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Ruteo de Vehículos en el Transporte de Materiales Peligrosos

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Abstract

Abstract (English)

The main objective of this thesis is to study the hazardous materials (HazMat) transportation problem considered as a heterogeneous fleet vehicle routing problem. HazMat transportation decisions comprise different and sometimes conflicting objectives. Two are considered in this work, the total routing cost and the total routing risk. The first task undertaken was the formulation of a mathematical model for the routing risk minimization, which depends on the type of vehicle, the material being transported, and the load change when the vehicle goes from one customer to another. A piecewise linear approximation is employed to keep a mixed integer linear programing formulation.

Hybrid solution methods based on neighborhood search are explored for solving the routing risk minimization. This includes the study of neighborhood structures and the development of a Variable Neighborhood Descent (VND) algorithm for local search, and a perturbation mechanism (shaking neighborhoods). A post-optimization procedure is applied to improve the solution quality. Finally, two different solution approaches, a multi-objective dominance-based algorithm and a meta-heuristic ϵ-constraint method are employed for addressing the multi-objective version of the problem. Two performance metrics are used: the hypervolume and the Δ-metric. The front approximations show that a small increment in the total routing cost can produce a high reduction in percentage of the expected consequences given the probability of a HazMat transportation incident.

Keywords : Mathematical models, Hazardous Substances - Transport, Hazardous Substances - Risk Assessment, Variable neighborhood search, Traveling salesman Problem

Résumé (Français)

L'objectif de cette thèse est d'étudier le problème du transport de matières dangereuses (HazMat) vu comme un problème de tournées de véhicules à flotte hétérogène. Les décisions pour ce type de transport comportent des objectifs différents, parfois antagonistes. Deux sont pris en compte dans ce travail, le coût et le risque. La première tâche entreprise a été la formulation d'un modèle mathématique pour la minimisation du risque, qui dépend du type de véhicule, du matériel transporté et du changement de charge lorsque le véhicule passe d'un client à un autre. Une approximation linéaire par morceaux est utilisée pour conserver une formulation de programmation linéaire en nombres entiers mixtes.

Des méthodes hybrides basées sur des explorations de voisinages sont proposées pour traiter la minimisation du risque. Cela comprend l'étude des structures de voisinages et le développement d'un algorithme de descente à voisinages variables (VND) pour la recherche locale, ainsi qu'un mécanisme de perturbation des solutions. Une post-optimisation est appliquée pour améliorer la qualité des solutions obtenues. Enfin, deux approches, un algorithme basé sur la dominance multi-objectif et une méta-heuristique de type ϵ- contrainte, sont développes pour traiter la version multi-objectif. Deux mesures de performance sont utilisées : l'hypervolume et la Δ-métrique. Les approximations de fronts montrent qu'une légère augmentation du coût total des tournées peut entraîner une forte réduction en pourcentage des risques.

Mots clés: Modèles mathématiques, Substances dangereuses - Transport, Substances dangereuses - Évaluation du risque, Recherche à voisinage variable, Problème du voyageur de commerce.

Resumen (Español)

El objetivo principal de esta tesis es estudiar el problema del transporte de materiales peligrosos (HazMat *hazardous materials*) modelado como un problema de ruteo de vehículos con flota heterogénea (HVRP *heterogeneous fleet vehicle routing problem*). Las decisiones en el transporte de HazMat comprenden considerar objetivos diferentes y a veces contradictorios. Dos son los objetivos considerados en este trabajo, el costo y el riesgo total de ruteo. La primera tarea realizada fue la formulación de un modelo matemático para la minimización del riesgo de ruteo, que depende del tipo de vehículo, el material que se transporta y el cambio en el tamaño de la carga cuando el vehículo pasa de un cliente a otro. Se emplea una aproximación lineal por partes de la función objetivo para mantener una formulación de programación lineal entera mixta.

Se exploran métodos híbridos de solución basados en búsqueda por vecindarios para resolver el problema de minimización del riesgo total de ruteo. Esto incluye el estudio de las estructuras del vecindario y el desarrollo de un algoritmo de descenso de vecindario variable (VND *variable neighborhood descent*) para realizar la búsqueda local, y de mecanismos de perturbación (estructuras de vecindario para perturbar las soluciones). Se aplica un procedimiento post-optimización (SP *set partitioning*) para mejorar la calidad de las soluciones. Finalmente, se emplean dos enfoques de solución diferentes para abordar la versión multi-objetivo del problema, un algoritmo basado en la dominancia Pareto y un método ϵ-*constraint* heurísticos. Se utilizan dos indicadores de rendimiento para algoritmos multi-objetivo: el *hypervolumen* y la métrica Δ. Las aproximaciones del frente Pareto obtenidas muestran que un pequeño incremento en el costo total de ruteo puede producir una gran reducción en el porcentaje de las consecuencias esperadas dada la probabilidad de un incidente de transporte de materiales peligrosos.

Palabras claves: Modelos Matemáticos, Substancias peligrosas - Transporte, Substancias - Evaluación del riesgo, Búsqueda con vecindarios variables, Problema del agente viajero.

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Chapter 1

Introduction

1.1 Introduction (English)

Today not only efficient transportation is important, environmental and safety concerns have become significant drivers towards more efficient and responsible transportation. Examples of the former are the transportation of hazardous materials (HazMat) or dangerous goods and green logistic. HazMat shipments are integral part of our industrial life style. These shipments, in most of the instances, originates and terminates at many different locations all around the world, what underlines the importance of the role that transportation plays for HazMat. What differentiates HazMat transportation problems from transportation of other materials is the risk associated with an accidental release of these materials during uploading, transportation and downloading. HazMat could pose an unreasonable risk to people, environment, and property when transported in commerce. Most of the shipments of these products use road networks (national routes and street network routes), and they are crucial for country economies and provide revenues to the shippers and fright owners.

Transportation using the road system represents an increasingly pressing problem due to the constant augmentation of the shipments number and amount. The road HazMat incidents represents the vast majority of incidents, indicating the importance of safety for HazMat transportations on roads. Even though, the number of vehicles involving in accidents when transporting HazMat is a small minority, HazMat transportation incidents have greater average consequences, this illustrates the low frequency-high consequence nature of road transportation risk. Assessing the risk events in HazMat transportation is a difficult task; the frequency of these events is very low, crashes on roadways are uncertain, but these incidents have a large impact on people and buildings and other traffic by the explosion or spill of

HazMat. There is no consensus on the best way to model risk but, it is generally agreed that any formulation will include two elements: the probability of an accidental HazMat release, and its associated consequences.

HazMat transportation seeks to reduce the risk involved in it for the purpose of improving the safety of the human, infrastructure and natural environment. The objective of the HazMat transportation problem is to move a quantity of a material considered as HazMat from the origins to the destinations through the most economic and safest routes. Transportation of HazMat involves multiple interested parties such as shippers, carriers, manufacturers, residents, insurers, governments, and emergency responders. Who usually have different priorities for cost and risk, among the possible objectives. HazMat transportation routing problem has two main focuses: shortest path problems (associated with full truck load distribution) and vehicle routing problem (VRP) (associated with less than full truck load distribution). There have been more research effort related to the first type of problems than the second ones. In accordance with this last aspect, in this work emphasis is given to the HazMat transportation vehicle routing problem.

HazMat routing problems belong to *rich* VRP, in which homogeneous fleet assumption is non-realistic in practice. In heterogeneous fleet problems tactical decisions are made related to fleet composition to be acquired leading to unlimited version of the problem. Operational decisions can be also made relating to building the trips and the vehicles assigned to them, when a fleet is already acquired (often over a long period of time) and the vehicles have different characteristics (including carrying capacity), leading to the limited fleet problem. Heterogeneous fleet vehicle routing problem (HVRP) is one of the challenging combinatorial optimization problems (COP) that has seen limited study. HVRP are NP-hard, as they include the VRP as a special case, but it has also to be borne in mind that, when it comes to HazMat routing problems, they are also multi-objective in nature.

Recent years have seen a significant increase in solving real-life optimization problems in science, engineering, economics and other in the presence of trade-offs between two or more conflicting objective functions, leading to multi-objective optimization. In many multi-objective optimization problems, no single solution exists that simultaneously optimizes each one of these conflicting objective. They are trade-off solutions. For a solution to be interesting, there must exist a domination relation, such as Pareto dominance, between the solution considered and other solutions. That means, there is a set of non-dominated or Pareto optimal solutions. Obtaining this set it is difficult for many reasons, among them, it can exist possibly a huge number or infinite solutions, that is why a variety of approaches for approximating this set either partially or entirely have been proposed. Minimizing the total routing cost while maximizing route balance, or minimizing the total routing cost while minimizing fuel consumption and emission of pollutants of VRP are examples of multi-objective routing optimization problems. In this work, first it is shown that the total routing risk and the total routing cost are indeed conflicting objectives. Then, it aims at an approximation of the behavior of the trade-off function between this two objective functions, when they are simultaneously optimized in the context of the HazMat vehicle routing problem using heterogeneous fleet.

The presence of several objectives usually does not allow decision makers to identify an universal best decision, meaning they need to make a choice among all possible alternatives to reach the best decision. As it is too difficult to find all possible decision alternatives or even their subset, potential choices are identified (approximation of Pareto-optimal set) and decision makers select the best among them. In response to the growing interest in approximating the set of Pareto optimal solutions in multi-objective vehicle routing problems, this research investigates developing a methodology for approximating this solution set for HVRP in HazMat transportation. In this work a combination of optimization techniques with a risk analysis model is employed to approximate the Pareto-optimal set and/or the Pareto-optimal front. Alongside, a mathematical framework is developed to formally consider and evaluate the potential of the proposed approach. The departure point is to propose a mathematical model for the routing risk assessment that incorporates variables whose values depend on routing decisions. This model allows a more realistic computation of the expected routing risk, which takes into account different vehicle and route segment characteristics, as the type of vehicle, the load size, the type of material, and the neighboring population of road segment. The aspects hereby developed are a contribution towards a more efficient and responsible transportation of HazMat and, they are intended to support the routing decisions made in the transportation of these materials using road and street networks.

For further guidance, a brief outline of the general organization of Chapter 1 follows. A statement of the research problem and the research objectives is included in Section 1.1, while the research contributions for each specific goal can be found in Section 1.2. The content of Chapters 2 through 5 is summarized in Section 1.3, with concluding comments together with ideas and research directions of this work being presented in Section 1.4.

1.1.1 Research Problem and Objectives

Research Problem

Truck or vehicle routing is considered as a major proactive risk mitigation measure in HazMat transportation. This measure aims at reducing incident probability and its consequences. Storage and transportation of HazMat are regulated by laws, guides and norms elaborated by local governments, international organizations and topic experts. In addition, the risk in HazMat transportation can be minimized improving the driver training and the vehicle maintenance, even though, operational research can be useful in risk minimization. This work focuses on applications of operational research models and methods to routing problems in HazMat transportation to obtain effective methods for identifying routes that will give lowest costs and risks. In Figure 1.1. the research problem is presented, multi-objective optimization of vehicle routing problem using an heterogeneous fleet through a road network and considering different routing associated critical variables in risk assessment.

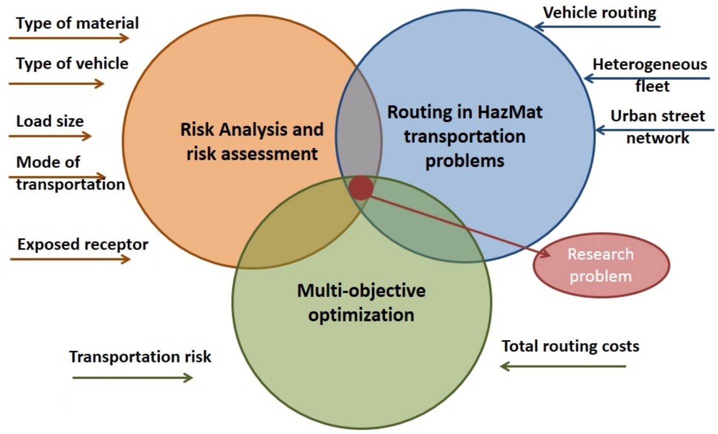


Figure 1.1: Research Problem

Minimizing a risk on a HazMat transportation route is highly sensitive to its definition. Given a quantitative method for route segment risk estimation, the next step is a function for evaluating the risk along a path or route. There are several path evaluation functions for HazMat transport. The most common risk evaluation function on a path is called the *traditional risk model*, which will be detailed in Chapter 3. Many other path evaluation functions have been proposed in addition to the traditional risk model. The risk model selected for path evaluation has effects on the path or route decisions. This poses the following research question:

- Which is the function risk to be used for evaluating the risk along a path or route present in HazMat transportation?

One of the HazMat transportation problems is the optimal transportation routing. Routing HazMat shipments involves a selection among alternative routes involving multiple customers. This leads to a particular VRP. In order to solve this problem, first, it is necessary to construct a mathematical optimization model that incorporates practical aspects of HazMat transportation such as: heterogeneous fleet of vehicles, route risk estimation, road network. How risk is incorporated into HazMat transportation problems is a main aspect in model formulation, further analysis is given in Chapter 3. Then, efficient and effective solution methods have to be developed and implemented. These methods could be exact mathematical, approximate mathematical, heuristics and meta-heuristics or a combination of those. The research questions associated to these aspects are:

- Which mathematical formulation approach is suitable for representing the heterogeneous vehicle routing problem in hazardous material transportation (HazMat-HVRP) in the mono-objective case and in the multi-objective case? Using the expected consequence for assessing the route segment risk in HazMat transportation is a convenient measure for operational research models. Most of the models use population exposure as the consequence measure, but this leads usually to nonlinear functions for the total routing risk objective. In this work, it is not intended start from scratch, but using as starting point the mixed integer linear programming formulation employed in the total routing cost minimization problems.

- What is the impact of using heterogeneous fleet of vehicles in the minimization of transportation risk for a single HazMat product when this risk depends on the type of vehicle and the load size? Different type of vehicles have different vehicle accident rates and different HazMat transportation incident outcomes, and they need to be taken into account when routing decisions are made. The change of the load carried by vehicle during each route between two customers in routing transportation problems also has to be considered.

- Are the solution methods used in minimizing routing costs equally efficient and effective in minimizing routing risks? Hybridized methods based on local or neighborhood search have given encouraging results when they are applied to solve the routing cost optimization problem. In this work, this approach also is studied for solving the routing risk optimization problem.

- Which is the most appropriated solution strategy for solving heterogeneous vehicle routing problems that incorporate risk minimization, both, independent and simultaneous? HazMat transportation problems are also multi-objective in nature, thus, it is necessary to deal at the same time with the convergence and diversity of the solutions belonging to the Pareto front. How to move from the mono-objective version of the solution method to the multi-objective, is another concern of this work.

- Which is the appropriated solution method according to the size of the HazMat-HVRP: exact mathematical method, approximate mathematical method, heuristics and meta-heuristic methods or a hybrid method? To approximate the Pareto front, several approaches are proposed in the literature but the nature of the problem, HazMat transportation, has to be considered. This problem is a multi-objective combinatorial optimization in which the number of the Pareto-front members could be large, and they may exist many non-supported solutions.

The objective of this study is to propose a mathematical model and to develop solution methods for HazMat transportation in urban areas. Several approaches to HazMat routing that have been reported in the literature involve various network modeling and routing techniques. But so far, they did not consider the use of a heterogeneous fleet of vehicles for transporting HazMat and a truck load dependent transportation risk evaluation simultaneously, which are important aspects of the problem that will be handled in this study.

This work aims to contribute in HazMat transportation by addressing the problem of determining the HazMat distribution routes in terms of cost and risk minimization when planning the delivery process executed by shippers and carriers. The results of this research could be useful in other scenarios as pollution-routing problem and energy-efficient routing problems.

General Objective

To develop optimization methods for vehicle routing problems (VRP) concerning the transportation (collection / distribution) of hazardous materials (HazMat) is the main target of this thesis.

Specific Objectives (SO)

To achieve the general objective three specific objectives are enumerated:

S01. To select a mathematical model for quantitative route risk assessment in HazMat transportation using road networks, and to propose a mathematical formulation for the heterogeneous vehicle routing problem (HVRP), Chapter 2 and Chapter 3.

S02. To design a new solution methodology for HVRP in the context of transport of hazardous materials and evaluate its performance, Chapter 4 and Chapter 5.

S03. To propose an algorithm for HazMat-HVRP multi-objective optimization problems, Chapter 6.

1.1.2 Research Contributions

As a result of investigating the research goals stated in the previous section, this study makes the following contributions to the field of multi-objective optimization and its applications.

Research Task 1. Risk assessment in routes

The first part of this work implies to make a comparative study of different risk assessment models for routes in HazMat transportation. Given a road network and, a model for assigning a value to HazMat transport risk associated with road segments that compose the network when an specific HazMat is transporting, the first step is to select a model for measuring risks for a specific route. A route is composed by a set of edges that are composed by road segments. It is supposed that each of these road segments have an homogeneous and known risk measure (population and/or infrastructure risk).

The goal of this task is to select a mathematical model to assess the transportation risk for a route in the transportation of a single HazMat commodity on a road network. The proposed model must to asses the risk for a specific receptor and for a given type of material. This task leads to two contributions (C).

- C 1.1. A literature review on mathematical models for routing risk estimation in HazMat transportation.
- C 1.2. Construction of a mathematical model for measuring the HazMat transport risk associated with a route.

