$  is the arc set. Each node  $i \in N$  corresponds to an intersection in the road network, and each arc  $(i, j) \in A$  corresponds to a road segment between two intersections.

Table 1: Mathematical notation

$A$	set of arcs
$C$	set of O-D shipments
$C_h$	set of O-D shipments of hazmat type $h$
$H$	set of hazmat types
$N$	set of nodes
$\alpha$	parameter converting distance in population exposure units
$\beta$	parameter converting population exposure in distance units
$c_{ij}$	the length of arc $(i, j) \in A$
$e_i^c$	equals 1, $-1$ , or 0 depending if node $i \in N$ is the origin, the destination or a transshipment node for shipment $c \in C$
$h(c)$	hazmat type for shipment $c \in C$
$M_{ij}^c$	big- $M$ constants
$n^c$	number of trucks needed by shipment $c \in C$
$\rho_{ij}^h$	number of people exposed on arc $(i, j)$ when hazmat type $h \in H$ is carried
$t_{ij}^h$	continuous variable that represents the toll on arc $(i, j) \in A$ for hazmat type $h \in H$
$x_{ij}^c$	binary variable that represents the flow on arc $(i, j) \in A$ for shipment $c \in C$
$y_{ij}^h$	binary variable that indicates if arc $(i, j) \in A$ is opened for hazmat type $h \in H$

Consider a set  $H$  of hazmat types and a set  $C$  of O-D shipments to be performed. For each O-D shipment  $c \in C$ , let  $h(c)$  be the type of hazmat transported and  $n^c$  be the number of trucks needed to complete the shipment (it is assumed that all trucks associated to the same shipment take the same path). For each arc  $(i, j) \in A$  and each hazmat type  $h \in H$ , let  $\rho_{ij}^h$  be the population exposure (number of people exposed). Let also  $c_{ij}$  be the cost of traveling on arc  $(i, j)$ . Note that throughout the paper, we use the terms ‘carriers’ cost’ and ‘traveled distance’ interchangeably. For each node  $i \in N$  and each shipment  $c \in C$ , let  $e_i^c$  take the value 1 (resp.  $-1$ ) if node  $i$  is the origin (resp. destination) of shipment  $c$ . Finally, let  $x_{ij}^c$  and  $y_{ij}^h$  be binary variables that take the value 1 if arc  $(i, j) \in A$  is used for shipment  $c \in C$  and if it can be used for hazmat type  $h \in H$ , respectively, and let  $t_{ij}^h$  be the toll set on arc  $(i, j) \in A$  for hazmat type  $h \in H$ . Table 1 provides a summary of the notation used in the formulations.

## 2.1 The Network Design Problem

The general network design problem can be modeled as the following bilevel program:

$$(ND) \quad \min_{y,x} \sum_{c \in C} \sum_{(i,j) \in A} n^c (\rho_{ij}^{h(c)} + \alpha c_{ij}) x_{ij}^c \quad (1)$$

$$\text{s.t. } y_{ij}^h \in \{0, 1\} \quad \forall (i, j) \in A, h \in H \quad (2)$$

$$\min_x \sum_{c \in C} \sum_{(i,j) \in A} n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) x_{ij}^c \quad (3)$$

$$\text{s.t. } \sum_{(i,j) \in A} x_{ij}^c - \sum_{(j,i) \in A} x_{ji}^c = e_i^c \quad \forall i \in N, c \in C \quad (4)$$

$$x_{ij}^c \leq y_{ij}^{h(c)} \quad \forall (i, j) \in A, c \in C \quad (5)$$

$$x_{ij}^c \in \{0, 1\} \quad \forall (i, j) \in A, c \in C, \quad (6)$$

where it is understood that in the outer (or leader) problem (1)-(2), the vector  $x$  must be an optimal solution of the inner (or follower) problem (3)-(6). The parameters  $\alpha$  and  $\beta$  allow the comparison between population exposure and carriers' costs. Their value is fixed by the regulator. If  $\alpha = \beta = 0$ , then the general ND problem reduces to that proposed by Kara and Verter (2004).

In ND, the leader (regulator) designs a network that minimizes a combination of population exposure and traveling costs, taking into account that carriers optimize their individual utility. What makes the problem hard is the fact that the trade-off value between risk and cost may differ for the leader and the follower, i.e.,  $\alpha \neq 1/\beta$ . While, for the sake of notational simplicity, the parameter  $\beta$  is identical for all carriers, one could make it dependent on the index  $c$ , without changing the nature of the problem. Note that ND is separable by hazmat type. Note also that, if ties between inner level solutions (routes) occur, the bilevel formulation implies that carriers adopt the one that minimizes the leader's objective, i.e., mainly risk.

### 2.1.1 Single-level MIP reformulations

For fixed design variables  $y_{ij}^h$ , the inner problem is a network flow problem. The binary requirement on  $x$  can thus be replaced by non-negativity constraints, and the bound  $x_{ij}^c \leq 1$ ,  $\forall (i, j) \in A, \forall c \in C$ , can be dropped since it is implied by the constraint  $y_{ij}^h \leq 1$ . Hence, the follower's linear problem can be replaced by its primal-dual optimality conditions. Let  $\pi_i^c, \forall i \in N, c \in C$ , and  $\mu_{ij}^c, \forall (i, j) \in A, c \in C$ , be the dual variables associated with constraints (4)-(5), respectively. With  $\alpha = \beta = 0$ , Kara and Verter (2004) reformulated ND as the following single-level program:

$$\min_{y,x,\pi,\mu} \sum_{c \in C} \sum_{(i,j) \in A} n^c (\rho_{ij}^{h(c)} + \alpha c_{ij}) x_{ij}^c \quad (7)$$

s.t.

$$\sum_{(i,j) \in A} x_{ij}^c - \sum_{(j,i) \in A} x_{ji}^c = e_i^c \quad \forall i \in N, c \in C \quad (8)$$

$$x_{ij}^c \leq y_{ij}^{h(c)} \quad \forall (i,j) \in A, c \in C \quad (9)$$

$$\pi_i^c - \pi_j^c - \mu_{ij}^c \leq n^c(c_{ij} + \beta \rho_{ij}^{h(c)}) \quad \forall (i,j) \in A, c \in C \quad (10)$$

$$\mu_{ij}^c (y_{ij}^{h(c)} - x_{ij}^c) = 0 \quad \forall (i,j) \in A, c \in C \quad (11)$$

$$x_{ij}^c (\pi_i^c - \pi_j^c - \mu_{ij}^c - n^c(c_{ij} + \beta \rho_{ij}^{h(c)})) = 0 \quad \forall (i,j) \in A, c \in C \quad (12)$$

$$\mu_{ij}^c \geq 0 \quad \forall (i,j) \in A, c \in C \quad (13)$$

$$x_{ij}^c \geq 0 \quad \forall (i,j) \in A, c \in C \quad (14)$$

$$y_{ij}^h \in \{0, 1\} \quad \forall (i,j) \in A, h \in H. \quad (15)$$

Constraints (8), (9), (14) and (15) ensure primal feasibility, constraints (10) and (13) ensure dual feasibility, while constraints (11) and (12) force complementary slackness. Resetting  $x$  to be binary, the latter two nonconvex groups of logical constraints can be linearized in the usual way. If  $M_{ij}^c$  are *big-M* constants, constraints (11), (12) and (14) can be replaced with the following constraints:

$$\mu_{ij}^c \leq M_{ij}^c (1 - (y_{ij}^{h(c)} - x_{ij}^c)) \quad \forall (i,j) \in A, c \in C \quad (16)$$

$$\pi_i^c - \pi_j^c - \mu_{ij}^c \geq n^c(c_{ij} + \beta \rho_{ij}^{h(c)}) - M_{ij}^c (1 - x_{ij}^c) \quad \forall (i,j) \in A, c \in C \quad (17)$$

$$x_{ij}^c \in \{0, 1\} \quad \forall (i,j) \in A, c \in C, \quad (18)$$

to yield a mixed integer program (MIP).