Once a route risk model have been defined, a mathematical model for the routing problem in HazMat transportation will be constructed. In this work will be assumed that in order to meet the demand a fleet of heterogeneous vehicles is available, each vehicle has a specific cost and capacity, and only one type of HazMat is transported. Information on risk (depending on the product, transported quantity, type of vehicle, arc used, etc.) will be included. Different objectives to be considered involve minimization of the total distance traveled and minimization of risk associated with this type of transportation. This problem could be then classified as a HazMat-HVRP. Problems characteristics are: a road network, no split delivering, and heterogeneous fleet of vehicles (fixed and unlimited).

The goals of this task is to present a mathematical formulation of the HazMat-HVRP and provide test instances for the road network used in HVRP problems.

This requires:

- C 1.3. A literature review on mathematical model formulations for routing problems in HazMat transportation.
- C 1.4. Definition of the HazMat-HVRP and presentation of a formulation considering cost minimization and risks minimization.
- C 1.5. Definition of test instances for vehicle routing network transportation.

Research Task 2. Solution Methods

A large size of the real problems or "rich" VRP problems is taken into account in order to construct and solve the model. The HVRP is a hard combinatorial optimization problem and only instances of certain size can be solved to optimality using exact methods. It is necessary to define solution strategies according to the problem size and to establish which approximate methods are appropriated to use. Approximate methods are usually based on a good construction of initial solutions and local improvement strategies. Here an exploration of combinations of different heuristics for constructing initial feasible solutions and for improving a given solution will be conducted. Experimentation on different approaches for constructing initial solutions and for defining different algorithms for exploding and exploring these solutions for this experimental design will be defined and conducted . This task mainly addresses the exploration and evaluation of several high-performance computing strategies that could be adopted in the implementation of the developed algorithms of the above tasks. The main problem related to this issue is that of finding minimum risk routes.

The goal of this task is to develop a new solution methodology that have two characteristics: accurate and computational efficient. This problem arises when logistics operational decisions are made and the solution method has to provide good solutions in a short period of time. This task gives:

- C 2.1. A literature review on solution methods for HVRP problems and HazMat routing transportation problems.
- C 2.2. Propose a new solution method for HazMat-HVRP.
- C 2.3. Apply the solution method to the previous defined problem instances.

Research Task 3. Multi-Objective Optimization

Once a solution method has been proposed for cost and risk routing minimization, a Pareto dominance based multi-objective optimization algorithm will be defined.

In this case two objectives will be considered. It is necessary to do a literature review about different methodologies to deal with approximating the Pareto front in multi-objective VRP.

The goal of this task is to propose an algorithm to approximate the Pareto front that minimize the distance to the optimal front (convergence) and maximize the diversity of the generated solutions (diversity).

- C 3.1. Literature review on multi-objective vehicle routing problem.
- C 3.2. Definition of the measures that will be used for comparing the different multi-objective optimization strategies.
- C 3.3. To propose and validate an algorithm for HazMat-HVRP multi-objectives problems.
- C 3.4. To develop a stand alone application for using and comparing the different algorithms.

1.1.3 Content of the Dissertation

For further guidance, a brief outline of the general organization of the dissertation is provided. The description of each of next six chapters in this dissertation is as follows:

Chapter 2 [C 1.1., C 2.1. and C 3.1.] Introduces the concept of HazMat transportation and its risk reduction when trucks are used for distributing these type of materials. It discusses the different approaches in routing HazMat transportation. It presents a review of selected literature and previous studies related to HazMat transportation, heterogeneous fleet vehicle routing problem and multi-objective HazMat transportation. It obtains sufficient background and understanding of these subjects, and their importance to industry, government and the public, and establish the basis for this research.

Chapter 3 [C 1.2., C 1.3., C 1.4. and C 1.5.] Introduces the optimization problem treated in this dissertation, HazMat-HVRP. The heterogeneous fleet vehicle routing problem variant is a combinatorial optimization problem of practical interest in HazMat transportation. A piece-wise linear single-objective formulation which tries to minimize the total routing risk is presented. This part is focused on improving risk analysis methodology by considering a probabilistic risk model in which the probability of accident is used instead of accident frequency. To facilitate more effective risk management and decision-making this option for route risk comparison is introduced.

A paper was presented in 8th IFAC Conference on Manufacturing Modeling, Management and Control MIM 2016, Troyes, France, 2016. The online article *Mixed Integer Linear Programming Model for Vehicle Routing Problem for Hazardous Materials Transportation* was published on line.

Chapter 4 [C 1.5. and C 2.1.] Offers general information about local or neighborhood search based optimization algorithm concepts. Here is also presented a study over the neighborhood structure used in vehicle routing problems and how this can be adapted to the particularities of the objective function of the proposed problem.

Chapter 5 [C 1.5., C 2.2. and C 2.3.] Introduces a neighborhood search based algorithm that is tested using the mono-objective version of the formulation introduced in the Chapter 3 and the local search structures studies and developed in the Chapter 4.

The work *Total Risk Routing Minimization for the Fleet Size and Mix Problem for Hazardous Materials Distribution* was presented in the annual workshop of the EURO working group on Vehicle Routing and Logistics optimization (VeRoLog), Nantes, France, 2016. An article Variable neighborhood search to solve the vehicle routing problem for hazardous materials transportation was published in *Journal of Hazardous Materials*

Chapter 6 [C 1.4., C 3.2., C 3.3., and C 3.4.] Presents two multi-objective hybrid algorithms based on generating methods. The advantages and disadvantages of a multi-objective neighborhood dominance-based algorithm, and an ϵ-constraint metaheuristic algorithm are also introduced, when approximating the Pareto-front in multi-objective combinatorial optimization problems. The proposed algorithms are tested using using a multi-objective formulation of the HVRP HazMath transportation problems described in Chapter 3.

The work *Bi-objective Fleet Size and Mix Vehicle Routing Problem for Hazardous Materials Transportation* was presented in the 18th ROADEF Conference of Société française de Recherche Opérationnelle et Aide à la Décision.

Chapter 7 Presents a summary of the work, the conclusions and the further perspectives.

1.1.4 Conclusion and Perspectives

Three main aspects form the core of this dissertation. First, a mathematical formulation of the hazardous materials routing problem using a heterogeneous fleet starting from the mixed integer linear programming model used for the routing cost minimization problem. In proposed model, the risk assessment depends on the type of vehicle, the material being transported, and the load change when the vehicle goes among customers. Also how to deal with the nonlinear nature of the total routing risk objective function needs to be considered.

Second, exploration of hybrid methods for solving the problem previously stated, conducting to develop an accurate and computationally efficient solution methodology.

Finally, a multi-objective approach to quantify effects of risk reduction on the total routing cost is developed. Because of routing cost and risk conflicting objective functions, the multi-objective problem solution is a set of solutions. Obtaining this set is difficult for many reasons, and, therefore, many approaches for approximating them have been proposed. In this research are addressed these observations and difficulties. Its primary contribution in this part focuses on the approximation of the Pareto set of multi-objective heterogeneous fleet vehicle routing problem (MHVRP) in HazMat transportation and its application in the field of HazMat transportation design, which has received limited study. The performance of each proposed algorithm is evaluated using an adaptation of heterogeneous vehicle routing test problems. Since multi-objective vehicle routing problems has many real-life applications, and in particular designing distribution networks, the new optimization proposed model for routing HazMat material, using road networks utilizing a heterogeneous fleet of vehicles, can be also used in other scenarios as green logistics and energy-efficient transportation where multi-objective optimization can be considered.

In summary, this dissertation introduces a mathematical framework to inform both private and public sector stakeholders regarding cost-effective approaches for reducing hazardous materials transportation risk. It provides tools that can be used to develop necessary information to better inform risk-based decision making. Furthermore, it offers a background for researchers interested in operations research analysis of hazardous materials transportation risk reduction options. This dissertation extends the investigation of multi-objective optimization, especially multi-objective combinatorial optimization (MOCO). It is hoped that the questions explored in this dissertation and the subsequent results and their implications add to the understanding of the field as well as open new areas of focus for further research.

1.2 Introduction (Français)

De nos jours, la logistique devient de plus en plus responsable. Non seulement elle est importante pour l'industrie, mais elle a aussi su prendre en compte les enjeux actuels tels que l'environnement ou les risques. La logistique des substances dangereuses (HazMat), le transport vert ou de matières dangereuses sont des exemples qui font d'ores et déjà partie de l'industrie de nos jours. C'est une problématique qui peut nécessiter le déplacement dans différents endroits à travers le monde. Aussi, ce qui la différencie du transport de matières régulières est l'effet du risque qui est pris en compte lors du chargement, transport et déchargement. HazMat peut en effet avoir des effets considérables sur l'humain, l'environnement ainsi que la propriété commerciale. La logistique de ces matières étant effectuée en utilisant le réseau national, leurs transports peuvent en effet générer des conséquences considérables sur leur environnement physique aussi bien que sur la population et l'environnement extérieur.

Le problème de HazMat dans le réseau routier ne cesse d'augmenter de nos jours où au nombre croissant de la flotte de transport ainsi que de son chargement. Par conséquent, le nombre d'accidents liés à ce transport représente la quasi-majorité des accidents routiers. Aussi, même si le nombre de véhicules causant des accidents transportant des matières dangereuses reste minime, leurs effets sont dévastateurs vis-à-vis de leur environnement. Ce qui prouve encore plus l'importance de la sécurité dans ce domaine de logistique, malgré les incertitudes liées à la fréquence ainsi qu'à la gravité des dégâts. Il s'avère donc nécessaire d'inclure ces deux facteurs dans toute évaluation du risque. En effet, le but du Hazmat est de réduire le risque associé au transport et à la logistique des matières dangereuses, en prenant en compte leurs risques sur l'humain, les infrastructures et l'environnement. De ce fait, l'objectif du problème du transport des matières dangereuses est de transporter ces matières d'un point à un autre en utilisant le chemin le plus économique et le plus sûr. Cette problématique fait interagir entre eux le transporteur, le donneur d'ordre, le résident, l'assureur, l'état et les forces de sûreté. Il est aussi à noter que chacun d'entre eux a généralement sa propre conception sur les coûts et les risques. Le problème du transport des matières dangereuses a donc deux intérêts majeurs: le problème du chemin le plus court (associé avec un chargement maximal du transport) et le problème de tournées de véhicules (associé avec un chargement moins maximal du transport). Dans la littérature, on s'est plus penché sur le premier problème que le second. De ce fait, dans cette thèse, on se penchera plus sur le problème de tournée de véhicules transportant du HazMat.

Le problème des tournées de véhicules transportant des matières dangereuses appartient à la riche section liée à la problématique des tournées de véhicules (VRP), où on considère en général une flotte homogène, chose qui n'est pas toujours réaliste de nos jours. Quand on considère une flotte hétérogène, le choix décisionnel de la composition génère une infinité de solutions. Aussi, le choix d'un véhicule (déjà acquis ou non) peut se faire suivant le type de route utilisée ou suivant sa capacité de chargement. De ce fait, le problème de tournée de véhicules utilisant une flotte hétérogène (HVRP) est un défi à relever et dont l'étude n'est pas aussi large et répandue que le VRP, qui est un cas spécial de ce dernier. C'est un problème d'optimisation combinatoire complexe (COP) et est NP-difficile. Il est aussi à noter que le problème de tournées de véhicules transportant des matières dangereuses pourrait être résout aussi en multi-objectif.

De nos jours, plusieurs problèmes d'optimisation de la vie réelle ont été proposés, que cela soit dans la science, l'ingénierie, l'économie tout en prenant en considération le conflit possible entre plusieurs fonctions objectives. Ceci rentre dans le cadre de l'optimisation multi-objectif, où on ne peut trouver une solution optimisant simultanément les différents objectifs. Dès lors, on devrait utiliser entres autre l'optimum du Pareto ou autres critères d'optimalité pour y remédier. Par conséquent, une approximation est nécessaire pour résoudre notre problème. On pourra ainsi considérer plusieurs choix tels que la minimisation du coût total de la tournée en maximisant le choix du chemin utilisé, ou la minimisation du coût total de la tournée ainsi que la consommation du carburant et les émissions polluantes générées par ce transport. De ce fait, la présence de plusieurs objectifs rend la tâche de la prise de décision compliquée vu qu'il n'y a pas de solution unique. Il faudrait donc choisir dans une liste de meilleures solutions alternatives proposées. Devant l'intérêt grandissant de l'utilisation de l'optimum du Pareto dans l'optimisation multi-objectif. Cette étude développe une méthodologie d'approximation d'ensembles de solutions du problème multi-objectif de la tournée des véhicules hétérogènes (HVRP) transportant des matières dangereuses. De ce fait, une combinaison de techniques d'optimisation avec un modèle d'analyse de risque est utilisée pour évaluer l'optimum du Pareto ou la frontière de l'efficacité du Pareto. Aussi, un modèle mathématique a été développé pour évaluer les approches proposées. Le point de départ de ce modèle est d'inclure des variables dépendantes de la tournée de véhicules, propose une simulation plus réaliste du risque lié au transport. Il prend aussi en compte la typologie des véhicules (type, capacité de chargement, type de matière transportée) ainsi que les caractéristiques des chemins parcourus (chemins avoisinants). Ces aspects développés représentent une contribution envers une logistique plus responsable des matières dangereuses. Ils représentent aussi un support d'aide à la prise de décision pour le transport de ce type de matières en utilisant le réseau routier.

Cette étude est structurée comme suit : le chapitre 1 résume le problème général d'optimisation. La problématique de recherche ainsi que les objectifs de la recherche sont inclus dans la section 1.1 , la contribution à la recherche pour chaque objectif est spécifiée dans la partie 1.2 . Les contenus des chapitres 2 à 5 sont résumés dans la section 1.3 . Finalement, une conclusion et des commentaires en perspectives futures sont présentés dans la section 1.4 .

1.2.1 Problème de recherche et objectifs

Problème de recherche

La tournée des camions est considérée comme une mesure pro-active majeure pour la mitigation du risque. Cette mesure a pour but de réduire la probabilité des accidents et leurs conséquences. La logistique et le stockage des matières HazMat sont régulés par la loi, normes et guides élaborés par le gouvernement, organisations internationales et experts dans le domaine. De plus, le risque lié au transport des HazMats pourrait être réduit en améliorant les compétences du conducteur et la maintenance du véhicule. Aussi, la recherche opérationnelle pourrait être utile pour la minimisation du risque. Ce travail est focalisé sur les applications de la recherche opérationnelle et de ses modèles pour le problème de la tournée de véhicules transportant des HazMats. Elle permet en effet de générer des méthodes efficaces pour identifier les chemins qui génèrent le minimum de coûts et de risques pour le transport des HazMat. Ce problème de recherche est présenté dans la Figure 1.1, où on présente le lien entre l'optimisation multi-objectif et son utilisation dans la tournée de flotte de véhicules hétérogènes, tout en utilisant le réseau routier connecté et présentant diverses variables.

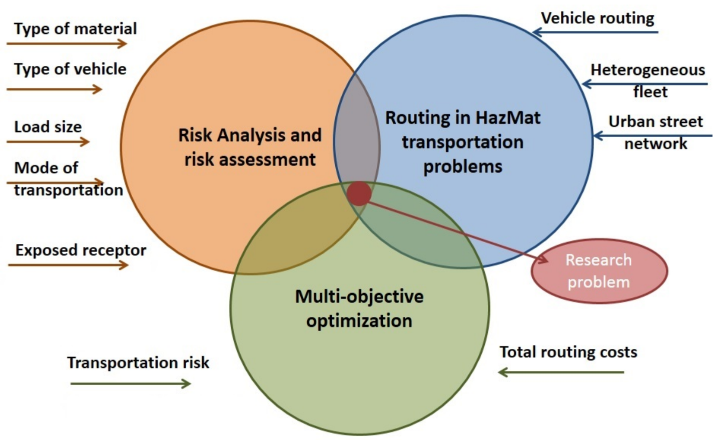


Figure 1.2: Problème de recherche (*Research problem*)

La minimisation du risque est hautement relative à sa définition. En prenant en compte une méthode quantitative pour estimer le risque dans un segment de route, la prochaine étape serait d'évaluer le risque tout au long d'un chemin parcouru. Il existe différentes fonctions d'évaluation du chemin parcouru en transportant du HazMat. Parmi elle se distingue une plus commune appelée modèle de risque traditionnel, qui sera développée dans le chapitre 3. D'autres fonctions d'évaluation ont été proposées en plus de cette dernière. Le modèle de risque sélectionné aura directement un effet sur l'évaluation et la décision sur le chemin parcouru. De ce fait, on a posé la question de recherche suivante:

- Quelle fonction de risque utiliser pour évaluer le risque sur un chemin parcouru en transportant du HazMat?