## An alternative MIP reformulation

Recall that when the design variables  $y_{ij}^h$  are fixed, the follower's problem is linear. The single-level network design problem can thus be modeled with constraints that impose the equality of the objective function values of the follower's primal and dual problems instead of complementary slackness conditions. In that case, constraints (11) and (12) can be replaced with the following constraints:

$$\sum_{(i,j) \in A} n^c(c_{ij} + \beta \rho_{ij}^{h(c)}) x_{ij}^c = \sum_{i \in N} e_i^c \pi_i^c - \sum_{(i,j) \in A} \mu_{ij}^c y_{ij}^{h(c)} \quad \forall c \in C. \quad (19)$$

One can observe that the latter constraints are nonconvex. Following the strategy described in Labbé et al. (1998), the bilinear terms can be linearized by introducing the variables  $\tau_{ij}^c = \mu_{ij}^c y_{ij}^{h(c)}$  in the model. The following linear constraints are added to ensure that  $\tau_{ij}^c = 0$

when  $y_{ij}^{h(c)} = 0$  and  $\tau_{ij}^c = \mu_{ij}^c$  when  $y_{ij}^{h(c)} = 1$ :

$$\tau_{ij}^c \geq 0 \quad \forall (i, j) \in A, c \in C \quad (20)$$

$$\tau_{ij}^c - M_{ij}^c y_{ij}^{h(c)} \leq 0 \quad \forall (i, j) \in A, c \in C \quad (21)$$

$$\mu_{ij}^c - \tau_{ij}^c \geq 0 \quad \forall (i, j) \in A, c \in C \quad (22)$$

$$\mu_{ij}^c - \tau_{ij}^c + M_{ij}^c y_{ij}^{h(c)} \leq M_{ij}^c \quad \forall (i, j) \in A, c \in C, \quad (23)$$

and constraints (19) can be replaced with the following linear constraints:

$$\sum_{(i,j) \in A} n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) x_{ij}^c = \sum_{i \in N} e_i^c \pi_i^c - \sum_{(i,j) \in A} \tau_{ij}^c \quad \forall c \in C, \quad (24)$$

to yield an alternative MIP formulation solely based on the integrality of  $y$ .

## 2.2 A Toll Approach

An alternative approach to inducing the use of safe routes can be achieved by a toll policy. Its mathematical formulation is as follows:

$$(TS) \quad \min_{t,x} \sum_{c \in C} \sum_{(i,j) \in A} n^c (\rho_{ij}^{h(c)} + \alpha (c_{ij} + t_{ij}^{h(c)})) x_{ij}^c \quad (25)$$

$$\text{s.t. } t_{ij}^h \geq 0 \quad \forall (i, j) \in A, h \in H \quad (26)$$

$$\min_x \sum_{c \in C} \sum_{(i,j) \in A} n^c (c_{ij} + t_{ij}^{h(c)} + \beta \rho_{ij}^{h(c)}) x_{ij}^c \quad (27)$$

$$\text{s.t. } \sum_{(i,j) \in A} x_{ij}^c - \sum_{(j,i) \in A} x_{ji}^c = e_i^c \quad \forall i \in N, \forall c \in C \quad (28)$$

$$x_{ij}^c \in \{0, 1\} \quad \forall (i, j) \in A, c \in C. \quad (29)$$

In TS, the leader sets tolls that minimize a combination of population exposure and travel costs, taking into account that the inner problem (27)-(29) minimizes the carriers' utility (with respect to the toll policy). As was the case for ND, TS is separable by hazmat type and one can use in the follower's objective function (27) parameters  $\beta^c$ ,  $\forall c \in C$ , that are specific to each carrier. Note again that, if ties between inner level solutions (routes) occur, the bilevel formulation implies that carriers adopt the one that minimizes the leader's objective. Actually, with TS as opposed to ND, ties could be broken through an arbitrarily small perturbation of the tolls.

### 2.2.1 Single-level MIP reformulations

Following our earlier strategy, the inner program can be replaced by its primal-dual optimality conditions. Upon the introduction of dual variables  $\pi_i^c$ ,  $\forall i \in N, c \in C$ , this yields the

single-level program

$$\min_{t,x,\pi} \sum_{c \in C} \sum_{(i,j) \in A} n^c (\rho_{ij}^{h(c)} + \alpha c_{ij}) x_{ij}^c + n^c \alpha t_{ij}^{h(c)} x_{ij}^c \quad (30)$$

s.t.

$$\sum_{(i,j) \in A} x_{ij}^c - \sum_{(j,i) \in A} x_{ji}^c = e_i^c \quad \forall i \in N, c \in C \quad (31)$$

$$\pi_i^c - \pi_j^c - n^c t_{ij}^{h(c)} \leq n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) \quad \forall (i,j) \in A, c \in C \quad (32)$$

$$x_{ij}^c (\pi_i^c - \pi_j^c - n^c t_{ij}^{h(c)} - n^c (c_{ij} + \beta \rho_{ij}^{h(c)})) = 0 \quad \forall (i,j) \in A, c \in C \quad (33)$$

$$t_{ij}^h \geq 0 \quad \forall (i,j) \in A, h \in H \quad (34)$$

$$x_{ij}^c \geq 0 \quad \forall (i,j) \in A, c \in C. \quad (35)$$

Again, after resetting the binary constraints on  $x$ , one may linearize the complementarity constraints (33):

$$\pi_i^c - \pi_j^c - n^c t_{ij}^{h(c)} \geq n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) - M_{ij}^c (1 - x_{ij}^c) \quad \forall (i,j) \in A, c \in C \quad (36)$$

$$x_{ij}^c \in \{0, 1\} \quad \forall (i,j) \in A, c \in C, \quad (37)$$

as well as the bilinear term of the leader's objective:

$$\tau_{ij}^c \geq 0 \quad (i,j) \in A, c \in C \quad (38)$$

$$\tau_{ij}^c - M_{ij}^c x_{ij}^c \leq 0 \quad \forall (i,j) \in A, c \in C \quad (39)$$

$$\tau_{ij}^c - t_{ij}^{h(c)} \leq 0 \quad \forall (i,j) \in A, c \in C \quad (40)$$

$$\tau_{ij}^c - t_{ij}^{h(c)} - M_{ij}^c x_{ij}^c \geq -M_{ij}^c \quad \forall (i,j) \in A, c \in C, \quad (41)$$

to yield a MIP formulation.

An alternative MIP formulation can be obtained by replacing constraints (36) with a constraints imposing the equality of the objective function values of the follower's primal and dual problems:

$$\sum_{(i,j) \in A} n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) x_{ij}^c + \sum_{(i,j) \in A} n^c \tau_{ij}^c - \sum_{i \in N} e_i^c \pi_i^c = 0 \quad \forall c \in C, \quad (42)$$

where the value of the variables  $\tau_{ij}^c$ ,  $\forall (i,j) \in A$ ,  $\forall c \in C$ , is already properly set by constraints (38)-(41).

Both MIP formulations require the same integer variables. When  $\alpha = 0$ , since the outer level objective is linear, variables  $\tau_{ij}^c$  and constraints (38)-(41) are redundant in the complementary slackness formulation.

### 2.3 The toll problem is not equivalent to the design problem

When there is only one O-D shipment, it can be easily shown that ND is equivalent to TS, in the sense that they yield the same optimal value and all suboptimal paths are made either unattractive (large tolls in TS) or unavailable (ND). Since the problem is separable by hazmat type, this also holds if there are more than one O-D shipments, provided that each carries a different type of hazmat. We next provide an example that illustrates the added flexibility of TS over ND, when more than one shipment carry the same type of hazmat.

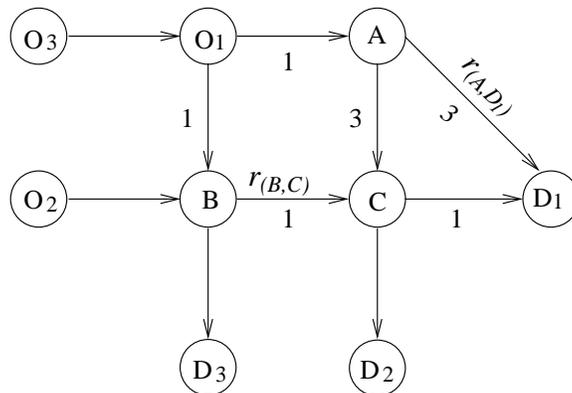


Figure 1: An example where toll-setting gives a lower optimal risk

Let us consider the example of Figure 1, that involves three O-D shipments,  $O_1 \rightarrow D_1$ ,  $O_2 \rightarrow D_2$  and  $O_3 \rightarrow D_3$ , comprised of only one truck each. One can notice that there is only one possible path for  $O_2 \rightarrow D_2$  and  $O_3 \rightarrow D_3$ , which is to go through intersections  $B, C$  and  $O_1, B$ , respectively. Suppose that the government's sole objective is to minimize the risk for the population ( $\alpha = 0$ ) and the carriers' sole objective is to minimize their traveling costs ( $\beta = 0$ ). Suppose also that the risk on arc  $(B, C)$  is larger than the one on arc  $(A, D_1)$ , i.e.,  $r_{(B,C)} > r_{(A,D_1)}$ , and that the risk on all other arcs is null (nobody lives within the evacuation limits). Suppose finally that the traveling cost on all arcs is one unit, except for arcs  $(A, D_1)$  and  $(A, C)$ , both having a traveling cost of three units. In that case, if the regulator does not interfere, then  $O_1 \rightarrow D_1$  would take the path going through intersections  $B, C$  (shortest path) and the total risk would be  $2r_{(B,C)}$  (recall that path  $O_2 \rightarrow D_2$  also uses  $(B, C)$ ).

With a network design policy, the regulator would close arc  $(C, D_1)$  since it is the only way to prevent the use of arc  $(B, C)$  for  $O_1 \rightarrow D_1$ . Arcs  $(B, C)$  and  $(O_1, B)$  cannot be closed since they must be used by  $O_2 \rightarrow D_2$  and  $O_3 \rightarrow D_3$ , respectively. Hence, the total risk would be  $r_{(B,C)} + r_{(A,D_1)}$  (path  $O_2 \rightarrow D_2$  uses  $(B, C)$  and path  $O_1 \rightarrow D_1$  uses  $(A, D_1)$ ). On the other hand, a solution to the toll problem would set the tolls so that path  $O_1 \rightarrow D_1$  uses neither arc  $(B, C)$  nor arc  $(A, D_1)$ . For instance, the regulator could put a toll of two units on arc  $(B, C)$  and one unit on arc  $(A, D_1)$ . The risk-free path  $O_1 \rightarrow D_1$  going through intersections  $A, C$  thus becomes as attractive for the carrier as the other more risky paths, and the total risk would be  $r_{(B,C)}$  (arc  $(B, C)$  must still be used for  $O_2 \rightarrow D_2$ ). In this example, if  $r_{(B,C)} \cong r_{(A,D_1)}$ , then a network design policy would thus only marginally reduce

risk ( $r_{(B,C)} + r_{(A,D_1)}$  vs  $2r_{(B,C)}$ ) whereas it would be halved with a toll policy ( $r_{(B,C)}$  vs  $2r_{(B,C)}$ ). Both risk mitigating policies are thus clearly not equivalent.

The main difference between the network design and the toll policies is that the latter can actually differentiate between carriers. A toll can be high enough to deter a carrier from using the corresponding arc, while another carrier moving the same type of hazmat might still use the arc. ND does not have the same flexibility since the design decisions have to be the same for all carriers moving the same type of hazmat.

### 3 Minimizing Hazmat Transport Risk via Toll-Setting

The previous section demonstrated that toll policies are more flexible than network design policies and can thus induce lower hazmat transport risk for the population. In this section, we will further show that it is always possible for a regulator to find a toll policy that induces minimum risk and that finding such a solution is an easy task.

A minimum risk flow is a solution corresponding to the minimum level of risk at which all shipments are delivered, i.e., a regulator's ideal solution. The problem of finding a minimum risk flow can be stated as follows:

$$(MR) \quad \min_x \sum_{c \in C} \sum_{(i,j) \in A} n^c \rho_{ij}^{h(c)} x_{ij}^c \quad (43)$$

s.t.

$$\sum_{(i,j) \in A} x_{ij}^c - \sum_{(j,i) \in A} x_{ji}^c = e_i^c \quad \forall i \in N, c \in C \quad (44)$$

$$x_{ij}^c \geq 0 \quad \forall (i,j) \in A, c \in C. \quad (45)$$

MR is comprised of the objective function of TS (25), where the value of  $\alpha$  is fixed to 0, and the flow conservation constraints. One can observe that MR is a pure network flow problem (one shortest path problem per carrier). Let  $\bar{x}$  denote the minimum risk flow obtained by solving MR. For  $\bar{x}$  to be the optimal solution to TS (i.e., for a toll policy to induce minimum risk for the population), then tolls have to be set on the road segments in such a way that  $\bar{x}$  becomes the carriers' optimal flow as well (an optimal solution to the inner problem (27)-(29)). This can be done by simply setting a toll on every arc with a value equal to the difference between the arc's coefficient in the objective function of MR and the one of the follower (27). This procedure is akin to marginal cost pricing (Pigou (1920)). In the present case, for a given arc  $(i,j) \in A$  and a given shipment  $c \in C$ , this marginal cost is  $(1-\beta)\rho_{ij}^h - c_{ij}$ . When tolls are set to these values, then the objective of the carriers matches of the leader and the carriers optimal flow obviously coincides with the minimum risk flow. However, nothing prevents a toll calculated in this fashion to be negative (population exposure can be null on some road segments). When subsidies are not permitted, some of the constraints (26) might thus be violated. In addition, all road segments can potentially be tolled in such a solution, which makes its implementation economically and technologically difficult, if not impossible.

Alternatively, the problem of finding a set of nonnegative tolls that yields the minimum risk flow can be solved by inverse optimization, which consists of inferring the values of some model parameters (in this case the tolls can be seen as a part of the cost coefficients) given the values of the decision variables. See Dial (1999) or Ahuja and Orlin (2001) for some other applications of inverse optimization. In our context, one might wish to minimize the sum of tolls raised from the carriers besides enforcing the minimum risk solution  $\bar{x}$ . This is achieved by the following linear mathematical program:

$$(IO(\bar{x})) \quad \min_t \sum_{c \in C} \sum_{(i,j) \in A} n^c t_{ij}^{h(c)} \bar{x}_{ij}^c \quad (46)$$

s.t.

$$\pi_i^c - \pi_j^c - n^c t_{ij}^{h(c)} \leq n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) \quad \forall (i, j) \in A, c \in C \quad (47)$$

$$\bar{x}_{ij}^c (\pi_i^c - \pi_j^c - n^c t_{ij}^{h(c)} - n^c (c_{ij} + \beta \rho_{ij}^{h(c)})) = 0 \quad \forall (i, j) \in A, c \in C \quad (48)$$

$$t_{ij}^h \geq 0 \quad \forall (i, j) \in A, h \in H, \quad (49)$$

where nonnegative tolls are chosen so that the complementarity slackness conditions of the follower's problem (carriers) are satisfied at  $\bar{x}$ . It is, in fact, the single-level model (31)-(35), where the variables  $x_{ij}^c$  are set at  $\bar{x}$ . One can notice that the flow conservation constraints and the non-negativity constraints on  $x$  are not necessary in  $IO(\bar{x})$  since they are trivially satisfied at  $\bar{x}$ .