L'un des problèmes de transport de HazMat est l'optimisation du chemin parcouru. Le chargement lors de la tournée de HazMat inclut la sélection de chemins alternatifs incluant de clients potentiels. Ceci mène classiquement à un problème de tournées de véhicules (VRP). Pour résoudre ce problème, il est d'abord nécessaire de construire un modèle mathématique d'optimisation qui inclut les aspects pratiques du transport du HazMat dont: flotte de véhicules hétérogènes, estimation du risque du chemin parcouru, le réseau routier urbain. Le chapitre 3 développe plus comment le risque a été incorporé dans le problème de transport de HazMat. Ensuite, des méthodes efficaces seront à développer en prenant en compte la taille de l'instance considérée. Ces méthodes pourraient être basées sur des modèles mathématiques exacts ou approximatifs, notamment basées sur des heuristiques ou méta-heuristiques ou une combinaison des deux. Les questions de recherche associées à ces aspects sont:

- Quelle formulation mathématique est appropriée pour représenter le problème de tournée d'une flotte hétérogène transportant des matières dangereuses (HazMat-HVRP), dans le cas mono-objectif et multi-objectif? En prenant en compte les conséquences prévisionnelles pour évaluer le risque sur un chemin transportant du HazMat, on peut mettre en évidence une mesure convenable pour les modèles de recherche opérationnelle. La plupart des modèles utilisent aussi comme indicateur d'évaluation de conséquence l'exposition de la population. Cependant, ceci mène à une fonction objectif non-linéaire du risque total de la tournée, ce qui n'est pas approprié pour l'optimisation. Dans ce travail, on ne sous-entend pas de commencer de zéro, mais on utilisera en premier de l'optimisation linéaire en nombres entiers pour minimiser le coût total du problème.

- Quel est l'impact de l'utilisation d'une flotte de véhicules hétérogènes dans la minimisation du risque dans le transport d'un produit dangereux en prenant en compte que le risque dépend du type de véhicule ainsi que de sa charge?

Différents types de véhicules ont différents taux d'accidents et diverses conséquences liées au transport du HazMat. On a donc besoin de prendre en compte ces données lors du choix du chemin parcouru. De ce fait, on doit considérer le changement de la charge du véhicule durant chaque chemin entre deux clients.

- Est-ce que les solutions utilisées pour réduire les coûts sont aussi efficaces pour réduire les risques? Des méthodes hybrides ont été en effet donné de résultats encourageants quand elles sont appliquées dans la résolution du problème d'optimisation du coût de la tournée. Dans ce travail, cette approche a aussi été étudiée pour résoudre le problème d'optimisation du risque lié à la tournée.

- Quelle est la stratégie de solution la plus appropriée pour résoudre le problème de tournée de flotte de véhicules hétérogènes qui inclut la minimisation du risque de manière indépendante et simultanée? Les problèmes multi-objectifs sont multi-objectifs de nature, il est donc nécessaire d'étudier en même temps la convergence et la diversité des résultats appartenant au front de Pareto. Il est aussi étudié dans ce rapport comment migrer de la version mono-objective de ce problème à la version multi-objective.

- Quelle est la méthode qui conviendrait le mieux à la taille du HazMat-HVRP: la méthode mathématique exacte, la méthode approximative, une heuristique, une méta-heuristique ou une méthode hybride? Pour approximer le front de Pareto, différentes approches ont été proposées dans la littérature. Cependant, la nature du problème; transport du HazMat; devrait être considérée. Ce type de problème est un problème d'optimisation combinatoire et multi-objectif dans lequel le nombre d'éléments du front de Pareto est large et dont la plupart des solutions sont irréalisables.

L'objectif de cette étude est de proposer un modèle mathématique et de développer des méthodes pour le transport de HazMat dans le réseau routier urbain. Différentes approches de tournées de HazMat ont été proposées dans la littérature incluant différentes configurations et techniques de tournées. Cependant, on n'a pas encore considéré l'utilisation de flotte hétérogène pour le transport de HazMat ainsi que la prise en compte du risque lié au chargement. Ces deux aspects ont été développés dans cette étude.

Ce travail a pour but de contribuer à la recherche sur la logistique des HazMat en modélisant la problématique du choix des routes en fonction du coût et de la minimisation du risque dans la planification du processus de livraison du HazMat par les affréteurs et les chargeurs. Les résultats de cette recherche auraient un grand intérêt d'utilisation dans d'autres scénarios tels que le problème de la tournée avec un minimum de pollution ou le problème de tournée avec une utilisation efficace d'énergie.

Objectif général

Le principal objectif de cette thèse est de développer des méthodes d'optimisation pour le problème de tournée de véhicule transportant (collecte/ distribution) des matières dangereuses (HazMat).

Objectifs spécifiques (OS)

Pour atteindre l'objectif général, quatre objectifs spécifiques ont été énumérés:

- OS1. Sélectionner un modèle mathématique pour une évaluation numérique du risque dans le transport de matières dangereuses en utilisant le réseau routier. Proposer ensuite un modèle mathématique pour le problème de tournée de véhicules hétérogènes (HVRP). Objectif développé dans les chapitres 2 et 3.

- OS2. Développer une nouvelle méthodologie pour le problème de tournée de véhicules hétérogènes (HVRP) dans le cas de transport de matières dangereuses. Evaluer ensuite ses performances. Objectif développé dans les chapitres 4 et 5.

- OS3. Proposer un algorithme pour le problème d'optimisation multi-objectif HazMat-HVRP. Objectif développé dans le chapitre 6.

1.2.2 Contributions à la recherche

Cette étude présente les résultats d'investigations des objectifs de recherche cités dans la section précédente. Elle contribue à la thématique d'optimisation multi-objectif et de ses applications.

Objectif de recherche 1. Évaluation du risque dans les routes

La première partie de ce travail a nécessité une étude comparative des différents modèles d'évaluation du risque dans le cadre du transport de matières dangereuses. En prenant un compte un réseau routier donné, un modèle d'affectation du risque de transport du HazMat associé à chaque segment de route composant le réseau routier a été développé. La première étape était de sélectionner un modèle de mesure du risque pour un chemin spécifique. Un itinéraire est composé de tranches qui sont composées à leurs tours de segments de routes. Il est supposé que chacun de ces segments de route a un risque donné et homogène (risque sur la population et/ou l'infrastructure). L'objectif de cette tâche est de sélectionner un modèle mathématique pour évaluer le risque lié au transport pour un itinéraire dans le cadre de transport d'une matière dangereuse dans un réseau routier urbain. Le modèle proposé devrait être capable d'examiner le risque de différents types de matières sur différents récepteurs exposés à ces dernières. Cette tâche a généré deux contributions:

- C.1.1. Un état de l'art sur les modèles mathématiques de l'estimation du risque dans le transport de HazMat.
- C.1.2. Construction d'un modèle mathématique pour mesurer le risque associé au transport d'une HazMat dans un itinéraire.

Une fois le modèle de risque défini, on a construit un modèle mathématique pour le problème de tournée lié au transport de HazMat. On a aussi considéré dans ce travail que pour satisfaire une demande donnée, une flotte hétérogène de véhicules est disponible. Chaque véhicule a un coût et une capacité spécifique, et que seul un type de HazMat peut y être transporté. On a calculé ensuite les informations liées au risque (en fonction du produit, sa quantité transportée, type de véhicule, chemin utilisé). Les objectifs pris en compte sont la minimisation de la distance totale parcourue ainsi que le risque associé à ce type de logistique. Ce problème est donc classé comme HVRP-HazMat. Les caractéristiques de ce dernier sont: un réseau routier urbain réel, pas de répartition de livraison et une flotte de véhicules hétérogènes (cas de flotte fixe et illimité).

Les objectifs de cette tâche sont donc de présenter un modèle mathématique pour le problème de tournée de véhicules hétérogènes transportant du matériel dangereux, ainsi que de proposer des tests pour un réseau traditionnel utilisé dans les problèmes de HVRP.

Ceci nécessite:

- C.1.3. Un état de l'art sur les modèles mathématiques pour formuler un problème de tournée transport du HazMat.
- C.1.4. Définition du problème de tournée de véhicules hétérogènes transportant du HazMat, et présentation d'une formulation du problème en minimisant le coût et le risque.
- C.1.5. Définition de tests pour le transport en tournée dans un réseau routier.

Objectif de recherche 2. Méthodes

Une grande taille de problèmes ou des problèmes VRP riches devraient être pris en compte pour construire et résoudre le modèle. Le problème HVRP est un problème combinatoire d'optimisation difficile, seules des instances d'une certaine taille peuvent être résolues en utilisant des méthodes exactes. Il est donc nécessaire de définir des solutions en fonction de la taille du problème et établir ensuite quelle méthode approximée est la plus appropriée. Les méthodes d'approximation sont généralement basées sur une bonne construction de solutions initiales ainsi qu'une stratégie d'amélioration locale. Dans ce travail, une exploration de combinaison de différentes heuristiques pour la construction de solutions initiales faisables dans le but d'améliorer une solution donnée a été menée. Aussi, une expérimentation a été définie et conduite sur les différentes approches pour construire des solutions initiales et pour définir différents algorithmes pour exploser et explorer ces solutions pour ce design expérimental. Cette tâche aborde principalement l'exploration et l'évaluation de différentes stratégies de calcul haute performance qui pourraient être adoptées pour implémenter et développer les algorithmes des tâches précédentes. Le problème principal lié à cette tâche est de trouver le risque minimal des itinéraires.

L'objectif de cette tâche est de développer une nouvelle méthodologie ayant deux caractéristiques: précision et efficacité de calcul. Ce problème intervient lorsque les décisions opérationnelles de logistique sont données et qu'une méthode devrait générer de bons résultats dans un délai court. Cette tâche a généré:

- C.2.1. Un état de l'art des méthodes utilisées dans le problème HVRP ainsi que le problème de tournées de véhicules transportant de HazMat.
- C.2.2. Proposer une nouvelle méthode pour le HVRP-HazMat.
- C.2.3. Utiliser ces algorithmes pour minimiser le risque dans les problèmes de tournées transportant du HazMat.

Objectif de recherche 3. Optimisation multi-objectif

Une fois on a proposé une méthode pour minimiser le risque ainsi que le coût, un algorithme d'optimisation multi-objectif basé sur la dominance de Pareto sera défini. Dans ce cas, deux objectifs ont été considérés. Il est donc nécessaire de réaliser un état de l'art sur les différentes méthodologies qui abordent l'approximation du front de Pareto. L'objectif de cette tâche est de proposer un algorithme d'approximation du front de Pareto qui minimise la distance au front optimal (convergence), et maximise la diversité des solutions générées (diversité). Cette tâche a généré:

- C.3.1. Un état de l'art.

- C.3.2. Définition des mesures qui seront utilisées pour comparer les différentes stratégies.
- C.3.3. Proposer et valider un algorithme pour le problème multi-objectif HVRP-HazMat.
- C.3.4. développer une application autonome pour utiliser et comparer les résultats des algorithmes.

1.2.3 Contenu de cette dissertation

Dans un souci d'orientation, on proposera dans cette section un aperçu de l'organisation générale de cette dissertation. La description des cinq chapitres de cette thèse est comme suit:

Chapitre 2 (C.1.1., C.2.1 et C.3.1) introduit les concepts de la logistique du HazMat ainsi que la minimisation des risques associés lorsqu'un camion est utilisé pour distribuer ce type de matières. On a ensuite discuté les différentes approches utilisées dans la tournée de véhicules transportant du HazMat, puis présenté une sélection d'états de l'art ainsi que les études précédentes relatives à la logistique du HazMat et le problème multi-objectif de tournée de flotte de véhicules transportant du HazMat. On a finalement eu suffisamment de recul et d'informations sur ces sujets ainsi que leurs importances pour l'industrie, le gouvernement et le public. Ce qui nous a permis d'établir les bases de cette recherche.

Chapitre 3 (C.1.2., C1.3, C1.4 et C1.5) introduit le problème d'optimisation abordé dans cette thèse. Le problème de tournée de véhicules à flotte hétérogène est un problème combinatoire ayant un intérêt pratique dans la logistique du HazMat. Une formulation mono-objective linéaire par morceaux pour minimiser le risque total de la tournée a été présentée. Cette partie se focalise sur l'amélioration de la méthodologie d'analyse du risque en considérant un modèle de risque probabiliste dans lequel la probabilité d'un accident est utilisée au lieu de sa fréquence. Afin de faciliter le management du risque ainsi que la prise de décision, cette option a été introduite pour une comparaison des risques des itinéraires. Un article a été présenté dans ce sens à la 8ème conférence IFAC-MIM 2016 (Conference on Manufacturing, modeling, management and control- MIM 2016. Troyes, France). L'article est d'ores et déjà en ligne: Mixed Integer Linear Programming Model for Vehicle Routing Problem for Hazardous Materials Transportation.

Chapitre 4 (C.1.5 et C.2.1) offre des informations générales sur les concepts d'algorithmes d'optimisations basés sur la recherche locale. Dans ce chapitre, une étude sur la structure du voisinage utilisée dans les problèmes de tournées de véhicules a été présentée. Ensuite, une adaptation de cette dernière aux particularités du problème présenté dans le chapitre 3 a été présentée.

Chapitre 5 (C.1.5, C.2.2 et C.2.3) introduit l'algorithme basé sur la recherche de voisinage qui est testé en utilisant la version mono-objectif de la formulation introduite dans le chapitre 3, ainsi que les structures de recherches locale étudiées et développées dans le chapitre 4. Ainsi, la communication Total Risk Routing Minimization for the Fleet Size and Mix Problem for Hazardous Materials Distribution a été présentée au congrès annuel VEROLOG à Nantes, France en 2016. Ensuite, un article Variable neighborhood search to solve the vehicle routing problem for hazardous materials transportation a été publié dans Journal of Hazardous Materials.

Chapitre 6 (C.1.4, C3.2, C.3.3 et C.3.4) présente deux algorithmes hybrides et multi-objectifs basés sur les méthodes de génération. Les avantages et inconvénients de l'algorithme multi-objectif basé sur une dominance de voisinage ainsi que l'algorithme méta-heuristique ϵ-contrainte ont été présentés lors de son utilisation pour estimer le front de Pareto dans un problème d'optimisation multi-objectif et combinatoire. Ces algorithmes proposés sont testés en utilisant une formulation multi-objective de la problématique de la logistique du HVRP HazMat présentée dans le chapitre 3. Le travail Bi-objective Fleet Size and Mix Vehicle Routing Problem for Hazardous Materials Transportation a été présenté à la 18ème conférence de ROADEF.

1.2.4 Conclusion et perspectives

Trois aspects froment le cœur de cette thèse. Premièrement, la formulation mathématique du problème de tournées de de véhicules à flotte hétérogènes transportant des matières dangereuses en utilisant en premier lieu un modèle linéaire en nombre entiers pour minimiser le coût des tournées. Dans le modèle proposé, l'évaluation du risque dépend du type du véhicule, de matériel transporté ainsi que le changement de la cargaison (charge) d'un client à un autre. Elle a été aussi considérée la nature non linéaire de la fonction objective du risque total de la tournée.

En second aspect, une exploration des méthodes hybrides pour résoudre le problème précédent a été conduite, ce qui a mené à développer une méthodologie précise et efficace du point de vue calcul.

Finalement, une approche multi-objective pour quantifier les effets de la réduction de risques sur le coût total d'une tournée a été développée. La solution du problème multi-objectif est dans ce cas un ensemble de solution au lieu d'une solution unique pour ces problèmes, ceci est dû au conflit entre les deux fonctions objectives du risque et du coût. Obtenir cet ensemble de solution est difficile pour plusieurs raisons, ce qui a mené à proposer plusieurs approches d'approximation à ce problème. La recherche réalisée dans cette thèse a mené aux observations et contraintes suivantes: Sa première contribution s'est focalisée sur l'approximation du front de Pareto du problème de tournées de véhicules à flotte hétérogène (MHVRP) transportant du HazMat. Ces études étant limitées dans la littérature, notre contribution aurait un impact sur les applications et le design de la logistique HazMat. La performance de chaque algorithme a été évaluée en utilisant une adaptation aux problèmes tests de tournées de véhicules à flotte hétérogène. Aussi, vu que les problèmes de tournées de véhicules multi-objectifs ont de nombreuses applications dans la vie; et plus particulièrement dans le design de nouveaux itinéraires; le modèle d'optimisation traité dans cette thèse peut aussi être utilisé dans d'autres scénarios tels que la logistique verte ou la logistique avec efficacité énergétique.

Au final, cette thèse a introduit une structure mathématique pour informer les décideurs publics et privés quant à l'efficacité économique de leurs approches dans la réduction du risque lié au transport de matières dangereuses. Elle fournit un outil qui peut être utilisé pour générer les informations nécessaires pour une aide à la décision basée sur la compréhension du risque. De plus, elle offre un rapport pour les chercheurs sur l'application de la recherche opérationnelle sur l'analyse du risque lié au transport des matières dangereuses. Cette thèse a aussi développé la recherche dans le domaine d'optimisation multi-objectif, et plus spécifiquement l'optimisation multi-objectif combinatoire (MOCO). On espère que les questions explorées dans cette thèse ainsi que les résultats générés et leurs conséquences ajouteront une plus-value à la compréhension de ce champ de recherche aussi bien dans d'autres domaines pour plus de perspectives.

1.3 Introducción (Español)

Hoy en día no solo un transporte eficiente es importante, aspectos medioambientales y de seguridad también deben ser tenidos en cuenta como guías en el transporte, no solo para hacerlo de forma aún más eficiente sino más responsable. Como ejemplos de lo anterior se tienen, el transporte de materiales peligrosos (HazMat por las iniciales en inglés de *hazardous material*) y la logística verde. La mayoría de las veces, los envíos de los HazMat se originan y terminan en diferentes sitios ubicados por todo el mundo, lo que subraya el importante papel que el transporte juega para los HazMat. Lo que diferencia el transporte de HazMat del transporte de otros materiales es el riesgo asociado con una fuga accidental de estos materiales, esto puede ocurrir durante la carga, el transporte o bien la descarga. Por definición un HazMat es un material capaz de someter a un riesgo más allá de lo razonable a las personas, el medio ambiente, y a las propiedades cuando es transportado en actividades comerciales. En la mayoría de los casos, los envíos de estos productos son realizados a través de las redes de rutas (nacionales y redes urbanas), y constituyen una parte importante para las economías de los países, proveyendo una fuente de ingresos para los transportistas y los propietarios de este tipo de carga.