If one chooses to impose the equality of the objective function values of the follower's primal and dual problems instead of complementary slackness conditions, constraints (48) can be replaced with the following equivalent linear constraints:

$$\sum_{(i,j) \in A} n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) \bar{x}_{ij}^c + \sum_{(i,j) \in A} n^c t_{ij}^{h(c)} \bar{x}_{ij}^c - \sum_{i \in N} e_i^c \pi_i^c = 0 \quad \forall c \in C. \quad (50)$$

**Proposition 1.** *When all road segments are subject to tolls, there exists a set of nonnegative tolls that yields a minimum risk solution, i.e.,  $IO(\bar{x})$  is always feasible.*

*Proof.* First, we note that there always exists a cycle-free minimum-risk solution  $\bar{x}$ , since this solution is the solution of a linear program, and can therefore be assumed to be an extreme point of a flow polyhedron.

The proof is based on an argument of Yang and Huang (2004), initially proposed in the context of forcing the optimal use of a congested transportation network involving customers with different valuations of travel time. Let us consider the following auxiliary linear program:

$$(AP) \quad \min_x \sum_{c \in C} \sum_{(i,j) \in A} n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) x_{ij}^c \quad (51)$$

s.t.

$$\sum_{(i,j) \in A} x_{ij}^c - \sum_{(j,i) \in A} x_{ji}^c = e_i^c \quad \forall i \in N, c \in C \quad (52)$$

$$\sum_{c \in C^h} n^c x_{ij}^c \leq \sum_{c \in C^h} n^c \bar{x}_{ij}^c \quad \forall (i, j) \in A, h \in H \quad (53)$$

$$x_{ij}^c \geq 0 \quad \forall (i, j) \in A, c \in C, \quad (54)$$

where  $C^h$  is the set of O-D shipments carrying hazmat type  $h \in H$ .

Let  $\pi_i^c, \forall i \in N, c \in C$ , and  $\lambda_{ij}^h, \forall (i, j) \in A, h \in H$ , be the dual variables associated with constraints (52) and (53), respectively. For a feasible solution of AP to be optimal, then it must also satisfy the following primal-dual optimality conditions (after constraints (53) are multiplied by  $-1$ ):

$$\pi_i^c - \pi_j^c - n^c \lambda_{ij}^{h(c)} \leq n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) \quad \forall (i, j) \in A, c \in C \quad (55)$$

$$x_{ij}^c (\pi_i^c - \pi_j^c - n^c \lambda_{ij}^{h(c)} - n^c (c_{ij} + \beta \rho_{ij}^{h(c)})) = 0 \quad \forall (i, j) \in A, c \in C \quad (56)$$

$$\lambda_{ij}^{h(c)} \geq 0 \quad \forall (i, j) \in A, h \in H. \quad (57)$$

One can notice that the complementary slackness conditions stating that either a constraint (53) is active, or the corresponding dual variable  $\lambda_{ij}^h$  is null, are not included in the latter optimality conditions. Since all coefficients are nonnegative in the objective function of MR (used to obtain  $\bar{x}$ ), constraints (53) are, in fact, always active in AP. Otherwise, a feasible solution to MR with a lower risk than  $\bar{x}$  would exist, which is impossible since  $\bar{x}$  is an optimal solution to MR.

One can also observe that the optimal value of AP (51) is  $\sum_{c \in C} \sum_{(i,j) \in A} n^c (c_{ij} + \beta \rho_{ij}^{h(c)}) \bar{x}_{ij}^c$  (the total flow on every arc for every hazmat type is known since all constraints (53) are active in AP for every feasible solution). Hence  $\bar{x}$ , which satisfies constraints (52)-(54), is an optimal solution of AP. The optimality conditions of AP are thus satisfied at  $\bar{x}$  and  $\text{IO}(\bar{x})$  is feasible ( $\text{IO}(\bar{x})$  constraints (47)-(49) are equivalent to AP optimality conditions (55)-(57), where the toll variables correspond to the nonnegative dual variables  $\lambda_{ij}^h$ ). Therefore, there always exists a solution to TS where all tolls are nonnegative and for which the corresponding cost is equal to the minimum risk.  $\square$

Hence, when the regulator only wishes to minimize risk, i.e., when  $\alpha = 0$  in the leader's objective function (25), TS is not a bilevel problem. However, the more general toll problem where the regulator rather wishes to minimize a combination of population exposure and traveling costs (including paid tolls) cannot be solved by inverse optimization and is thus a true bilevel problem. Nevertheless, when  $\bar{x}$  is an optimal solution to MR where the objective function (43) is replaced with:

$$\min_x \sum_{c \in C} \sum_{(i,j) \in A} n^c (\rho_{ij}^{h(c)} + \alpha c_{ij}) x_{ij}^c, \quad (58)$$

$IO(\bar{x})$ , although not equivalent to TS, can be used as a proxy. The latter inverse optimization problem indeed finds a set of minimum tolls yielding a solution itself minimizing a combination of population exposure and distance traveled. It has the advantage of being very easy to solve and providing solutions with a reduced combination of risk and traveled distance for the carriers, but may mean higher paid tolls compared to directly solving one of the MIP formulations for TS.

## 4 Solution Methodology

As demonstrated in the previous section, the toll problem is efficiently solved by inverse optimization when the sole objective of the regulator is to minimize hazmat transport risk. However, the general toll problem is, like the network design problem, truly bilevel. The MIP formulations proposed in Section 2 for TS and ND can be solved directly with a powerful linear programming software, but some enhancements are required to obtain optimal solutions in reasonable computing times.

### 4.1 Bounding the Big- $M$ constants

In all MIP formulations presented, large constants are used. It is well known in the integer programming field that the value of such constants has an impact on the solution process, and our formulations are no exception to the general rule.

#### 4.1.1 MIP formulation with equality of the primal and dual objectives

Dewez et al. (2006) have proposed tight and valid bounds for toll problems where the formulation imposing the equality of the primal and dual objectives of the follower's problem is used. Among other valid bounds, the authors propose to calculate, for a given arc  $(i, j) \in A$  and a given shipment  $c \in C$  (an O-D pair), the difference between the shortest distance from the origin of shipment  $c$  ( $O^c$ ) to its destination ( $D^c$ ) on a toll-free path (a path comprised of non-tollable arcs), and the shortest distance from  $O^c$  to  $D^c$  using arc  $(i, j)$  (when all tolls are fixed to 0). The idea is to compute the maximum tolls that could be set on every arc for every carrier. A similar procedure could be applied to network design problems. From constraints (20)-(23) and the binary constraints on  $y$ , for a given arc  $(i, j) \in A$  and a given shipment  $c \in C$ :

- i) if  $y_{ij}^{h(c)} = 0$ , then  $\tau_{ij}^c = 0$  and  $M_{ij}^c \geq \mu_{ij}^c$
- ii) if  $y_{ij}^{h(c)} = 1$ , then  $M_{ij}^c \geq \tau_{ij}^c$  and  $\tau_{ij}^c = \mu_{ij}^c$ .

Hence, the dual variables associated with constraints (5),  $\mu_{ij}^c$ , are valid upper bounds for  $M_{ij}^c$ , and, since  $\mu_{ij}^c$  represents the increase in the carriers' costs of shipment  $c$  when arc  $(i, j)$

is closed, they are themselves bounded by the value of the shortest distance from  $O^c$  to  $D^c$  on a path comprised of non-closable arcs.