El constante aumento del número de embarques y de la cantidad enviada en el transporte terrestre ha dado como resultado un problema que crece cada día. La gran mayoría del total de incidentes, en el caso del transporte de HazMat, se da por accidentes en las vías, un indicativo del interés en la seguridad en el transporte de estos materiales. A pesar de que el número de vehículos involucrados en accidentes cuando están transportando HazMat es una pequeña minoría, los incidentes en el transporte de estos materiales tienen un gran impacto esperado; lo que ilustra la naturaleza del riesgo en el transporte de HazMat, una baja frecuencia pero un alto impacto o consecuencia. Evaluar los riesgos a los que se puede llegar a estar expuesto por eventos ocurridos en el transporte de HazMat es una tarea nada fácil; la frecuencia de estos eventos es muy baja, los choques en las vías son inciertos; sin embargo estos incidentes tienen un gran impacto sobre las personas, propiedades y otro tipo de tráfico debido a una explosión o derrame del HazMat transportado. No existe un consenso sobre la mejor manera de modelar el riesgo en el transporte, sin embargo, es aceptado en general que cualquier formulación debe incluir dos elementos: la probabilidad de un escape accidental del HazMat y las consecuencias asociadas a este evento.

En el transporte de HazMat se busca reducir el riesgo a fin de mejorar la seguridad de las personas, la infraestructura y el medio ambiente natural. El objetivo del transporte de HazMat es mover una cantidad de material considerado HazMat desde el origen de la carga hasta su destino, a través de las rutas más económicas y más seguras. El transporte de HazMat involucra múltiples partes interesadas, como por ejemplo, expedidores, transportistas, fabricantes, residentes, aseguradoras, gobiernos y organismos de emergencia. Las diferentes partes involucradas en el transporte por lo general tienen diferentes prioridades en lo referente al costo y el riesgo, dentro de los posibles objetivos a plantear. El transporte de HazMat tiene dos enfoques principales: los problemas de ruta más corta (asociados con distribución usando vehículos a carga completa) y los problemas de ruteo de vehículos (VRP por las siglas en inglés de *vehicle routing problem* (asociados a la distribución de carga compartida entre varios clientes). Hay existido un mayor esfuerzo de investigación relacionado con el primer tipo de problemas que con el segundo tipo. Es por ello que el énfasis de este trabajo se encuentra en el transporte de HazMat bajo el enfoque de problema de ruteo de vehículos.

Los problemas de ruteo de HazMat hacen parte de los problemas *rich* VRP, en los cuales una flota homogénea no es un supuesto realista. En el problemas del transporte con flota heterogénea se toman decisiones tácticas relacionadas con la composición de la flota a ser adquirida, lo que se conoce como la versión no limitada del problema. Y, cuando se cuenta con una flota ya adquirida (por lo general para un periodo de tiempo lo suficientemente largo) y los vehículos tiene diferentes características, se toman decisiones operacionales relacionadas con los viajes y los vehículos que les son asignados; lo que se conoce como la versión con flota limitada del problema. Los problemas de ruteo de vehículos con flota heterogénea (HVRP por sus siglas en inglés *Heterogeneous Vehicle Routing Problem*) es uno de los problemas de optimización combinatoria (COP por *Combinatorial Optimization Problem*) más desafiantes, que no han tenido un amplio estudio en comparación con otras variantes del VRP. El HVRP es un problema tipo *NP-hard*, dado que es un tipo especial de los problemas VRP, pero también debe tenerse en cuenta, que en lo que tiene que ver con los problemas de ruteo involucrado HazMat, estos también son de naturaleza multi-objetivo.

En los últimos años se ha visto un incremento significativo en tratar de resolver problemas de optimización de la vida real relacionados con la ciencia, la ingeniería, la economía entre otras, teniendo en cuenta la presencia de negociaciones (*trade-offs*) entre dos o más funciones objetivos conflictivas entre sí, lo que conduce a una optimización multi-objetivo. En muchos problemas de optimización multi-objetivo, una única solución, que de forma simultánea optimice cada una de los objetivos conflictivos, no existe. Hay varias soluciones del tipo *trade-off*. Para que una solución sea de interés debe existir una relación de dominancia, como la de dominancia Pareto, entre la solución considerada y otras soluciones. Lo anterior significa, que lo que se busca es un conjunto de soluciones no dominadas u óptimas Pareto. Obtener este conjunto es una tarea difícil por muchas razones, entre ellas, puede existir la posibilidad de un gran número o infinitas soluciones de este tipo, por lo que se ha propuesto una variedad de enfoques para aproximar este conjunto de forma total o parcial. Minimizar el costo total de ruteo mientras se maximiza el balance de las rutas, o minimizar el costo total de ruteo mientras se minimiza el consumo de combustible y la emisión de contaminantes del vehículo en problemas de VRP, son ejemplos de problemas de ruteo multi-objetivos. En este trabajo de investigación, se busca primero mostrar que las funciones objetivos de minimización del costo total de ruteo y minimización del riesgo de ruteo son de verdad conflictivas. Luego, se busca una aproximación del comportamiento de la función que representa las soluciones tipo *trade-offs* cuando se optimizan simultáneamente múltiples funciones objetivos en el contexto del ruteo de vehículos usando flota heterogénea y transportando HazMat.

La presencia de varios objetivos por lo general no permite a los decisores identificar una mejor decisión universal, lo cual quiere decir, que ellos necesitan tomar una decisión entre todas las posibles alternativas para alcanzar la que se consideraría la mejor de todas. Dado que puede llegar a ser muy difícil encontrar todas las posibles alternativas de decisiones o incluso un subconjunto de ellas, se trata de identificar un conjunto posible y que los decisores seleccionen la mejor dentro de estas. Como respuesta al creciente interés en la aproximación del conjunto de soluciones óptimas Pareto en los problemas de optimización multi-objetivo en VRP, este estudio investiga el desarrollo de metodologías para la aproximación de conjuntos de soluciones multi-objetivo para los problemas HVRP en el transporte de HazMat. En este trabajo una combinación de técnicas de optimización junto a un modelo de análisis de riesgo se emplean para aproximar el conjunto Pareto óptimo (espacio de soluciones) como también el conjunto de soluciones en el frente óptimo Pareto (espacio de las funciones objetivo). Conjuntamente se desarrolla un marco matemático para formalmente considerar y evaluar el potencial del enfoque propuesto. El punto de partida del estudio es proponer un modelo matemático para la evaluación del riesgo de ruteo que incorpore variables cuyos valores dependen de las decisiones de ruteo. Este modelo debe permitir un cálculo más realista del riesgo esperado del ruteo; tomando en cuenta diferentes características de los vehículos y de los tramos de ruta, como es el caso del tipo de vehículo utilizado, el tamaño de la carga transportada, el tipo de material y la población que se encuentra alrededor del tramo de ruta considerado. Los aspectos aquí desarrollados son una contribución en camino a un transporte más eficiente y responsable de los HazMat y un soporte a la toma de decisiones cuando estos materiales se transporte usando las redes de carreteras y calles.

Para una mejor ilustración, a continuación se realiza una descripción general de la organización de este capítulo. La definición del problema y los objetivos de investigación se incluyen en la Sección 1.1, las contribuciones de la investigación, de acuerdo a cada objetivo específico, se muestran en la Sección 1.2. Los contenido de los Capítulos 2 al 7 se resumen en las sección 1.3. En la sección 1.4 se dan las conclusiones generales de este capítulo junto a las ideas que guían la investigación en este trabajo.

1.3.1 Problemas y objetivos de investigación

Problema de investigación

El ruteo vehículos o camiones en el transporte de HazMat se considera una de las principales medidas pro-activas de mitigación del riesgo. Este medida busca reducir la probabilidad de los accidentes y sus consecuencias. El almacenamiento y transporte de los HazMat están regulados por leyes, guías y normas elaboradas por los gobiernos locales, organizaciones internacionales y expertos en el área. Además, el riesgo en el transporte de HazMat puede ser minimizado mejorando la capacitación de los conductores y con el mantenimiento del vehículo, sin embargo, las herramientas de investigación de operaciones pueden ser usadas también para la minimización de este riesgo. Este trabajo se enfoca en el uso de modelos y métodos de investigación de operaciones para los problemas de ruteo en el transporte de HazMat a fin de desarrollar métodos efectivos para identificar las rutas que provean el menor costo y el menor riesgo. En la Figura 1.1 se muestra la delimitación del problema de investigación, optimización multi-objetivo del problema de ruteo de vehículos usando flota heterogénea en el transporte de materiales peligrosos a través de redes de rutas urbanas y considerando diferentes variables críticas en la valoración del riesgo.

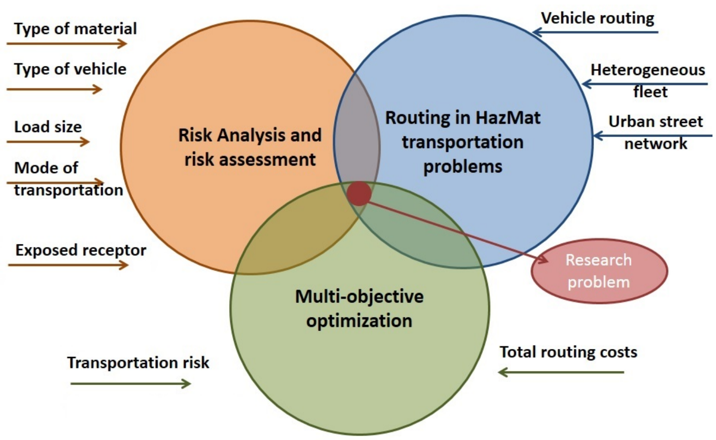


Figure 1.3: Problema de investigación

El modelo de riesgo seleccionado para la evaluación de la ruta tiene efectos sobre las decisiones del camino o ruta a tomar en el transporte. La minimización del riesgo en el transporte es muy sensible a su definición. Partiendo de un método cuantitativo para la estimación del riesgo de un segmento de ruta, el siguiente paso es una función para evaluar el riesgo a lo largo de una ruta. Hay varias funciones de evaluación del riesgo para ruta en el transporte de materiales peligrosos. La función de evaluación de riesgo para una ruta más común se llama *modelo de riesgo tradicional*, el cual será detallado en el Capítulo 3. Si embargo se han propuesto muchas otras funciones para la evaluación del riesgo de una ruta además del modelo de riesgo tradicional. Esto plantea la siguiente pregunta de investigación:

- Cuál es la función que se utilizará para evaluar el riesgo presente a lo largo de una ruta presente en el transporte de materiales peligrosos?

Uno de los problemas en el transporte de HazMat es el ruteo óptimo. El ruteo de los envíos de HazMat implica una selección entre rutas alternativas que involucran a múltiples clientes. Esto conduce clásicamente a un problema particular de ruteo de vehículos (VRP). Para resolver este problema, primero, es necesario construir un modelo de optimización matemático que incorpore los aspectos prácticos del transporte de materiales peligrosos, tales como: flota heterogénea de vehículos, estimación del riesgo de ruta, el uso de la red de rutas urbanas. Cómo se incorpora el riesgo en los problemas de transporte de materiales peligrosos es un aspecto principal en la formulación del modelo; en el Capítulo 3 se ofrece un análisis adicional. Luego, se deben desarrollar métodos de solución eficientes y efectivos de acuerdo con el tamaño de las instancias del problema considerado para la minimización del riesgo de transporte. Estos métodos podrían ser matemáticos exactos, matemáticos aproximados, heurísticos y meta-heurísticos o una combinación de ellos. Las preguntas de investigación asociadas a estos aspectos son:

- Qué enfoque de formulación matemática es adecuado para representar el problema de ruteo de vehículos heterogéneos en el transporte de materiales peligrosos (HazMat-HVRP) para los casos mono-objetivo y multi-objetivo? La utilización de la consecuencia esperada para evaluar el riesgo del segmento de ruta en el transporte de materiales peligrosos es una medida conveniente cuando se usan modelos de investigación operacional. La mayoría de los modelos para obtener la consecuencia esperada usan la exposición a la población como la medida de la consecuencia, pero esto generalmente conduce a funciones no lineales para la función objetivo de riesgo total de ruteo, para los propósitos de optimización es mejor contar con funciones lineales. En este trabajo, no se pretende comenzar desde cero, sino que se usa como punto de partida la formulación de programación lineal mixta entera empleada en los problemas de minimización del costo total de ruteo.

- Cuál es el impacto del uso de una flota heterogénea de vehículos en la minimización de riesgos en el transporte de materiales peligrosos de un solo producto cuando estos riesgos dependen del tipo de vehículo y del tamaño de la carga? Diferentes tipos de vehículos tienen diferentes índices de accidentalidad, y diferentes resultados pueden darse como resultado de los incidentes en transporte de materiales peligrosos. Todo lo anterior debe tenerse en cuenta cuando se lleva a cabo el ruteo. Otro aspecto a considerar es el cambio en la cantidad transportada por el vehículo cuando se desplaza entre dos clientes en una misma ruta.

- Los métodos de solución usados para minimizar los costos de ruteo son igualmente eficientes y efectivos para minimizar los riesgos? Los métodos híbridos basados en búsqueda local han dado resultados alentadores cuando se aplican para resolver el problema de optimización del costo del ruteo. En este trabajo, este enfoque también se estudian estos métodos para resolver el problema de optimización del riesgo del ruteo.

- Cuál es la estrategia de solución más apropiada para resolver problemas de ruteo de vehículos heterogéneos que incorporan la minimización de riesgos, tanto de forma independiente como simultánea? Los problemas de transporte de HazMat también tienen objetivos múltiples, lo que hace necesario tratar al mismo tiempo la convergencia y la diversidad de las soluciones perteneciente al frente Pareto. Cómo pasar de la versión del método de solución mono-objetivo a la multi-objetivo, es otra preocupación de este trabajo.

- Cuál es el método de solución apropiado de acuerdo con el tamaño de la instancia del HazMat-HVRP: método matemático exacto, método matemático aproximado, métodos heurísticos y meta-heurísticos o un método híbrido? Para aproximarse al frente de Pareto varios enfoques son propuestos en la literatura, pero debe considerarse la naturaleza del problema, el transporte de materiales peligrosos. Este problema es una optimización combinatoria multi-objetivo en la que el número de miembros de frente de Pareto es grande y existen muchas soluciones no-soportadas.

El objetivo de este estudio es proponer un modelo matemático y desarrollar métodos de solución para el transporte de materiales peligrosos en áreas urbanas. Varios enfoques del ruteo de materiales peligrosos que se han informado en la literatura incluyen diversas técnicas de ruteo y modelado de las redes de rutas. Pero hasta ahora no se han considerado el uso de una flota heterogénea de vehículos para transportar materiales peligrosos con riesgo dependiente de la carga, que son dos de los importantes aspectos del problema que se manejará en este estudio.

Este trabajo también tiene como objetivo contribuir al transporte de materiales peligrosos abordando el problema de determinar las rutas para la distribución de materiales peligrosos considerando la minimización de costos y riesgos de forma simultánea cundo se planifica el proceso de entrega por parte de despachadores y transportistas. Los resultados de esta investigación podrían ser útiles en otros escenarios como el problema de ruteo considerando la contaminación y los problemas de ruteo energético-eficientes.

Objetivo General (OG)

El principal objetivo de esta tesis es desarrollar métodos de optimización para los problemas de ruteo de vehículos relacionados con el transporte (recolección / distribución) de materiales peligrosos (HazMat).

Objetivos específicos (OE)

Para alcanzar el objetivo general, cuatro objetivos específicos son planteados:

OE1. Seleccionar un modelo matemático para la evaluación cuantitativa de riesgos de las rutas en el transporte de materiales peligrosos utilizando redes de rutas, y proponer una formulación matemática para el problema de ruteo de vehículos con flota heterogénea (HVRP), Capítulo 2 y Capítulo 3.

OE2. Diseñar una nueva metodología de solución para el problema de ruteo de vehículos con flota heterogéna (HVRP) en el contexto del transporte de materiales peligrosos y evaluar su desempeño, Capítulo 4 y Capítulo 5.

OE3. Proponer un algoritmo para problemas de optimización multi-objetivo de HazMat-HVRP, Capítulo 6.

1.3.2 Contribuciones de la investigación

Como resultado de los objetivos de investigación establecidos en la sección anterior, este estudio hace las siguientes contribuciones al campo de optimización multi-objetivo y sus aplicaciones.

Tarea de investigación 1. Evaluación del riesgo en las rutas

La primera parte de este trabajo implica hacer un estudio comparativo de diferentes modelos de evaluación de riesgos para rutas en el transporte de materiales peligrosos. Dada una red de carreteras urbanas y un modelo para asignar un valor al riesgo de transporte de materiales peligrosos, asociado con segmentos de carreteras que componen la red cuando se está transportando un HazMat específico, el primer paso es seleccionar un modelo para medir los riesgos para una ruta específica. Una ruta está compuesta por un conjunto de segmentos de carretera. Se supone que cada uno de estos segmentos viales tiene una medida de riesgo homogénea y conocida (población o infraestructura).

El objetivo de esta tarea es seleccionar un modelo matemático para evaluar el riesgo de transporte de una ruta en el transporte de un solo producto básico en el transporte de materiales peligrosos en una red de carreteras urbanas. El modelo propuesto debe poder analizar los riesgos de un receptor expuesto y para un tipo de material. Esta tarea lleva a dos contribuciones.

- C 1.1. Una revisión de la literatura sobre modelos matemáticos para la estimación del riesgo de ruteo en el transporte de materiales peligrosos.

- C 1.2. Construcción de un modelo matemático para medir el riesgo en el transporte de materiales peligrosos asociado a una ruta.

Una vez que se haya definido un modelo de riesgo de ruta, se construirá un modelo matemático para el problema de ruteo en el transporte de materiales peligrosos. En este trabajo se supone que para satisfacer la demanda existe una flota de vehículos heterogéneos, cada vehículo tiene un costo y capacidad específico, y solo se transporta un tipo de material peligroso. Se incluirá información sobre el riesgo (dependiendo del producto, cantidad transportada, tipo de vehículo, segmento de ruta utilizado, etc.). Los diferentes objetivos considerados son la minimización del costo total de transporte y la minimización del riesgo asociado con este tipo de transporte. Este problema podría entonces clasificarse como HazMat-HVRP. Las características de los problemas son: una red de rutas urbanas, sin dividir las entregas, y una flota heterogénea de vehículos (limitada e ilimitada).

El objetivo de esta tarea es presentar una formulación matemática del problema de ruteo de vehículos con flota heterogénea de materiales peligrosos y proporcionar instancias de prueba para las redes de rutas utilizadas en problemas de HVRP.

Lo anterior da como resultado:

- C 1.3. Una revisión de la literatura sobre formulaciones de modelos matemáticos para problemas de ruteo en el transporte de materiales peligrosos.

- C 1.4. Definición del problema de ruteo de vehículos con flota heterogénea de materiales peligrosos y presentación de una formulación considerando minimización de costos y minimización de riesgos.

- C 1.5. Definición de instancias de prueba para el problema transporte de de ruteo de vehículos en el transporte de materiales peligrosos.

Tarea de investigación 2. Métodos de solución

Se debe tener en cuenta el gran tamaño de los problemas VRP reales o *rich* VRP en la construcción y solución del modelo. El HVRP es un problema de optimización combinatoria difícil y solo las instancias de cierto tamaño se pueden resolver de forma óptima usando métodos exactos. Es necesario definir estrategias de solución de acuerdo con el tamaño del problema y establecer qué métodos aproximados se utilizaran. Los métodos aproximados generalmente se basan en una buena construcción de soluciones iniciales y estrategias de mejora local. Aquí se realizará una exploración de combinaciones de diferentes heurísticas para construir soluciones factibles iniciales y para mejorar una solución dada. Se definirá y conducirá una experimentación sobre los diferentes enfoques para construir soluciones iniciales y para definir los diferentes algoritmos para explotar y explorar estas soluciones. Esta tarea se dirige principalmente a la exploración y evaluación de varias estrategias de cómputo de alto rendimiento que podrían adoptarse en la implementación de los algoritmos desarrollados de las tareas anteriores. El principal problema relacionado con este aspecto es encontrar las rutas de riesgo mínimas.

El objetivo de esta tarea es desarrollar una nueva metodología de solución que tenga dos características: precisa y computacionalmente eficiente. Este problema surge cuando se toman decisiones operativas en logística y el método de solución tiene que proporcionar buenas soluciones en un corto período de tiempo. Esta tarea proporciona:

- C 2.1. Una revisión de literatura sobre métodos de solución para problemas de HVRP y problemas de transporte de ruteo de materiales peligrosos.
- C 2.2. Proponer un nuevo método de solución para HazMat-HVRP.
- C 2.3. Aplicar el método de solución a las instancias de problema definidas anteriormente.

Tarea de investigación 3. Optimización multi-objetivo

Una vez que se ha propuesto un método de solución para la minimización de costos y riesgos, se definirá un algoritmo de optimización multi-objetivo basado en la dominancia de Pareto.

El objetivo de esta tarea es proponer un algoritmo para aproximar el frente de Pareto que minimice la distancia al frente óptimo (convergencia) y maximice la diversidad de las soluciones generadas (diversidad).

- C 3.1. Revisión de la literatura sobre el problema de ruteo de vehículos multi-objetivo.

- C 3.2. Definición de las medidas que se utilizarán para comparar las diferentes estrategias de optimización multi-objetivo.
- C 3.3. Proponer y validar un algoritmo para problemas HVRP Hazmat multi-objetivo.
- C 3.4.Desarrollar una aplicación independiente para usar y comparar los diferentes algoritmos.

1.3.3 Contenido de la disertación

Para mayor orientación, se proporciona un breve resumen de la organización general del documento de tesis. La descripción de cada uno de los siguientes seis capítulos en este documento es la siguiente:

Capítulo 2 [C 1.1., C 2.1. y C 3.1.] Presenta el concepto de transporte de materiales peligrosos y la reducción de riesgos cuando camiones se utilizan para distribuir este tipo de materiales. Discute los diferentes enfoques en el ruteo en el transporte de materiales peligrosos. Presenta una revisión de la literatura seleccionada y estudios previos relacionados con el transporte de materiales peligrosos, el problema de ruteo de vehículos con flota heterogéneas y el problema transporte de sustancias peligrosas multi-objetivo. Obtiene suficientes antecedentes y comprensión de estos temas, y su importancia para la industria, el gobierno y el público, y establece las bases de esta investigación.

Capítulo 3 [C 1.2., C 1.3., C 1.4. y C 1.5.] Presenta el problema de optimización tratado en esta disertación. La variante del problema de ruteo de vehículos con flota heterogénea es un problema de optimización combinatoria de interés práctico en el transporte de materiales peligrosos. Se presenta una formulación mono-objetivo lineal por partes del problema de minimización del riesgo total de ruteo. Esta parte se enfoca en mejorar la metodología de análisis de riesgos al considerar un modelo de riesgo probabilístico en el que se usa la probabilidad de accidente en lugar de la frecuencia del accidente. Para facilitar una gestión de riesgos y una toma de decisiones más eficaces, se introduce esta opción para la comparación del riesgo de las rutas.

Un artículo fue presentado en *8th IFAC Conference on Manufacturing Modeling, Management and Control MIM 2016, Troyes, France, 2016*. Un artículo en línea fue publicado: *Mixed Integer Linear Programming Model for Vehicle Routing Problem for Hazardous Materials Transportation*.

Capítulo 4 [C 1.5. y C 2.1.] Ofrece información general sobre conceptos de algoritmos de optimización basados en búsquedas locales. Aquí se presenta un estudio sobre la estructura de los vecindarios utilizados en los problemas de ruteo de vehículos y cómo se pueden adaptar a las particularidades de la función objetivo del problema propuesto en el Capítulo 3.

Capítulo 5 [C 1.5., C 2.2. y C 2.3.] Presenta un algoritmo basado en la búsqueda de vecindarios que se prueba utilizando la versión la formulación mono-objetivo presentada en el Capítulo 3 y los estudios de estructuras de búsqueda locales y se desarrolló en el Capítulo 4.

El trabajo *Total Risk Routing Minimization for the Fleet Size and Mix Problem for Hazardous Materials Distribution* fue presentado en el *the annual workshop of the EURO working group on Vehicle Routing and Logistics optimization (VeRoLog), Nantes, France, 2016*. El artículo *Variable neighborhood search to solve the vehicle routing problem for hazardous materials transportation* fue publicado en el *Journal of Hazardous Materials*

Capítulo 6 [C 1.4., C 3.2., C 3.3., and C 3.4.] Presenta dos algoritmos híbridos multi-objetivo basados en métodos generativos. Se presentan las ventajas y desventajas de un algoritmo de vecindarios basado en dominancia de Pareto y de un algoritmo metaheurístico ϵ-*constraint*, utilizados para aproximar el frente de Pareto en problemas de optimización combinatoria multi-objetivo. Los algoritmos propuestos se prueban utilizando una formulación multi-objetivo de los problemas de transporte HVRP HazMat descritos en el Capítulo 3.

El trabajo *Bi-objective Fleet Size and Mix Vehicle Routing Problem for Hazardous Materials Transportation* se presentó en la *18th ROADEF Conference of Société française de Recherche Opérationnelle et Aide à la Décision*.

Capítulo 7 Presenta un resumen del trabajo, las conclusiones y las perspectivas adicionales.

1.3.4 Conclusiones y Perspectivas

Tres son los aspectos principales que forman el corazón de esta disertación. En primer lugar, una formulación matemática del problema de ruteo de materiales peligrosos utilizando una flota heterogénea a partir del modelo de programación lineal entera mixta utilizado para el problema de minimización del costo de ruteo. En el modelo propuesto, la evaluación del riesgo depende del tipo de vehículo, el material que se transporta y el cambio de carga cuando el vehículo pasa de un cliente a otro. También se considera cómo tratar con la naturaleza no lineal de la función objetivo de riesgo de ruteo total.

En segundo lugar, la exploración de métodos híbridos para resolver el problema mencionado anteriormente, conduciendo a desarrollar una metodología de solución precisa y computacionalmente eficiente.

Finalmente, se desarrolla un enfoque multi-objetivo para cuantificar los efectos de la reducción del riesgo en el costo total del ruteo. Debido a que el costo de ruteo y el riesgo son funciones objetivos conflictivas, la solución del problema multi-objetivo es un conjunto de soluciones en lugar de una solución única. La obtención de este conjunto es difícil por muchas razones y, por lo tanto, se han propuesto muchos enfoques para aproximarlas. La investigación presentada en esta disertación aborda estas observaciones y dificultades, la contribución principal en esta parte se centra en la aproximación del conjunto de Pareto de problema de ruteo de vehículos de flota heterogénea multi-objetivo (MHVRP) en el transporte de materiales peligrosos. Este tipo de problemas ha recibido un estudio limitado, lo mismo que su aplicación en el campo del diseño de transporte de HazMat. El rendimiento de cada algoritmo propuesto se evalúa usando una adaptación de problemas de pruebas de ruteo de vehículos con flota heterogénea. Debido a que los problemas de ruteo de vehículos multi-objetivos tienen muchas aplicaciones reales, en particular en el diseño de redes de distribución, el nuevo modelo propuesto de optimización para transportar material HazMat, utilizando redes viales que utilizan una flota heterogénea de vehículos, también se puede usar en otros escenarios como logística verde y transporte energético-eficiente.

En resumen, esta disertación introduce un marco matemático para informar a las partes interesadas del sector público y privado sobre aproximaciones rentables para reducir el riesgo de transporte de materiales peligrosos. Proporciona herramientas que se pueden utilizar para obtener la información necesaria para una mejor toma de decisiones basada en el riesgo. Además, ofrece una base para los investigadores interesados en el análisis de las opciones que la investigación de operaciones puede aportar en la reducción del riesgo de transporte de materiales peligrosos. Esta disertación amplía la investigación de la optimización multi-objetivo, especialmente la optimización combinatoria multi-objetivo (MOCO por sus siglas en inglés *multi-objective combinatorial optimization*). Se espera que las preguntas exploradas en esta disertación y los resultados y sus implicaciones subsiguientes aumenten la comprensión del campo, así como también abran nuevas áreas para futuras investigaciones.

Chapter 2

Routing Problem in Hazardous Material (HazMat) Transportation

Abstract (English)

This chapter presents the hazardous material vehicle routing problem. After an introduction (Section 2.1) draws a shape on hazardous material (HazMat) transportation, Section 2.2 details the two main approaches used in the literature for studying the HazMat routing problem, with focus on the distribution problem using road networks. Section 2.3 presents the heterogeneous vehicle routing problem as a model for HazMat distribution using road networks. The last section provides an introduction to the multi-objective nature of the HazMat distribution problem and the solutions methods implemented so far. The materials reviewed in this part provide the critical ideas and the rationale for this research work described in the upcoming chapters.

Résumé (Français)

Ce Chapitre présente le problème de tournées de véhicules transportant des substances dangereuses. Après une introduction, Section 2.1, qui décrit le transport de substances ou matières dangereuses (HazMat hazardous materials), la Section 2.2 détaille les deux principales approches utilisées dans la littérature pour étudier le problème de routage de HazMat, en mettant l'accent sur le problème de distribution utilisant des réseaux routiers. La Section 2.3 présente le problème de tournées de véhicules à flotte hétérogène en tant que modèle mathématique pour la distribution de HazMat utilisant des réseaux routiers. La dernière Section donne *une introduction à la nature multi-objective du problème de distribution de HazMat et aux méthodes de solutions mises en œuvre jusqu'à présent. Les matériaux examinés dans cette partie fournissent les idées critiques et la justification de ce travail de recherche qui est décrit dans les prochains chapitres.*

Resumen (Español)

En este Capítulo se presenta el problema de ruteo de vehículos en el transporte de materiales peligrosos. Después de la descripción dada en la introducción, Sección 2.1, del transporte de materiales peligrosos (HazMat hazardous materials), la Sección 2.2 detalla los dos enfoques principales utilizados en la literatura para estudiar los problemas de ruteo en el transporte de materiales peligrosos, centrándose en el problema de distribución utilizando redes de carreteras. La Sección 2.3 presenta el problema de ruteo de vehículos con flota heterogénea como modelo apropiado para la distribución de materiales peligrosos usando redes de carreteras. La última sección da una introducción a la naturaleza multi-objetivo del problema de distribución de materiales peligrosos y a los métodos de soluciones implementados hasta ahora. Los aspectos descritos en este Capítulo proporcionan las ideas críticas y la justificación para este trabajo de investigación, el cual se desarrolla en los siguientes capítulos.

2.1 Introduction

The United States (US) Department of Transportation defines a hazardous materials (HazMat) (or dangerous goods) as follows "*a substance or material that the Secretary of Transportation has determined is capable of posing an unreasonable risk to health, safety, and property when transported in commerce*". According to 49 US Code of Federal Regulations (CFR) 105.5 Term "Hazardous Materials" includes all of the following: (1) Hazardous Substances, (2) Hazardous Wastes, (3) Marine Pollutants, (4) Elevated Temperature Material (5) Materials identified in 172.101, and (6) Materials meeting the definitions contained in Part 173. For its part, the United Nations (UN) categorized hazardous materials into nine classes, according to their physical, chemical, and nuclear properties: explosives and pyrotechnics; gases; flammable and combustible liquids; flammable, combustible, and dangerous-when-wet solids; oxidizers and organic peroxides; poisonous and infectious materials; radioactive materials; corrosive materials (acidic or basic); and miscellaneous dangerous goods, such as hazardous wastes.

HazMat shipments are integral part of our industrial life style. In almost all instances, HazMat originate at a location other than their destination, and therefore transportation plays a significant role for these type of materials. The magnitude of this role depends on the size of a country and its level of industrialization. What makes the HazMat (or dangerous goods) transportation different from other transportation problems is the risk ingredient associated with this activity. Among these risks are those related to events as spills, fires and explosions. HazMat transportation accidents do happen, and they can happen during transportation as well as during their treatment and disposal. An accident is called an incident when there is a release of the HazMat (Erkut et al., 2007). An incident may bring severe consequences on the people and the environment nearby the affected site: fatalities, injuries, evacuation, property damage, environmental degradation, and traffic disruption.

HazMat transportation can be classified according to the mode of transport, namely: road, rail, water, air, and pipeline. In the case of inter-modal transport HazMat shipments are switched from one mode to another during its carriage. Among the different means used to transport HazMat, the usage of road system by trucks represents an increasingly pressing problem due to the constant augmentation of the shipments number and amount. Most of all individuals HazMat shipments in countries like Colombia are transported using trucks, three quarters (75.5%) of inland freight transport in the EU-28 was transported over roads (Eurostat), and 67% of total weight shipments in USA was moved by trucks (Bureau of Transportation Statistics U.S. DOT). Vehicular accident and human error are the most frequent cause of a serious HazMat transportation incidents on roads, and flammable-combustible liquid and corrosive materials classes account for the majority of HazMat accidents/incidents. While people benefiting from HazMat shipments are usually those who live near the production facility or the delivery points, the exposed population to the transport risks are those living along the route connecting the HazMat origin and destinations, whether or not they benefit from the HazMat shipments.

Research in HazMat transportation using vehicles on roads focuses on two main issues: the first one is related to assessing the risk induced on the population, the environment and/or infrastructure by HazMat vehicles traveling on various segments of the road network, and the second one involves the selection of the safest routes among the alternative paths between origin-destination pairs. One possible classification for HazMat transportation problem is given by Erkut et al. (2007):

- risk assessment,
- routing,
- combined facility location and routing,

- network design.