In the case of the hazmat transportation problem, the existence of toll-free paths (or paths only comprised of non-closable arcs), is not guaranteed. Unlike other toll problems, the leader's objective in TS is not to maximize revenues raised from tolls, but to minimize population exposure (and even minimize a fraction of the paid tolls since they contribute to the carriers' costs). Hence, the problem is bounded without having to suppose that there exist toll-free paths between each origin-destination pairs. A valid upper bound on the shortest distance between an O-D pair, although less tight, can however be given by the longest path between the O-D pair. Yet, the problem of finding longest paths is NP-complete (unless it is on a directed acyclic graph, which is not the case here since arcs can represent two-way roads). Nevertheless, one can efficiently generate valid bounds by solving, for every O-D pair, a maximum cost flow problem (minimum cost flow where where all cost are multiplied by  $-1$  in the objective function), which is linear and bounded (every arc has a capacity of 1 unit of flow). Let  $B1_{ij}^c$  be the upper bound on  $M_{ij}^c$  obtained by calculating the difference between the value of the maximum cost flow problem from  $O^c$  to  $D^c$  (upper bound on the longest path) and the shortest distance from  $O^c$  to  $D^c$  using arc  $(i, j)$ . Although valid, these bounds are obtained from solutions which are not necessarily paths since they can contain cycles, both attached to the O-D paths or disjoint. For example, Figure 2 shows the solution of a maximum cost flow problem where a unit of flow goes from O to D. One can observe that the cycles  $(2 \rightarrow 3 \rightarrow 2)$  and  $(4 \rightarrow 5 \rightarrow 4)$  are present in the solution since they contribute to increasing the cost of the solution, but they break up the path. Yet, just removing both cycles  $(O \rightarrow 1 \rightarrow 2 \rightarrow D)$  may yield an invalid bound. On the other hand, one can improve the bounds by limiting the flow to one at every node and thus eliminating the cycles attached to the O-D paths (like  $(2 \rightarrow 3 \rightarrow 2)$ ). One can observe that this can be done without breaking the network structure, by splitting in two every node that are afterward linked together with a capacity of one unit. Let  $B2_{ij}^c \leq B1_{ij}^c$  be the upper bounds on the longest path obtained from these modified maximum cost flow problems.

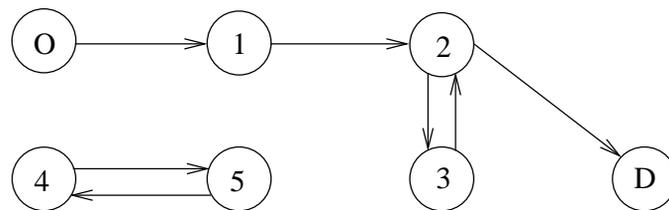


Figure 2: A maximum cost flow solution that does not correspond to a path

When one wishes to further improve the bounds through the incorporation of cycle elimination constraints (disjoint cycles like  $(4 \rightarrow 5 \rightarrow 4)$ ), then the network structure collapses and the solution process has to be embedded within a branch-and-bound procedure. Our numerical results show that when even the simplest such constraints are added (2-cycle constraints), the improved quality of the bounds is offset by the CPU time required for their

computation. Nonetheless, the linear relaxation of these constrained problems yields valid upper bounds (maximization problem), denoted by  $B3_{ij}^c$ , which improve on  $B2_{ij}^c$ . Our computational experiments show that the value of the linear relaxation and the total CPU time required to solve the network design problem are indeed improved by using  $B3_{ij}^c$  compared to using  $B1_{ij}^c$  and  $B2_{ij}^c$ , but also compared to a *best empirical bound* obtained by gradually decreasing a unique  $M$  appearing in every constraints (21) and (23) until the objective value stops being optimal.

#### 4.1.2 MIP formulation with complementary slackness conditions

From constraints (16)-(18) and the binary constraints on  $y$ , for a given arc  $(i, j) \in A$  and a given shipment  $c \in C$ , we may write:

- i) if  $x_{ij}^c = 0$  and  $y_{ij}^{h(c)} = 1$ , then  $M_{ij}^c \geq \pi_j^c - \pi_i^c + n^c(c_{ij} + \beta\rho_{ij}^{h(c)})$ ;
- ii) if  $x_{ij}^c = 0$  and  $y_{ij}^{h(c)} = 0$ , then  $M_{ij}^c \geq \mu_{ij}^c + \pi_j^c - \pi_i^c + n^c(c_{ij} + \beta\rho_{ij}^{h(c)})$ ;
- iii) if  $x_{ij}^c = 1$ , then  $y_{ij}^{h(c)} = 1$  and  $M_{ij}^c \geq \mu_{ij}^c$ .

Hence, the constant  $M_{ij}^c - n^c(c_{ij} + \beta\rho_{ij}^{h(c)})$  is bounded by  $\mu_{ij}^c + \pi_j^c - \pi_i^c$ , where  $\mu_{ij}^c$  is the increase in the carriers' costs when arc  $(i, j)$  is closed for shipment  $c$ , and  $\pi_j^c - \pi_i^c$  is the difference between the shortest distance from  $O^c$  to  $j$  and the shortest distance from  $O^c$  to  $i$ . When the existence of a toll-free path (or a path comprised of non-closable arcs) is not guaranteed for every pair of nodes, a valid upper bound on  $\pi_j^c - \pi_i^c$  is given by the longest path between  $O^c$  and  $D^c$ , which is also a valid upper bound for  $\mu_{ij}^c$  (see Section 4.1.1).  $M_{ij}^c$  can thus be set to  $2B3_{ij}^c + n^c(c_{ij} + \beta\rho_{ij}^{h(c)})$ , where  $B3_{ij}^c$  is the upper bound provided by the LP value of a maximum cost flow problem augmented with the  $k$ -cycle constraints (see Section 4.1.1). When the formulation including complementary slackness conditions is used, upper bounds on  $M_{ij}^c$  can be more than twice larger than the bounds corresponding to the equality formulation.

## 4.2 Warm-starting with a toll scheme

In some cases, the regulator can be more interested in network design solutions than in toll solutions if it feels that the former are easier to implement. Nevertheless, the toll problem (or its proxy) can be used to construct a feasible solution to the network design problem to accelerate the solution process. This is particularly true when the computing time is limited and a good feasible solution is needed rapidly (e.g., when evaluating different scenarios).

A feasible solution to ND can be found by solving a minimum cost flow problem on a reduced network where all arcs that are tolled in the optimal solution of TS, but unused by a carrier, are removed. This latter solution  $(x, y)$  can be used, after the value of the remaining variables  $(\pi, \mu, f)$  have been computed, as an upper bound in a branch-and-bound procedure. It is

interesting to add that a solution obtained with the toll problem proxy can also be used to warm-start the general bilevel toll problem.

The computational experiments found in Section 5 show that this enhancement is helpful in reducing computing times. This latter statement is true even when the improved solution process is compared to a solution process using CPLEX 10.0, which includes MIP heuristics that have been known to efficiently find integer solutions.

## 5 Computational Experiments

In this section, we present computational experiments that were carried out on the data found in Kara and Verter (2004). We first provide a description of these instances, followed by a summary of our computational experiments.

### 5.1 The data set

The test data is based on the highway system of Western Ontario, Canada. Geographical information systems were used to obtain a description of highway segments and information on population exposure within the region of interest. Artificial nodes were added to the real road network to ensure that the density of the population along any given arc is constant. The records of Statistics Canada (1998) provided the list of hazmat shipments with corresponding origin, destination, hazmat type and the number of trucks used. Four different hazmat types, accounting for 56% of all the hazmat transported, are considered: gasoline, fuel oil, alcohol, and petroleum and coal tar. However, since the first three types pose the same exposure (evacuation of the people within 800 meters, according to Transport Canada, 1996), they were grouped together. Therefore, the data set is comprised of 287 shipments of either one of two hazmat types. The road network is comprised of 48 nodes and 114 arcs (57 two-way links) affecting 31 population centers. In the study of Kara and Verter (2004), only the 53 shipments with an annual volume of 500 trucks or more were kept in the data. In the present paper, our tests are done on the same subset of shipments (*500+ trucks*), but also on all 287 shipments (*all shipments*). The partial data set is included in our computational experiments for the reader to appreciate the increased difficulty of solving the complete data set.

### 5.2 Computational experiments

To evaluate the benefits of solving TS versus ND, we solved both formulations of each problem: the formulation with complementary slackness conditions (*CS*) (used by Kara and Verter (2004) for ND) and the alternative formulation involving the equality of the primal and dual objectives (*PD*). For TS (with positive  $\alpha$ ) and for ND, the single-level MIP formulations were solved, using CPLEX 10.0. The big- $M$  constants were set to  $B3_{ij}^c$  (see Section 4.1). TS was also solved by inverse optimization (*IO*) and we warm-started the solution process of

ND with a feasible solution constructed from the optimal set of tolls ( $IS$ ) obtained by IO. All experiments were performed on a AMD Opteron Processor 248, 2191 MHz computer, using two processors. When  $IS$  is used (and only in that case), the heuristics used by CPLEX 10.0 to generate integer solutions became unnecessary and were thus deactivated.