According to Taniguchi et al. (2010) risks are not fully taken into account in modeling city logistics and implementing city logistics schemes in urban areas. The reasons given by the authors are:

- *assessing the risks related to city logistics is hard due to uncertainty of these events*,
- *incorporating risks of natural and man-made hazards incurs additional costs logistical operations, and*
- *natural and man-made disasters are not regarded as being within the logistics managers' responsibility.*

HazMat transportation concerns about the safety of people, the natural environment and public and private properties, and it is an important issue, especially in large cities where transportation of fuel or industrial, biological or, radioactive waste can cause considerable harm to population and environment immediate to an accident. Reduction of HazMat transportation risks can be achieved in many different ways. Transportation risk management can be both proactive and reactive, and truck routing is considered a major proactive risk mitigation measure. This measure aims at reducing accident probability and reducing accident consequences. Operational research can be useful in providing effective methods for truck routing and, thereby, identifying routes that will give lowest costs and risks for HazMat transportation.

2.2 Hazardous Material Routing

Routing HazMat shipments implies to apply a selection criteria for choosing the safest paths among the alternative ones linking origin-destination. The risk factors pertaining to each alternative route (such as accident probability and population exposure) can vary with the level of different critical factors, among them, the type of material and vehicle (truck). A shipment typically involves multiple vehicles that have to be scheduled. Routing in HazMat transportation has two main focuses: shortest path problems and vehicle routing problem. *While the first class is dominated with large volume of the literature, research relating to second class is very limited* (Pradhananga et al., 2014a).

Related to **shortest risk path**, in recent works, Carotenuto et al. (2007) study the generation of minimal risk paths for the road transportation of HazMat between an origin-destination pair of a given regional area. They add to the main objective of selecting a set of paths of minimum total risk, risk equity, by bounding the maximum risk sustained by the population living along (in the proximity of) each populated arc of the network. Kang et al. (2014) determine routes that minimize the global Value-at-Risk value while satisfying equity constraint. Bronfman et al. (2015) present an exact model for the HazMat routing problem from an origin to a destination in a urban area, they maximize the minimum weighted distance between a vulnerable center and its assigned link.

Shortest path problems also are the base for the transportation network design problem. This problem integrates decisions pertaining to manufacturing plant and distribution center location, product distribution between different echelons of the supply chain, as well as customers' assignment to distribution centers. In HazMat transportation network design (HTNDP) a given set of HazMat shipments has to be sent over a road transportation network in order to transport a given amount of HazMat from specific origin points to specific destination points (Amaldi et al., 2011). Kara and Verter (2004) study the HTNDP and propose a bi-level integer programming model by considering the roles of carriers and a government authority. Erkut and Gzara (2008) generalize Kara and Verter (2004) model to the undirected case. Verter and Kara (2008) provide a path-based formulation for network design problem. Amaldi et al. (2011) consider a generalization of the HTNDP where a subset of roads can be forbidden by the government. Xin et al. (2013) use the absolute deviation criterion (maximum regret criterion) to deal with the risk uncertainty in HTNDP.

Vehicle routing problem (VRP) is one of the most frequently faced logistical decisions in distribution management; it belongs to operational decisions in logistics management, where it often arises in transportation decisions as collection of raw materials, and distribution of intermediate and final products to customers (Prins, 2009). The complexity of this problem causes a heavy computational burden for its solution, especially in cases of large scale distribution networks.

The vehicle fleet used to transport goods have different capacities, fixed costs, and/or variable costs. The associated type of VRP in this transportation case is called **Heterogeneous Fleet Vehicle Routing Problem (HVRP)** in which customers are served by a heterogeneous fleet of vehicles. Although it is more general, the HVRP has only attracted very few consideration and its solution method is still a topic of interest (Hoff et al., 2010), specially in the case of HazMat routing problem. Using this type of variant of VRP is a way to incorporate the complexity of real-life routing problems (Sörensen et al. (2008)).

There are a few routing studies with a single objective for the VRP in HazMat transportation. Tarantilis and Kiranoudis (2001b) propose a risk based technique to solve a capacitated vehicle routing problem (CVRP) in the HazMat distribution. They focus on population exposure risk mitigation via construction of truck routes.

They employ a List Based Threshold Accepting (LBTA) algorithm that minimizes risk by minimizing the total distance traveled by trucks in the so-called risk space. The risk of a point is defined as the product of population of an aggregate population point (city, town, ward) and distance length between this point and the aggregate population point. Pradhananga et al. (2011) apply a genetic algorithm to solve a typical HazMat routing problem in Thailand. The routing problem is solved for a single cost based objective, minimizing the economic and risk costs.

2.3 Heterogeneous Fleet Vehicle Routing Problem

The heterogeneous fleet VRP with unlimited number of each vehicle type, also called fleet size and mix VRP (FSMVRP), was first considered by Golden et al. (1984). This problem is an extension of the CVRP that accommodates a heterogeneous fleet and takes vehicle costs into consideration in addition to travel costs. This variant of VRP arises when a fleet of vehicles characterized by different capacities and costs is available for distribution activities. Taillard (1999) introduced the version of HVRP that considers a heterogeneous fixed fleet of vehicles, with a limited number of available vehicles of each type.

There is a strong dependency between fleet composition and routing. When solving heterogeneous fleet VRP, it has to take into account that routing decisions are strongly dependent on the available fleet. Also, fleet composition decisions may be based on a too simplified view on transportation demand if routing aspects are ignored. In HazMat transportation problem this point is crucial, as it will be shown in the next chapter, the type of vehicle and its load size are among the critical factors for estimating the transportation risk.

Golden et al. (1984) suggest several heuristics for HVRP with unlimited fleet. The authors also develop a procedure to calculate the lower bound that trades off the fixed costs against the routing costs. They define 20 test instances with $12-100$ nodes and $3-6$ vehicle types, generally used as benchmark instances for the standard FSMVRP. Taillard (1999) proposes a heuristic column generation method for the HVRP. Combining tabu search and linear programming to solve the problem, and considering the set of test problems proposed by Golden et al. (1984), the method is tested on the eight largest instances of the set, including variable costs c_{ij}^k dependent of the type of vehicle used on arc (i, j).

Baldacci et al. (2008) review the main solution approaches proposed for the VRP with heterogeneous fleet and defined five different variants for the problem. They compare different heuristic algorithms on some benchmark instances, identifying lower bounds. Hoff et al. (2010) made a survey focusing on operational research technique combining fleet composition and vehicle routing. They establish two classes for HVRP: the heterogeneous fixed fleet (HFF) problem and the fleet size and mix (FSM). They reviewed the literature on fleet composition and routing related to industrial aspects.

Tarantilis and Kiranoudis (2001a) present a paper in which they formulated the problem of distributing fresh milk in Greece as HVRP and solved it with an algorithm call backtracking adaptive threshold accepting (BATA). This is a meta-heuristics threshold accepting algorithm in which the value of the threshold is lowered, raised or backtracked depending on new accepted solutions. Prins (2002) presents heuristic solution methods for HVRP dealing with multi-trips. Prins considers two objectives, the main one is to minimize the total duration of trips and the second one is to minimize the number of trucks. Chu (2005) addresses the problem of routing a fixed number of trucks with limited capacity from a central warehouse to customers with known demand. He developed a mathematical model and a heuristic algorithm. First the selection of a group of customers is carried out and a modification of Clarke and Wright's savings algorithm is used to obtain the initial solution. Then a refining procedure composed of a succession of intra-route and inter-route arc exchanges is applied to initial solution. Tavakkoli-Moghaddam et al. (2007) present a mix-integer linear model of a CVRP with split services and heterogeneous fleet. They used hybrid simulated annealing method to solve the model. Li et al. (2007) adapt their record-to-record travel algorithm for the VRP to handle the HVRP. They compare the results on eight benchmark problems used by Taillard (1999).

Prins (2009) presents two memetic algorithms (genetic algorithms hybridized with a local search) able to solve HVRP. Both algorithms use solutions encoded without trip delimiters, which can be evaluated with a splitting procedure. The evaluation is pseudo-polynomial for the HVRP. He compared his results with those of the best published algorithms using the 20 instances from Golden et al. (1984). Li et al. (2010) propose a multistart adaptive memory programming (MAMP) and path relinking algorithm to solve HVRP. They use MAMP for constructing several provisional solutions at each iteration, these provisional solutions are further improved by a modified tabu search. Path relinking is integrated to enhance the performance of MAMP as intensification strategy. Tütüncü (2010) propose a visual interactive approach based on a new greedy randomized adaptive memory programming search (GRAMPS) algorithm. The algorithm is used to solve the heterogeneous fixed fleet vehicle routing problem (HFVRP) and the heterogeneous fixed fleet vehicle routing problem with backhauls (HFVRPB). Brandão (2011) proposes a tabu search algorithm and tested it on several benchmark problems. The initial solution is obtained by constructing a travelling salesman problem (TSP) tour including all the customers and by performing a partition of the tour into feasible routes. He overcomes local optima by using several different route improvement proce-

Table 2.1: Heterogeneous VRP Problems and Solution Methods

Heterogeneous Fleet Vehicle Routing Problems			
Fleet Size and Mix		Heterogeneous Fixed Fleet	
Authors	**Method**	**Authors**	**Method**
Golden et al. (1984)	Heuristics	**Taillard (1999)** (19)	Heuristics Column Generation
Salhi and Rand (1993)(6)	Heuristics	Tarantilis et al. (2004)(15)	Deterministic Simulated Annealing (Threshold Accepting) (Record to record)
Taillard (1999)(3,4,14,15,19)	Heuristics Column Generation	Li et al. (2007)[7/8]	Deterministic Simulated Annealing (Threshold Accepting) (Record to record)
Gendreau et al. (1999)(5)	Tabu Search		
Brandão (2009)(17,18)	Tabu Search	Prins (2009)[6/8]	Memetic Algorithm
Choi and Tcha (2007) (13,16)	Exact Methods (B&Bound + CG)	Subramanian et al. (2012)[7/8]	Hybrid algorithms
Prins (2009)[9/12]	Memetic Algorithms	Duhamel et al. (2012)[6/8]	Hybrid algorithms
Subramanian et al. (2012)[12/12](20)	Hybrid algorithms		

Best know solution (BKS) found for this instances by the first time, Number of BKS found over the number of studied instances

dures. Duhamel et al. (2012) present a hybrid evolutionary local search for heterogeneous fleet vehicle routing problems based on the application of split strategies and propose a set of new HVRP instances from 50 to more than 250 nodes. Subramanian et al. (2012) propose a hybrid algorithm based on the Iterated Local (ILS) Search metaheuristic, that uses Variable Neighborhood Descent (VND) with random neighborhood ordering (RVND) in the local search phase, combined with a Set Partitioning (SP) formulation. Their results are quite competitive with those found in the literature and new improved solutions are reported. See in Table 2.1 the literature review summary.

Kwon et al. (2013) use tabu search algorithms to obtain solutions for the heterogeneous fixed fleet vehicle routing with carbon emission to minimizing the sum of variable operation costs. They consider three neighborhood generation methods for tabu search; insertion, swap and hybrid. Penna et al. (2013) propose an algorithm based on the iterated local search (ILS) metaheuristic which uses a variable neighborhood descent procedure, with a random neighborhood ordering (RVND), in the local search phase. They consider five different HVRP variants involving limited and unlimited fleets. Naji-Azimi and Salari (2013) propose an integer linear programming-based heuristic approach for the HFVRP it is intended for been used as a complementary tool to improve the performance of the existing methods of solving this problem. The method follows a destruct-and-repair paradigm in which the initial solution is destroyed and repaired by solving an ILP-based model to optimality. The proposed method follows four major phases to check for any possible improvement: selection phase, extraction phase, recombination phase and reallocation phase.

Considering hybrid methods for solving HVRP problems have proved to provide good solutions. These heuristic approaches consider cooperation between meta-heuristics and exact methods. Tours, constructed by the meta-heuristics, are given to the exact algorithm which works on a subspace (partitioning). The hybrid methods implemented by Penna et al. (2013) and Subramanian et al. (2012) are a sequential implementation where the components work on only on a part search space (Jourdan et al. (2009)). Also, as pointed out by Sörensen et al. (2008) multiple neighborhood search is one of the best-performing approaches when designing the meta-heuristic component.

To the best of our knowledge no publication deals with HVRP in HazMat transportation. Çağri et al. (2016) make a classification and review of the literature on heterogeneous vehicle routing problems. They claim that no exact algorithm has specifically been designed for the standard HVRP, and present hybrid heuristics including local search as having a good performance solving the unlimited and limited version of HVRP. They also review some variants and extensions of HVRP in recent works but HazMat transportation is not mentioned.

2.4 Multi-objective vehicle routing HazMat transportation works

Total transportation cost and risk are not only conflicting objective functions, but also they are measured in different units. Transportation risk is generally expressed as the expected consequences (population exposure) of a hazardous materials accident, the road segment hazardous materials accident probability times the exposed population. This last term is defined as the population that is contained in a given distance from roadway segment where the HazMat incident can happen. Usually, the hazardous materials accident probability is assumed constant independently of the truck load. That means that the road segment risk is an input parameter of the problem.

2.4.1 Overview of multi-objective vehicle routing problem (MO-VRP)

Demir et al. (2014) note that the multi-objective variant of the VRP has not been extensively studied. Also, they point out the infrequent use of Pareto dominance based methods and/or of multi-objective metrics for comparing algorithms performance when solving MO-VRP. Jozefowiez et al. (2008) find in their overview of the research about MO-VRP that the three most common objectives are minimization of: the cost (distance or time), the length of the longest tour (makespan), and route balance. Also, They present two strategies as the most preferred by the researchers for solving the multi-objective routing problem, scalar methods, as weighted aggregation, and evolutionary algorithms. Labadie and Prodhon (2014) complement the previous work reaching similar conclusions. They also identify MO-VRP with time windows (TW) as the most investigated variant.

The above mentioned can be verified with a brief description of some relevant past works related to MO-VRP. Starting with the objectives concerned and the solution methods applied, most of the latter are developed to solve a MO-VRPTW, including the total travel time (length) as an optimization objective. Multi-objective evolutionary algorithms are used in the works of Ombuki et al. (2006), Jozefowiez et al. (2009), Tan et al. (2006), Ghoseiri and Ghannadpour (2010), Garcia-Najera and Bullinaria (2011), and Lacomme et al. (2015a). Multi-objective versions of meta-heuristics based on trajectory approach are used by Norouzi et al. (2009) (particle swarm) and Baños et al. (2013) (simulated annealing). While, Demir et al. (2014) employ a multi-objective version of the adaptive large neighborhood search (ALNS) algorithm, considering the minimization of fuel consumption and the minimization of driving time as objectives. In most of these works the objectives considered are connected in one way or another, among them, the number of routes or vehicles, the total travel distance, the total travel time, the route balance. Although in the work of Demir et al. (2014), objective functions are to some extent related, they are measured in different units and their computations are independently conducted.

Regarding the most used metrics in the previously described works, hypervolume is the preferred measure to conduct the comparison of the results, but not all of works utilize a multi-objective performance metric.

2.4.2 Multi-objective vehicle routing problem in HazMat transportation

Concerning the HazMat multi-objective VRP, Jozefowiez et al. (2008) present hazardous product distribution as an example of multi-objective VRP where a specific real-life situation is studied, that is, decision-makers define the objectives to be optimized. In this study, the work of Zografos and Androutsopoulos (2004) is presented as an example of multi-objective HazMat distribution.

Zografos and Androutsopoulos (2004) define a bi-objective vehicle routing problem with time windows, the two objective considered are risk and cost minimization. The transportation risk is expressed as the expected consequences. They solve a mono objective problem weighting the two objectives (scalarization approach). They propose an insertion heuristic that builds the routes step by step by inserting in the already existing routes a new demand point at each iteration. They compare the results of alternative constructive algorithms with the results of their proposed heuristic for the mono-objective case, the number of vehicles used, the travel time, and the schedule time. They present some non-dominated solutions for the bi-objective application of the heuristics but they do not use any multi-objective performance measure for assessing the results.

Later, Zografos and Androutsopoulos (2008) use again the traditional risk measure. Here the exposed population is estimated by simulating and assessing a wide range of HazMat incident scenarios, using a geographic information system (GIS) functionality that estimates the total population within a specific designated area. The hazardous materials accident probability on any road segment is computed through a discrete choice model. Nevertheless, these two values are given as problem input. They use multiple compartment trucks. Each compartment can be loaded with only one type of products. Also in this work, the solution approach is based on the weighting method and use an insertion heuristic algorithm for approximating the set of non-dominated solutions (Zografos and Androutsopoulos, 2004).

Following their previous works, Androutsopoulos and Zografos (2010) incorporate time-dependent cost and risk attributes of each arc of the underlying transportation network. They suppose the population exposure and the accident probability may vary considerably for different parts of a day. However, in their work, the sequence of stops for a truck is known in advance but multiple-objectives are considered. They define the problem as a bicriterion shortest time-dependent path problem with fixed mandatory intermediate stops constrained within specified service time windows.

Androutsopoulos and Zografos (2012) present a bi-objective time-dependent vehicle routing problem with time windows. The objective function is expressed by the weighted sum of the two objectives under consideration, routing cost and transportation risk. A route-building heuristic algorithm is presented for addressing each of the constituent single-objective problems, it takes into account explicitly the bi-objective path-finding problems between any pair of stops. They retake the problem in Androutsopoulos and Zografos (2010) but in this case identification of the truck routes is also part of the problem.

Table 2.2: Multi-objective VRP in HazMat Transportation

Authors	**Problem**	**Solution method**	**Risk function model**	**Multi-objective approach**
(Zografos and Androutsopoulos, 2004)	Vehicle routing problem with time windows	Insertion based heuristic	Traditional risk model	Weighted Method.
(Zografos and Androutsopoulos, 2008)	Vehicle routing problem with time windows	Insertion based heuristic.	Traditional risk model	Weighted Method
(Tanguchi et al., 2010).	Vehicle routing problem with time windows	Ant colony system (ACS)	Traditional risk model	**Non dominated paths**
(Lozano et al., 2011)	Vehicle routing problem		The length and the population exposure.	Weighted Method
(Pradhananga et al., 2014b)	Vehicle routing problem with time windows	Multi-objective ant colony system (MOACS)	Traditional risk model	**Non-dominated path**

Tanguchi et al. (2010) present an Ant Colony System (ACS) based meta-heuristic algorithm that is supported by a labeling algorithm for solving a multi-objective optimization vehicle routing problem with time windows (VRPTW) in HazMat transportation. The simultaneous minimization of three conflicting objective functions are considered: total number of vehicles in use, total scheduling time of all the vehicles in operation, and total risk exposure associated with the transportation process. The risk associated with a path due to a HazMat incident is a measure of probability of occurrence of the event and its consequence. Exposed population for each arc segment is used as a consequence of HazMat incident. In Table 2.2 are presented some relevant works in multi-objective HazMat VRP.

2.5 Conclusions

2.5.1 Conclusions (English)

The vehicle routing problem in the context of hazardous material transportation that includes enriching elements as a heterogeneous fleet is an interesting study subject. It has attracted less attention when compared with the shortest path problem in hazardous material transportation. Hazardous material transportation has multiple stakeholders with different objectives, thus, not only the risk routing minimization should be considered, but the total transportation minimization when optimization is undertaken.

Analysis and assessment of the route risk is the starting point in order to undertake a study of the hazardous material transportation. In this case, the interest is placed on the routing hazardous material transportation problem, thus, assessing the risk induced on the population, the environment and/or infrastructure by hazardous materials vehicles traveling on various segments of the road network is a necessary previous step for the selection of the safest routes. The impact of routing decision variables as the type of vehicle, the transported material and the arch composing the path to travel must be considered when assessing the route risk. A quantitative risk assessment approach seems to be the path to follow to applicate operational research models and methods. There are several path evaluation functions for hazardous materials transportation. It should always be borne in mind that the risk model selected for path evaluation has effects on the path or route decisions, and two are the main model components to take into account, the incident probability estimation and the consequence assessment.

Multi-objective optimization of vehicle routing problem belongs to multi-objective combinatorial optimization, where the focus has been on vehicle routing problem with time windows and using evolutionary algorithms as solution methods. Exploring the use of solution methods based on local search appears to be a promising and interesting approach to solve the multi-objective vehicle routing problem.

There is an opportunity in study the multi-objective optimization of vehicle routing problem using an heterogeneous fleet, through an urban street network, transporting hazardous materials considering different routing variables in risk assessment. Firstly, it is necessary to propose a mathematical optimization model that incorporates the practical aspect of hazardous materials transportation such as: heterogeneous fleet of vehicles, route risk estimation, urban street network. How risk is incorporated into hazardous transportation problems must be a main aspect in model formulation. Then, efficient and effective solution methods have to be developed according to the size of the instance of the problem considered. In the next chapter, a quantitative risk analysis approach for hazardous material transportation using a road network is introduced, and a mixed integer linear programming formulation for the heterogeneous fleet vehicle routing problem is presented.

2.5.2 Conclusions (Français)

Le problème de tournées de véhicules dans le contexte du transport de matières dangereuses incluant l'utilisation d'une flotte hétérogène est un sujet d'étude intéressant. Cependant, il a attiré moins d'attention par rapport au problème de plus court chemin pour le transport de matières dangereuses. Dans ce type de problème, on retrouve de multiples parties prenantes ayant des objectifs différents. Ainsi, pour entreprendre une démarche d'optimisation, non seulement la minimisation du risque doit être considérée, mais aussi la minimisation du coût total de transport.

L'analyse et l'évaluation du risque dans les tournées de véhicules sont le point de départ pour entreprendre une étude du transport des matières dangereuses. Dans le problème de transport des matières dangereuses, l'évaluation des risques induits sur la population, l'environnement et / ou l'infrastructure par les véhicules circulant sur diffrents tronçons du réseau routier est une étape préalable nécessaire pour la sélection des routes les plus sûres. L'impact des variables portant sur les décisions comme le choix du type de véhicule ou des arcs composant la trajectoire à parcourir doit être pris en compte lors de l'évaluation du risque des tournées. Une approche quantitative de l'évaluation des risques semble être la voie à suivre pour appliquer les modèles et méthodes de recherche opérationnelle. Il existe plusieurs fonctions d'évaluation de chemin pour le transport de matières dangereuses. Il faut toujours garder à l'esprit que le modèle du risque sélectionné pour l'évaluation des tournées a des effets sur les décisions des routes empruntées, et que les deux principales composantes du modèle à prendre en compte sont l'estimation de la probabilité d'incident et l'évaluation des conséquences.

L'optimisation multi-objectif du problème de tournées de véhicules appartient à l'optimisation combinatoire multi-objectif, où la littérature montre que l'accent a surtout été mis sur le problème de tournées avec fenêtres de temps et en utilisant des algorithmes évolutifs comme méthodes de résolution. Explorer l'utilisation de méthodes basées sur la recherche locale semble être une approche prometteuse et intéressante dans notre cas: l'étude de l'optimisation multi-objectif du problème de tournées de véhicules utilisant une flotte hétérogène, à travers un réseau routier, transportant des matières dangereuses en tenant compte les différentes variables de tournées dans l'évaluation des risques.

2.5.3 Conclusiones (Español)

El problema de ruteo de vehículos en el contexto del transporte de materiales peligrosos que incluya elementos enriquecedores como una flota heterogénea es un tema de estudio interesante. Este problema ha atraído menos atención cuando se compara con el problema de ruta más corta, para el caso del transporte de materiales peligrosos. Múltiples son las partes interesadas en el transporte de materiales peligrosos, las cuales pueden llegar a tener diferentes objetivos. Por lo anterior, no solo se debe considerar la minimización del del riesgo de ruteo, sino la minimización del costo total del transporte cuando se lleva a cabo la optimización.

El análisis y la evaluación del riesgo sobre una ruta es el punto de partida para realizar un estudio del transporte de materiales peligrosos. Dado que en ese trabajo el interés se centra en el problema del transporte de materiales peligrosos, un paso previo es evaluar el riesgo inducido en la población, el medio ambiente o bien la infraestructura por vehículos transportando materiales peligrosos que viajan a través de varios segmentos de una red vial; para después realizar la selección de las rutas más seguras. Al evaluar el riesgo de ruta, deben considerarse el impacto de variables de decisión de ruteo como el tipo de vehículo, el material transportado y los segmentos que componen la ruta de viaje. Un enfoque cuantitativo de evaluación de riesgos parece ser el camino a seguir para aplicar los modelos y los métodos de investigacin operacional. Varias son los modelos de funciones que existen para la evaluación del riesgo de ruteo en el transporte de materiales peligrosos. Debe tenerse en cuenta al elegir una ellos, que el modelo de riesgo seleccionado para la evaluación de ruta tiene efectos sobre la ruta o las decisiones de ruta, y que dos son sus principales componentes a tener en cuenta, la estimación de probabilidad de incidente y la evaluación de las consecuencias.

La optimización multi-objetivo del problema de ruteo de vehículos pertenece al tipo de problemas de optimizacin combinatoria, donde el enfoque ha estado en los problema con ventanas de tiempo y métodos de solución basados en algoritmos evolutivos. Explorar el uso de métodos de solución basados en la búsqueda local parece ser un enfoque prometedor e interesante para resolver el problema de ruteo de vehículos multi-objetivo dado los buenos resultados en la variante mono-objetivo.

Existe una oportunidad para estudiar el problema multi-objetivo de optimización del ruteo de vehículos utilizando una flota heterogénea, a través de una red de calles urbanas, transportando materiales peligrosos y considerando diferentes variables de ruteo en la evaluación de riesgos. En primer lugar, es necesario proponer un modelo de optimización matemática que incorpore aspectos prácticos del transporte de materiales peligrosos, tales como: una flota heterogénea de vehículos, estimación del riesgo de ruta, red de calles urbanas, entre otros. Cómo se incorpora *el riesgo a los problemas de transporte peligrosos debe ser un aspecto principal en la formulación del modelo. Paso seguido, se deben desarrollar métodos de solución eficientes y efectivos acordes con el tamaño de la instancia del problema considerado. En el siguiente capítulo, se presenta un enfoque de análisis cuantitativo de riesgos para el transporte de materiales peligrosos utilizando una red de carreteras, y se presenta una formulación de programación lineal mixta para el problema de ruteo de vehículos de la flota heterogénea.*

Chapter 3

Hazardous Materials (HazMat) Transportation Risk Modeling

Abstract (English)

This Chapter focuses on a quantitative risk analysis in hazardous material (HazMat) transportation using a road network, and the use of this model in a mixed integer linear programming formulation for the heterogeneous fleet vehicle routing problem. The Chapter is organized as follows. In Section 3.1 an introduction about HazMat transportation risk is presented. Section 3.2 presents a review about quantitative risk analysis (QRA) studies of transportation of HazMat as flammable liquids (gasoline). Section 3.3 deals with the risk route evaluation, with special emphasis on HazMat transportation using road networks. In the Section 3.4., the focus is on the mathematical mixed integer linear programming model for the risk routing minimization in the context of HazMat transportation.

Résumé (Français)

Dans ce Chapitre l'accent est mis sur une analyse quantitative de risque dans le transport de substancess dangereuses (HazMat hazardous material) utilisant un réseau routier, et l'utilisation de ce modèle dans une formulation de programmation linéaire en nombres entiers pour le problème du tournée des véhicules à flotte hétérogène. Le Chapitre est organisé comme suit. Dans la section 3.1, une introduction sur le risque de transport de HazMat est présentée. La section 3.2 présente une revue de littérature des études d'analyse quantitative des risques (QRA quantitative risk analysis) portant sur le transport des HazMat en tant que liquide inflammable (essence). La section 3.3 traite de l'évaluation des risques sur les routes, en mettant l'accent sur le transport de matières dangereuses en util-

isant les réseaux routiers. Dans la section 3.4., le focus est possé sur le modèle de programmation linéaire mixte mathématique pour la minimisation des risques du routage dans le contexte du transport de HazMat.

Resumen (Español)

Este capítulo se centra en un análisis cuantitativo de riesgos en el transporte de material peligrosos (HazMat hazardous material) utilizando una red de carreteras, y el uso de este modelo en una formulación de programación lineal mixta entera para el problema de ruteo de vehículos con flota heterogénea. El capítulo está organizado de la siguiente forma. En la Sección 3.1, se presenta una introducción sobre el riesgo de transporte de materiales peligrosos. La Sección 3.2 presenta una revisión sobre los estudios de análisis de riesgos cuantitativos (QRA quantitative risk analysis) en el transporte de materiales peligrosos, como por ejemplo líquidos inflamables (gasolina). La Sección 3.3 trata sobre la evaluación del riesgo en la ruta, con especial énfasis en el transporte de materiales peligrosos utilizando redes de carreteras. En la Sección 3.4., La atención se centra en el modelo matemático de programación lineal entera mixta para la minimización del riesgo de ruteo en el contexto del transporte de materiales peligrosos.

3.1 Introduction

The transportation risk is a measure of the probability and severity of harm to an exposed receptor due to potential undesired events involving hazardous materials (HazMat) (Alp, 1995), (Erkut et al., 2007). When assessing the risk in HazMat transportation many variables need to be considered, see Figure 3.1 (Kazantzi et al., 2011b), where the type of material being transported, the load size and the type of truck used are among the critical variables to be considered.

As it has been mentioned previously, two are the key elements in the HazMat transportation, one is **the estimation and analysis of risk**, and the other element is the **routing problem** (Erkut et al., 2007). Assessing the risks caused by events in HazMat transportation is a difficult task, the frequency of the initiating events is very low, crashes on roadways are uncertain, and incidents have a large impact on people and buildings and other traffic by the explosion or spill of hazardous material. There is no consensus on the best way to model risk but, it is generally agreed that any formulation should include two elements: the probability of an accidental HazMat release, and its associated consequences. The routing problem for HazMat can be described as the minimum risk path selection problem. Considerable attention should be paid to the risk modeling in HazMat transportation routing. When

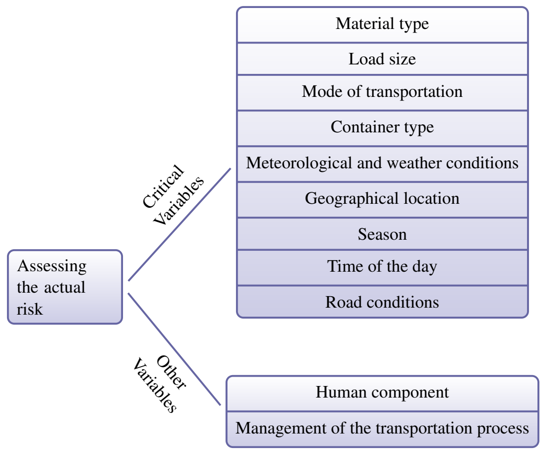


Figure 3.1: Variables in HazMat transportation assessment

selecting the route between a given origin-destination pair for a given HazMat, transportation mode, and vehicle type, the alternatives routes generated depends critically on the model adopted for the quantification of risk (Bell, 2006). The risk model has effects on the path or route decisions, and the optimal path for certain criterion can perform poorly under another (Erkut et al., 2007).

3.2 Quantitative Risk Analysis in HazMat Transportation

According to Kazantzi et al. (2011b), there is a number of papers that have pointed out the uncertainties and pitfalls in assessing accident and release rates as well as characterizing consequential risk incidents. This is because incident occurrences in HazMat transportation are very low and reported incident data are very scarce. Some use historical frequencies for estimating truck accident rates and release probabilities in accidents from truck accident data. Other alternative way of estimating probability HazMat release incidents is the use of fault tree and event tree analysis methods. These techniques sometimes are combined with Monte Carlo simulations, especially when an examination of the impact of different input variables on risk occurrences wants to be carried out. The consequences of a HazMat transportation incident are economic losses, injuries, fatalities, environmental pollution, damage to wildlife, traffic interruption. These consequences are a function of the population, property, and environmental assets within the impact area (Erkut et al., 2007). The shape and size of an impact area depends on many factors, such as the substance being transported, the topology, the weather, and the speed and direction of the wind.

Risk analysis can be qualitative or quantitative. In the case of the qualitative risk assessment possible accident scenarios are identified and the consequences are estimated. Back in 1971, the National Transportation Safety Board (NTBS) was strongly recommending a quantitative risk-based approach in order to establish regulations for HazMat transportation (List et al., 1991). Since then, several techniques have been developed for estimating risks associated with HazMat transportation. Quantitative Risk Analysis (QRA) has matured to the point that it is considered an effective tool that is used to support stakeholders decisions. One of the critics in the work of List et al. (1991) was about the availability of data supporting the detailed estimates of the probability that a specific type of vehicle will be involved in an accident with a consequent release of HazMat. According to Erkut et al. (2007) the quality of this data has improved, nowadays there is more access to huge amount of historical data on accident frequencies, specially in developed countries, and more accurate models for estimating the consequences after an accident.

QRA results in a numerical assessment of risks involved. At the end this risk analysis can be summarized by using a single measure of risk as the expected consequences, or by the FN-curve (or risk profile) which expands the point estimate of the expectation to the entire distribution, (List et al., 1991) and (Erkut et al., 2007). The expected consequence is a convenient measure for mathematical programming models, while FN-curve is a richer multiple-measure method. Both measures can be derived from the use of the general framework for risk analysis in transportation proposed by Ang (1979). It decomposes the problem into three different stages: (a) determining the probability of an undesirable event; (b) determining the level of potential receptor exposure, given the nature of the event; and (c) estimating the magnitude of consequences, given the level of exposure. Each of these stages produces one or more probability distributions, with the two last stages involving conditional distributions. The probability distribution of accident event that involves a HazMat transportation and the conditional distributions can be combined to produce a resulting distribution of potential consequences from a specified activity. In the Figure 3.2 is displayed the framework.

One example of an expected consequences measure is to compute the expected number of impacted individuals by multiplying the probability of impact per person with the number of persons present in the affected zone (societal risk). This means, the multiplication of the *individual risk* for a person in the neighborhood of the impacted road segment al_{ij} (Equation 3.1) by the population located in the neighborhood of road segment al_{ij}, PD_{ij}.