Table 2: Notation (numerical experiments)

$CS$	Formulation including complementary slackness conditions
$IO$	Inverse optimization solving process
$IS$	Network design problem with an initial solution constructed from TS
$ND$	Network design problem
$PD$	Formulation where primal and dual objectives are equal
$TS$	Toll-Setting problem
$\% \text{ chg}$	Change, in percentage, from a specified ND model to a TS model
$CPU$	Total CPU time (in minutes)
$BBn$	Total number of nodes in B&B tree
$Cuts$	Number of cuts generated by CPLEX 10.0
$PopExp$	Total population exposure (in millions of persons)
$Dist$	Total distance traveled (in millions of kilometers)
$ObjVal$	Optimal value of the function combining risk and traveled distance
$ObjVal+$	Optimal value of the function combining risk, traveled distance and paid tolls
$Tpaid$	Total amount of tolls paid by the carriers (in millions of dollars)
$Nc-Nt$	Number of arcs closed or number of arcs tolled

We first present numerical results for the case where the leader’s objective is solely to minimize the population exposure, and then for the more general case where a fraction of the carriers’ costs is also minimized in the leader’s objective function. Population exposure ( $PopExp$ ), traveled distance ( $Dist$ ) and computational effort ( $CPU$ ) needed to solve both data sets with the different approaches are compared. We also indicate, for all approaches, the number of cuts generated by CPLEX ( $Cuts$ ), the number of nodes evaluated in the branch-and-bound tree ( $BBn$ ) and the number of closed, or tolled, arcs ( $Nc-Nt$ ) out of the 228 possibilities (114 arcs and two hazmat types). For the toll problem, we also report the total amount of tolls paid by the carriers ( $Tpaid$ ). Finally we computed the percentage change in population exposure and traveled distance between ND and TS ( $\% \text{ chg}$ ). The notation is displayed in Table 2.

### 5.2.1 Minimizing population exposure

Even when the government’s sole objective is to minimize population exposure, it is advantageous to set  $\alpha$  to a small positive value in order to favor, among minimum risk solutions, one that minimizes carriers’ cost. For both data sets tested,  $\alpha = 1$  was suitable. ND and TS were solved for  $\alpha = 0$  and  $\alpha = 1$ . The results are presented in Table 3.

For ND, the alternative PD formulation is faster than the current CS formulation, with the exception of the smallest data set ( $\alpha = 1$ ), where the optimal solution is found at node 0<sup>+</sup> of the branch-and-bound procedure, i.e., exploiting CPLEX heuristics and/or cuts at node

0. Recall that, in CS, binary constraints are required on  $x$ , whereas they are not in PD (see Section 2.1.1). Formulation CS could not even solve the data set involving all shipments, within 36 hours of computing time, unless warm-started (IS). The warm-start procedure actually improves the running time of both CS and PD, either with  $\alpha = 0$  or  $\alpha = 1$ .

Table 3: Network design problem vs toll problem<sup>†</sup>

	<i>CPU</i>	<i>BBn</i>	<i>Cuts</i>	<i>PopExp</i>	<i>Dist</i>	<i>Tpaid</i>	<i>Nc-Nt</i>
<b><i>500+ trucks</i></b>							
<i>ND</i> ( $\alpha = 0$ )							
1. <i>CS</i>	1.28	190	356	481.38	27.88		140
2. <i>CS IS</i>	1.27	211	373	481.38	27.88		140
3. <i>PD</i>	0.49	18	5	481.38	27.88		14
4. <i>PD IS</i>	0.34	19	5	481.38	27.86		14
<i>ND</i> ( $\alpha = 1$ )							
5. <i>CS</i>	0.04	0	9	481.38	27.86		140
6. <i>CS IS</i>	0.05	0	9	481.38	27.86		139
7. <i>PD</i>	1.04	31	5	481.38	27.86		17
8. <i>PD IS</i>	0.30	18	5	481.38	27.86		14
<i>TS</i> ( $\alpha = 0$ )							
9. <i>IO</i>	0.01	0	0	481.25	27.81	0.012	26
<i>TS</i> ( $\alpha = 1$ )							
10. <i>IO</i>	0.01	0	0	481.25	27.81	0.012	26
11. <i>PD</i>	0.02	0	0	481.25	27.81	0.012	26
<i>% chg 9 vs 8</i>				-0.03	-0.18		
<b><i>All shipments</i></b>							
<i>ND</i> ( $\alpha = 0$ )							
1. <i>CS</i>	+36h						
2. <i>CS IS</i>	1503.33	25531	2200	656.87	35.02		87
3. <i>PD</i>	21.58	118	6	656.87	35.62		40
4. <i>PD IS</i>	16.05	175	9	656.87	35.81		48
<i>ND</i> ( $\alpha = 1$ )							
5. <i>CS</i>	880.94	8086	229	656.87	34.58		85
6. <i>CS IS</i>	176.80	2000	29	656.87	34.58		86
7. <i>PD</i>	17.92	76	9	656.87	34.58		35
8. <i>PD IS</i>	13.06	84	10	656.87	34.58		44
<i>TS</i> ( $\alpha = 0$ )							
9. <i>IO</i>	0.02	0	0	652.64	34.57	0.282	44
<i>TS</i> ( $\alpha = 1$ )							
10. <i>IO</i>	0.02	0	0	652.64	34.56	0.282	41
11. <i>PD</i>	0.27	0	170	652.64	34.56	0.282	41
<i>% chg TS vs 8</i>				-0.64	-0.06		

<sup>†</sup> Unless otherwise specified, all CPU times are in minutes.

In Table 3, one observes that the number of arcs closed is significantly reduced under PD. The latter MIP formulation thus yields, in a reduced computing time, more attractive solutions for the regulator (less expensive to implement). When the leader's objective function is perturbed to allow the minimization of the number of arcs closed, as a second objective, the problem becomes much harder to solve, without achieving a significant improvement. For

instance, PD closes 14 arcs for *500+ trucks* while the minimum possible is 11 arcs. For this reason, the results of the latter problem are not reported. If, in order to gain more control on the carriers, one is interested in a solution involving a large number of closed arcs, then one simply has to close all arcs that carry no flow in the ND PD IS solutions. The same result can be achieved under TS by setting the tolls on all unused arcs to arbitrarily large values.

When  $\alpha = 0$ , the distance traveled by the carriers can vary for the same level of risk, up to 3.6% higher for ND in *all shipments*, i.e., 35.81 million kilometers compared to the minimum of 34.58 million. Since the inclusion of a fraction of the carriers' traveling costs within the leader's objective function actually makes ND easier to solve, PD IS with  $\alpha = 1$  (model 8) seems to be the best choice for ND when the government's objective is to minimize population exposure.

TS is solved very quickly and it yields the minimum risk flow while minimizing the distance traveled (with  $\alpha = 1$ ) and setting positive tolls on a small number of arcs. When  $\alpha = 1$ , it is interesting to note that for both data sets, the solution given by TS IO provides the same optimal value than the true bilevel model where the traveling costs include the paid tolls on top of the traveling distance (TS PD), i.e., there is no solution yielding the minimum risk while reducing a combination of traveled distance and paid tolls compared to the solution provided by the proxy. For these instances, the proxy is thus equivalent to TS when the traveling costs are only minimized as a second objective. When comparing TS to the best ND (model 8), one can observe that the total population exposure is only reduced by 0.03% for *500+ trucks*, but by a higher percentage (0.64%) when all shipments are considered. The total traveled distance can also be slightly reduced under TS. For *500+ trucks*, the increase in total cost related to the tolls *actually* paid is slightly smaller than the decrease in total traveling costs (0.14%), while it is slightly higher when all shipments are considered (0.76%). It is important to note that this last statement applies no matter what the traveling costs per kilometer are. Depending on the size of the truck and on the annual utilization, the operating costs of a liquid tanker in Ontario lies between 1.40\$ and 2.30\$ per kilometer (Transport Canada (2005)). Since arc costs are constants in the models, modifying the traveling costs only scales the models, as long as the large constants  $M_{ij}^c$  are scaled proportionally. Algorithmic efficiency is the same and the toll vectors are only scaled.

### Bounding the Big- $M$ constants

As described in Section 4.1, the big- $M$  constants used in the single-level MIP formulations can be set to the difference between the shortest distance from  $O^c$  to  $D^c$  using arc  $(i, j)$ , and an upper bound on the longest distance from  $O^c$  to  $D^c$ . Recall that  $B1_{ij}^c$  is obtained by solving a maximum cost flow problem from  $O^c$  to  $D^c$ , while  $B2_{ij}^c$  is obtained by solving a modified problem where the flow is limited to one at every node and  $B3_{ij}^c$ , when  $k$ -cycles are forbidden in the linear relaxation of the latter modified maximum cost flow problems. In our numerical results, the addition of  $k$ -cycles constraints did not improve  $B3_{ij}^c$  for  $k > 2$ .

Table 4 compares the different bounding methods on the basis of the total CPU time required

to solve ND PD IS, with  $\alpha = 1$ , and the linear relaxation value (*LP value*) they yield. Besides the bounds described in Section 4.1 ( $B1_{ij}^c$ ,  $B2_{ij}^c$  and  $B3_{ij}^c$ ), two other methods were tested. *Total arc costs* uses a common  $M$ , that is set equal to the value of the sum, for all carriers, of all arc costs in the network (it is valid since every arc has a capacity of one for every carrier). This trivial bound was then decreased empirically until the optimal value of the resulting problem stopped being optimal. The latter bound (*Best empirical M*), for which the optimal value needs to be known a priori, only served as a comparison point. The methods are ranked on the basis of their corresponding LP relaxation. One observes in Table 4 that the CPU time decreases significantly with every slight improvement in the LP value (with  $\alpha = 1$ , the optimal integer objective function value is 691.45) and that  $B3_{ij}^c$  is clearly the best choice. It is interesting to note that the LP value with the best empirical  $M$  (common constant) can be lower than with other bounding methods with a specific large constant for every arc and every carrier ( $M_{ij}^c$ ).

Table 4: Comparison of bounding methods for  $M_{ij}^{c,\dagger}$ 

<i>ND PD IS</i> ( $\alpha = 1$ )	<i>LP value</i>	<i>CPU</i>
1. $B3_{ij}^c$	687.33	13.06
2. $B2_{ij}^c$	687.30	22.14
3. <i>Best empirical M</i>	687.26	27.17
4. $B1_{ij}^c$	687.25	42.32
5. <i>Total arc costs</i>	687.19	+36h

† Unless otherwise stated, CPU times are in minutes.

Our numerical experiments have also shown that the LP value of the existing MIP formulation (ND CS IS based on  $B3_{ij}^c$ ) is equal to the one obtained with the best empirical  $M$  (687.20). Even though the upper bounds based on  $B3_{ij}^c$  can be more than twice as large under CS as under PD, they are nevertheless quite good for CS, and the comparison between formulations CS and PD found previously remains relevant. The fact that the LP value obtained under PD is better than the one obtained under CS provides numerical evidence that PD is more efficient.

### 5.2.2 The general hazmat transportation problem

For the problem where the leader's objective function involves a carrier term, Figure 3 illustrates the compromise between the population exposure and the traveled distance when the parameter  $\alpha$  is gradually increased in TS (*all shipments*), i.e., the Pareto boundary.

One can notice in Figure 3 that the population exposure only slowly increases at first, when the carriers' costs rapidly decrease, and then more rapidly (when the population exposure goes beyond about 850 millions). This turning point corresponds to a value of  $\alpha = 70$ . A similar curve is found when  $\alpha$  is gradually increased in the smaller data set.

Table 5 presents a comparison of the population exposure, the traveled distance and the computational effort needed to solve ND and TS on both data sets for the turning point  $\alpha$

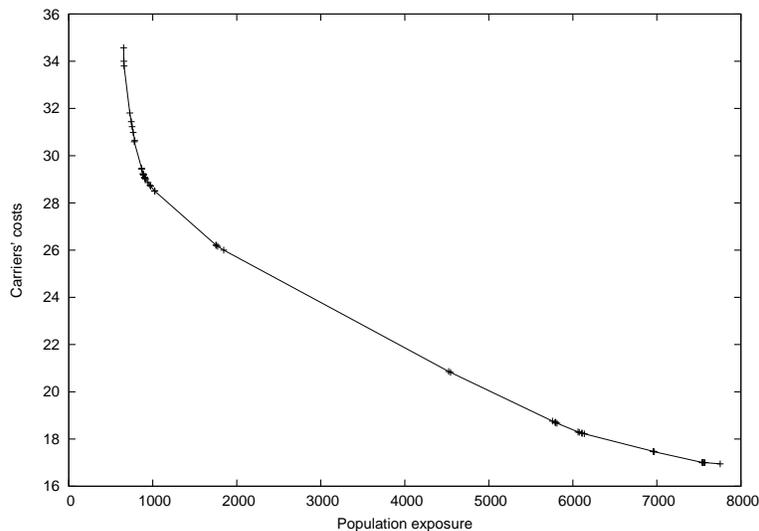


Figure 3: How the population exposure increases as the carriers' costs decrease

value. For TS and ND, both single-level MIP formulations were solved (PD and CS), but since PD was again clearly the best choice, only the results with PD are included in the table. As a comparison to the true bilevel TS, we also solved a proxy of TS by inverse optimization (IO) (see Section 3). The solution to the latter problem also served to warm-start ND and TS. For this general problem, we indicate the leader's objective function value when it combines risk and traveled distance ( $ObjVal$ ), but also when it combines risk, traveled distance and the paid tolls ( $ObjVal+$ ). The abbreviations for all the given solution characteristics are defined in Table 2.

The same conclusions as the minimum risk problem can be drawn for the general network design problem, i.e., the proposed alternative formulation warm-started from an initial solution constructed from a set of tolls (model 2, PD IS) is clearly the best choice for ND. It is solved efficiently and the solutions contain a small number of closed arcs. For the smaller data set, one can observe that when TS is approximated with IO (model 3), the solution obtained is equivalent to the one given by the true bilevel model (model 4, PD IS). When all shipments are considered, the decrease in the combination of risk and traveling costs ( $ObjVal$ ) is higher with the proxy than with the true model ( $-0.34\%$  for TS IO and  $-0.19\%$  for TS PD IS, compared to ND). On the other hand, when the paid tolls are taken into account, the proxy actually increases the combination of risk and total carriers' costs ( $ObjVal+$ ), compared to ND, whereas the true model does not. The bilevel TS is a lot harder to solve than its proxy, but not significantly harder than ND. The different methodologies can provide different scenarios to be analyzed by the regulator.

Table 5: General network design problem vs general toll problem ( $\alpha = 70$ )<sup>†</sup>

	<i>CPU</i>	<i>BBn</i>	<i>Cuts</i>	<i>PopExp</i>	<i>Dist</i>	<i>ObjVal</i>	<i>Tpaid</i>	<i>ObjVal+</i>	<i>Nc-Nt</i>
<b><i>500+ trucks</i></b>									
<i>ND</i>									
1. <i>PD</i>	0.90	10	3	623.59	24.43	2333.37			9
2. <i>PD IS</i>	0.19	18	5	623.59	24.43	2333.37			12
<i>TS</i>									
3. <i>IO</i>	0.01	0	0	623.46	24.38	2329.83	0.012	2330.67	27
4. <i>PD IS</i>	0.01	0	28	623.46	24.38	2329.83	0.012	2330.67	16
<i>% chg TS vs 2</i>				-0.02	-0.20	-0.15		-0.12	
<b><i>All shipments</i></b>									
<i>ND</i>									
1. <i>PD</i>	10.41	160	5	855.76	29.76	2938.95			27
2. <i>PD IS</i>	4.64	147	5	855.76	29.76	2938.95			26
<i>TS</i>									
3. <i>IO</i>	0.02	0	0	867.41	29.45	2928.87	0.546	2967.08	39
<i>% chg 3 vs 2</i>				+1.36	-1.04	-0.34		+0.96	
4. <i>PD IS</i>	8.71	353	81	857.40	29.66	2933.29	0.029	2935.32	34
<i>% chg 4 vs 2</i>				+0.19	-0.35	-0.19		-0.12	

<sup>†</sup> All CPU times are in minutes.

### 5.3 Summary of computational experiments - Constrained case

In the models presented in the previous sections, it was assumed that all road segments were subject to restrictions (tolls or curfew). In real-world situations, however, it is possible that some of them are free of restrictions for economical, political or technical reasons, irrespective of the actual risk. When it is the case, TS becomes a combinatorial program that cannot be solved any more as a linear program. In contrast, the corresponding network design problem can be facilitated since the number of feasible combinations is reduced. When some road segments have to stay toll-free, the optimal value of the objective function is likely to deteriorate (second-best pricing).

A weakness of the toll problem is that tolls are not necessarily set on the risky arcs. For instance, one of the optimal solutions to the example shown in Figure 1 sets tolls on arcs  $(A, D_1)$  and  $(O_1, B)$  (instead of  $(A, D_1)$  and  $(B, C)$ ). The solution, although equivalent for the regulator, can be viewed as inequitable since  $O_3 \rightarrow D_3$  has to pay a toll although it uses a risk-free path, while  $O_2 \rightarrow D_2$  is toll-free, even though it uses a risky arc! This weakness also arises in the network design problem, as nothing prevents risk-free arcs to be closed and thus lengthen a path for a carrier that would not have gone through a populated area, but can be partially dealt with by restricting the set of arcs subject to tolls or curfew, according to their associated risk. Some rules might allow an arc to be tolled, or closed, only if the corresponding population exposure exceeds a given threshold value, yielding solutions that may be more acceptable to the carriers. For the numerical results presented in this section, this minimum level of risk ( $Rmin$ ), given by a minimum number of people exposed,

was gradually increased, and Table 6 compares ND and TS for the different values, when all shipments are considered and  $\alpha = 1$ . The single-level MIP formulation imposing the equality of the objective function values of the follower’s primal and dual problems (PD) was solved (with  $M_{ij}^c = B3_{ij}^c$ ) for ND and TS. We also tried to improve the solution process of ND by warm-starting it from a feasible solution constructed with an optimal toll scheme and the total CPU time of the latter solution process (including the computing time for solving TS) is given in the table (*CPU IS*). We also indicate, for every level of risk, the percentage of arcs that are subject to restrictions among all arcs in the network (*arc%*) and the percentage decrease in population exposure ( $\downarrow R\%$ ) obtained with TS as opposed to ND. The abbreviations for all other solution characteristics are defined in Table 2.

Table 6: Network design problem vs toll problem - Constrained case<sup>†</sup>

		<i>Network Design (ND PD)</i>					<i>Toll-Setting (TS PD)</i>					
<i>Rmin</i>	<i>arc%</i>	<i>PopExp</i>	<i>Dist</i>	<i>Nc</i>	<i>CPU</i>	<i>CPU IS</i>	<i>PopExp</i>	<i>Dist</i>	<i>Tpaid</i>	<i>Nt</i>	<i>CPU</i>	$\downarrow R\%$
0	100	656.87	34.58	35	17.92	13.08	652.64	34.56	0.28	41	0.02	0.64
1	45	656.87	34.58	30	2.34	1.00	652.64	34.56	0.28	37	0.24	0.64
500	40	656.87	34.58	27	1.22	0.94	652.64	34.56	0.28	35	0.24	0.64
1500	37	659.44	34.58	32	1.09	1.16	652.64	34.56	0.28	37	0.19	1.00
3000	32	659.44	34.58	30	1.12	0.76	652.64	34.56	0.42	34	0.15	1.00
5000	25	695.79	34.30	28	0.79	0.57	691.03	34.33	0.21	26	0.20	0.68
7000	23	699.46	33.73	24	0.41	0.35	694.70	33.76	0.21	31	0.11	0.68
10000	18	699.46	33.73	22	0.33	0.29	699.46	33.73	0.00	23	0.10	0.00

<sup>†</sup> All CPU times are in minutes.

One can see, from Table 6, that 55% of the network’s arcs do not involve any population exposure. Once these arcs are taken out of the subset of arcs which are subject to restrictions, i.e., when  $Rmin = 1$ , the number of closable combinations is reduced and ND becomes much easier to solve. The opposite phenomenon can be observed for TS as it stops being linear when  $Rmin \geq 1$ . As  $Rmin$  increases, ND continues to get easier to solve while the CPU time for TS is more stable. The fact that TS is harder to solve when  $Rmin \geq 1$  makes the use of its solution as a starting point for ND less attractive, but one can observe that ND PD IS is nevertheless generally slightly faster to solve than ND PD (recall that CPU TS is already included in CPU IS).

One can also observe in Table 6 that from  $Rmin = 0$  to 1500, the total carriers’ costs (distance traveled and tolls) and the total population exposure do not increase for TS, while the number of tolled arcs decreases as  $Rmin$  increases. In addition, the set of tolled arcs in the solutions also changes. Hence, the solution with  $Rmin = 1500$  is as interesting for the regulator as the one with  $Rmin = 0$ , while being perceived as more fair from the carriers. It has the advantage of not restricting the use of less risky arcs and thus preventing situations where a carrier pays a toll even if it does not go through any populated area (just to prevent another carrier to use a risky path). For the network design problem, the population exposure starts increasing when  $Rmin = 1500$ . At that minimum risk level, there is, in fact, a 1% difference in population exposure when the design problem is solved instead of the toll problem, which is solved about six times faster than ND. One can finally observe

that when  $R_{\min} = 10000$ , TS becomes equivalent to ND. When only the most risky arcs are subject to restrictions, no tolls are paid by the carriers (they only serve to discourage the carriers to use the corresponding arcs) and the optimal risk for the population and costs for the carriers are the same in TS and in ND. It is interesting to add that when the optimal value is the minimum risk, i.e., up until  $R_{\min} = 3000$ , it was always possible to solve TN with inverse optimization, in a fraction of TS PD CPU, which makes warm-starting ND with TS even more advantageous.

In summary, these constrained hazmat problems are interesting since they produce solutions which can be more acceptable to the carriers. For these problems, toll-setting still finds better solutions than network design in a reduced computing time.

## Conclusion

This paper has introduced toll-setting as an efficient policy tool for mitigating the public and environmental risks associated with dangerous goods shipments. We compared the hazmat TS problem, where tolls are imposed on road segments in order to channel the hazmat shipments toward less populated roads, with the more popular hazmat ND problem, where certain road segments are closed to hazmat transportation. We demonstrated that TS, by being able to differentiate between carriers, can achieve higher reductions in the associated transport risks while only slightly increasing the carriers' costs, and can be used by a regulator to obtain minimum risk solutions very efficiently. The paper has also proposed a more efficient ND formulation necessitating a reduced number of integer variables and introduced an improved solution methodology where the toll problem is used to construct an initial solution. Finally, this paper has proposed valid and easily calculated bounds for the value of the large constants used in the MIP formulations. The bounds that are proposed in the literature for other toll problems always rely on the existence of a toll-free path, which is not the case for this hazmat transportation problem. Together, the proposed enhancements have permitted to solve a much larger instance of the network design problem in reasonable computing time whereas the former approach proposed by Kara and Verter (2004) could not. The paper further proposed to limit the set of road segments subject to restrictions to improve the buy-in received from the hazmat carriers. Future developments of our approach will consider both risk equity among the different population centers and cost equity among the carriers.

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