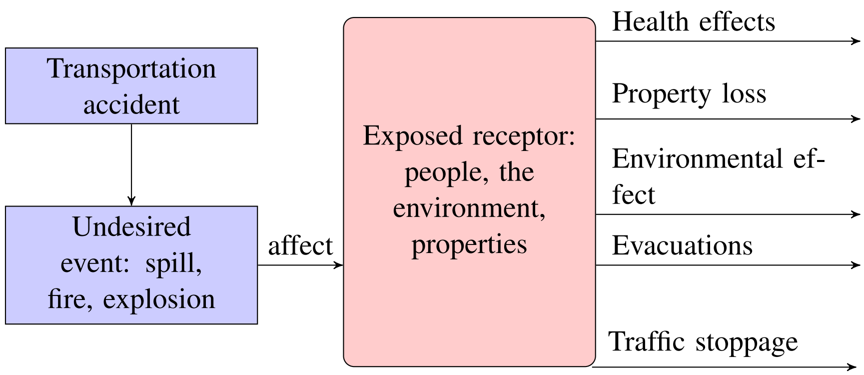


Figure 3.2: Risk Assessment Framework

$$p_{al_{ij}}(A, M, I, D) = p_{al_{ij}}(D|A, M, I)p_{al_{ij}}(I|A, M)p_{al_{ij}}(M|A)p_{al_{ij}}(A) \quad (3.1)$$

where $p_{al_{ij}}(A, M, I, D)$ is the probability of an injury to an individual (D) given than an outcome (I) was the result of the HazMat release initiating event (M) as a result of the vehicle accident event (A) that involves a HazMat transporter. The greater the number of people present around the hazardous activity the greater the societal risk (Erkut et al., 2007).

3.2.1 The probability of a HazMat transportation incident

The first stage of the framework presented by Ang (1979) requires, according to List et al. (1991), the estimation of the probabilities of various types of incidents generally based on:

1. estimates of accident rates involving vehicles carrying HazMat, and
2. estimates of the probability of release of material (or of the probabilities of releasing various amounts of material) in an accident of a given type.

The probability that a vehicle (henceforth truck) of the type being considered will be involved in an accident with a consequent release of hazardous material is replaced normally by the estimation of the accident/incident truck rates. Every truck carries HazMat in its fuel tank, however, this work specifically addresses vehicles carrying HazMat type 3 (flammable liquids as gasoline) loads additional to that carried in their fuel tank. A "release" is defined as a spill or leak of the HazMat load, and an "accident" is defined as an event involving one or a combination of a collision, an overturn or the truck running off the road (Button and Reilly, 2000). The analysis of accident rates is out of the scope of this research. Here, it is assumed that the required accident rates are available from observed data or from estimates specific to the road network being considered. Kazantzi et al. (2011b) present a review of some works about assessing accident and release rates. Their work focuses on accident-related incidents for highway transportation. First, they consider the accident rates of a truck of type k ($TTAR^k$) expressed in terms of the number of accidents per Million Vehicle-Kilometers traveled ($MVKm$). The $TTAR^k$ varies between $0.164MVKm$ and $2.238MVKm$ for accident rates in different countries and different type of roads (urban and rural). The probability PR_{ij} , it is defined as the probability of a release event (or incident) on an arc (i, j) that connects two network nodes i and j, and it is computed as:

$$PR_{ij} = TTAR^k \times al_{ij} \times P_{release} \tag{3.2}$$

where, al_{ij} is the arc length, and $P_{release}$ is the probability of HazMat release given a truck accident, each arc (i, j) of the road network consists of segments that are assumed to be homogeneous in the probability of a release event. The $TTAR^k$ can be estimated using available data on truck accident rates with respect to the road network being considered (e.g. rural, urban, etc) by the following equation Chakrabarti and Parikh (2011):

$$TTAR^k = \frac{YATT^k}{TTK^k} \tag{3.3}$$

$YATT^k$ is the yearly number of accidents of the truck tank type k on the route network studied, and TTK^k is the annual truck tank kilometers of travel on the route network. The types of accidents involving trucks transporting HazMat include overturn and collision, overturn with no collision, collision with no overturn, and no overturn and no collision. HazMat accidents resulting into loss of containment (LOC) or release is accounted in terms of what is known as the *Releasing Accident Truck Tank Rates* (RATTRs) which is obtained by multiplying the TTARs with the default release probabilities for the road network (Chakrabarti and Parikh, 2011).

The conditional probability that a HazMat release will occur following an accident, $P_{release}$, is estimated based on model developed in the work of Button and Reilly (2000), also applied in the work of Kazantzi et al. (2011b). The model output can be used to estimate release and fire incident rates for specific truck routes (rural or urban), types of trucks (tanker or non-tanker), and types of loads (type of HazMat, large or small load), but in this work the model is only used for computing the probability of a HazMat release or LOC after a truck tank accident. At the end the objective is to compute $TTAR^k \times P_{release}$ that represents the release or spillage probability per $truck\ tank - Km$, as detailed in the work of Chakrabarti and Parikh (2011). However in this last study the authors use default release probabilities taken from the work of Harwood et al. (1993).

3.2.2 The probability of incident outcomes

After defining the frequency of an initiating event (the spill of a hazardous material) it is necessary to define the probability of a certain outcome arising as a consequence, such as a fire, explosion, or toxic gas cloud (Ronza et al., 2007). The incident that follows a loss of containment event can lead to *no outcome* or a *major accident* such as an explosion or a large fire (Vílchez et al., 2011).

The volume of transported HazMat plays an important role in determining the likelihood of occurrence of an incident. In HazMat material distribution, the vehicle load is reduced by a quantity equals to the customer demand each time a client is visited, affecting the optimal path in risk minimization problems. Here we use the model proposed by Ronza et al. (2007). They use the *Hazardous Materials Incident Reporting System* (HMIRS) of the US Department of Transportation's HMIS (Hazardous Materials Information System) for estimating the probability of an outcome of the release of a HazMat as a function of the amount and substance spilled. This model is based on empirical approaches to predict ignition and explosion probabilities for land transportation spills as a function of the substance, the load, and the transportation mode. They determine that this function has a clearly exponential behavior with respect to $\log Q$, where Q is the quantity being transported.

$$P(outcome) = \beta \times Q^{\alpha} \tag{3.4}$$

The resulting coefficients α and β depend on the type of HazMat transported.

Given the previous results, the probability that an exposed receptor at a location within the impact area will experience an undesirable consequence given an outcome as a result of a release when the truck type k is traversing the route segment (i, j) is expressed as:

$$P(Hazmat\ release\ incident)_{al_{ij}} = TTAR^k \times al_{ij} \times P_{release} \times \alpha \times Q^{\beta} \tag{3.5}$$

3.2.3 The estimation of the consequences

Concerning the undesirable consequences of a HazMat transportation accident, it starts by estimating the area impacted by a HazMat accident. The estimate of the shape and size of the impact area of a potential accident is difficult for routing purposes, risks must be estimated for the infinite number of points on a road network (Zhang et al., 2000). Erkut et al. (2007) present a review about the different geometric shapes used to model the impact area. The most common approximation of the impact zone is the danger circle, and the fixed-bandwidth approximation with regard to the impact area along a route segment between two nodes, Figure 3.3. The bandwidth or radius is substance-dependent. The radius can be determined by considering the evacuation distance when a HazMat incident occurs, for example, 0.8 Km for flammable HazMat and 1.6 Km for flammable and explosive HazMat (Guidebook, 2016).

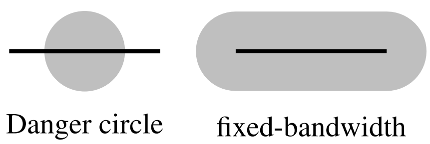


Figure 3.3: Possible shapes of impact area around the route segment.

After defining the impacted zone and given than an exposed receptor is identified (persons, environment, properties, or traffic), the next step is to make an inventory of this receptor within the zone and how this is going to be affected: fatalities, injury, or long-term effects due to exposure, property loss, environmental effect, population evacuation, or stoppage of traffic.

The modeling of an impact area can also be considered from the point of view of the affected population center. The population can be represented by using aggregation points or by using Geographic Information Systems (GIS) to represent the spatial distribution of population density. In this case a raster framework transforms a continuous space into a discrete one by modeling it as a tessellation of grid cells called pixels, with each cell storing a single value. It can be extended by using raster bands. Each pixel represents a location which might be impacted. Road network links are represented by strings of adjacent pixels. First, the exposure of a release at the route segment (i, j) on the population located at the points within the impact radius is computed. Next, the total expected exposure for a point on a road segment is the sum of expected population exposure for all landscape points. This is going to be a new pixel and finally the sum pixel by pixel total expected consequences and assign them to the road segment.

3.3 Risk Route Evaluation Models

Routing in HazMat transportation is a tool that has the potential impact of reducing the negative consequences of transporting this type of materials. Routing problems have as a fundamental requirement the assessment of the risk imposed by shipments traversing each link in a road network. The risk is assessed based on various factors, mainly the frequency of accident leading to hazardous substance release and its consequences. In Erkut et al. (2007), a survey is made about the risk model used for route evaluation, and how risk is incorporated into HazMat transport models, starting with the basic elements and moving our way into risk assessment along a route.

For routing purposes, risks must be estimated for all the links of the transportation network. The most common risk function in HazMat transportation is the so-called "traditional" risk model. In this model the risk is computed as an expected incident consequence, the multiplication of the probability of a release event (or incident) on a road segment or link times a measure of the consequence of a release event on the road segment. Population exposure is used as consequence measure. One common assumption is to consider that all people within impact zone will be affected equally and no one outside of the zone will be impacted at all. This zone is defined as the buffer area that can be impacted by the outcome of the release incident.

Let be σ^r a route composed of $(\sigma^r_1, \sigma^r_2), (\sigma^r_2, \sigma^r_3), \cdots, (\sigma^r_{|\sigma^r|-1}, \sigma^r_{|\sigma^r|})$ arcs, where σ^r_i represents the client visited on $i - th$ position on the route. To evaluate the risk associated to a route σ^r we use the total expected consequences expressed as:

$$R(\sigma^r) = \sum_{u=1}^{n-1} \left[\prod_{v=1}^{u-1} (1 - PI^k_{\sigma^r_v \sigma^r_{v+1}}) \right] PI^k_{\sigma^r_u \sigma^r_{u+1}} PD_{\sigma^r_u \sigma^r_{u+1}} \tag{3.6}$$

Where $PI^k_{\sigma^r_u \sigma^r_{u+1}}$ is the probability of occurrence of an incident using a type of vehicle k, and $PD\sigma^r_u \sigma^r_{u+1}$ is the exposed population within a buffer distance surrounding the arc $(\sigma^r_u \sigma^r_{u+1})$ (Erkut et al., 2007). To estimate $R(\sigma^r)$ we considered that $PI^k_{\sigma^r_u \sigma^r_{u+1}} PI^k_{\sigma^r_v \sigma^r_{v+1}} \cong 0$ for all pair of consecutive arcs $(\sigma^r_u \sigma^r_{u+1}), (\sigma^r_v \sigma^r_{v+1})$, given the fact that HazMat incident probability takes small values, Erkut et al. (2007). In consequence, (3.6) is reduced to:

$$R(r) = \sum_{u=1}^{n-1} PI^k_{\sigma^r_u \sigma^r_{u+1}} PD_{\sigma^r_u \sigma^r_{u+1}} = \sum_{(i,j) \in \sigma^r} PI^k_{ij} PD_{ij} \tag{3.7}$$

where the arc i represents σ^r_u and j σ^r_{u+1}. To evaluate the incident probability

PI_{ij}^k and consequence PD_{ij}^k it is necessary to consider that an accident occurs, generating a material release that could have several outcomes (jet-fire, pool fire, toxic cloud, explosion, etc.) affecting a population, as is presented on Figure 3.4. (y_{ij}^k is the material amount transported on arc (i, j)). All the events involved in a HazMat incident have an associated probability that is used to estimate the risk.

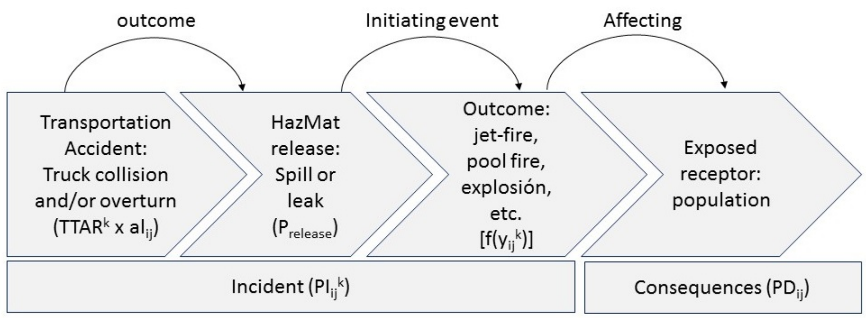


Figure 3.4: Risk assessment in HazMat Transportation

The population exposure in a radius (buffer size) is defined depending on the type of HazMat transported and the maximum volume that can be carried on a truck.

Combining (3.7)-(3.5), the route risk for a given route r is estimated as:

$$R(r) = TTAR^k \times P_{release} \times \beta \times \sum_{(i,j)\in r} (y_{ij}^k)^\alpha \times (al_{ij} \times PD_{ij}) \quad (3.8)$$

3.4 Mixed Integer Linear Programming Model for Vehicle Routing Problem for Hazardous Materials Transportation

In this part we focus on expected population exposure risk mitigation via selection of routes by solving a variant of heterogeneous vehicle routing problem (HVRP). This section provides a problem definition and presents the mixed integer linear programming (MILP) formulation of the HVRP in HazMat transportation.

3.4.1 Problem Definition

The vehicle routing problem for HazMat transportation using a heterogeneous fleet can be defined as the determination of the safest routes assigned to a fleet of different vehicles transporting a specific HazMat from a depot to a set of clients. This problem is characterized as the HVRP proposed by Golden et al. (1984) but with the introduction of the transportation risk objective function, that is expressed as the expected consequences of a hazardous materials accident.

To model the problem, a Mixed Integer Linear Programming (MILP) based on the proposal of Gheysens et al. (1984) and Baldacci et al. (2008) is proposed.

In this model the HVRP is defined on a complete directed graph $\mathcal{G}(\mathcal{N}, \mathcal{L})$. The node set $\mathcal{N} = \{0, 1, 2, \ldots, n\}$ includes the depot node 0, and a set of customer nodes (service stations), $\mathcal{C}$. Each client $i \in \mathcal{C}$ has a demand d_i and it is connected with other node $j \in \mathcal{N}$ by an arc $(i, j) \in \mathcal{L}$. Each arc is characterized by a length al_{ij}, a cost c_{ij}, and a number of persons exposed to the consequences of a HazMat release PD_{ij}. To satisfy the demands there is a set of $\mathcal{K}$ different types of trucks. A truck type $k \in \mathcal{K}$ is characterized by a maximal capacity Q_k, a fixed cost FC_k, and an accident rate $TTAR_k$.

A solution is composed of a set of routes $\mathcal{SR}$ satisfying all customer demands once. Each route $\sigma^r \in \mathcal{SR}$ starts and ends at the depot, and respects the vehicle capacity Q_k. Split deliveries are not allowed.

Two types of decision variables are defined:

y_{ij}^k : flow of goods from node i to node j in a vehicle of type k

$$x_{ij}^k : \begin{cases} 1 & \text{if a vehicle of type } k \text{ travels the arc } (i,j) \\ 0 & \text{otherwise} \end{cases}$$

The HVRP for HazMat transportation is formulated as follows:

$$minimize\ z = \sum_{r \in \mathcal{SR}} R(\sigma^r) \tag{3.9}$$

subject to:

$$\sum_{k \in \mathcal{K}} \sum_{i \in \mathcal{N}} x_{ij}^k = 1,\ \forall j \in \mathcal{N} \setminus \{0\} \tag{3.10}$$

$$\sum_{i \in \mathcal{N}} x_{ij}^k - \sum_{i \in \mathcal{N}} x_{ji}^k = 0,\ \forall k \in \mathcal{K}, \forall j \in \mathcal{C} \tag{3.11}$$

$$\sum_{k \in \mathcal{K}} \sum_{i \in \mathcal{N}} y_{ij}^k - \sum_{k \in \mathcal{K}} \sum_{i \in \mathcal{N}} y_{ji}^k = d_j,\ \forall j \in \mathcal{C} \tag{3.12}$$

$$d_j \sum_{k \in \mathcal{K}} x_{ij}^k \leq \sum_{k \in \mathcal{K}} y_{ij}^k \ \forall i, j \in \mathcal{N},\ i \neq j \tag{3.13}$$

$$y_{ij}^k \leq x_{ij}^k (Q_k - d_i) \ \forall i, j \in \mathcal{N} \ \ i \neq j,\ \forall k \in \mathcal{K} \tag{3.14}$$

$$y_{ij}^k \geq 0,\ \forall k \in \mathcal{K}, \forall (i, j) \in \mathcal{L} \tag{3.15}$$

$$x_{ij}^k \in \{0, 1\},\ \forall k \in \mathcal{K}, \forall (i, j) \in \mathcal{L} \tag{3.16}$$

Equation (3.9) expresses objective function for minimizing the total risk, being $R(\sigma_r)$ the risk associated to route σ_r. The set of constraints (3.10) ensures that each customer is visited exactly once, and the set (3.11) and (3.12) represents the conservation flux constraints. Additionally, (3.12) guarantees demand satisfaction. Constraints (3.13) and (3.14) state that goods are not transported from i to j if there is not a vehicle serving the arc (i, j), and (3.14) define the load of the vehicle k when traversing arc (i, j).

Based on the Equation 3.8 the objective risk function becomes:

$$\begin{aligned} z = \ & P_{release} \times \beta \times \\ & \sum_{(i,j) \in \mathcal{L}} \sum_{k \in \mathcal{K}} TTAR^k \times (y_{ij}^k)^\alpha \times al_{ij} \times PD_{ij} \end{aligned} \tag{3.17}$$

As this is a nonlinear function on, y_{ij}^k, a piecewise linear approximation is used.

3.4.2 Linear Approximation

Let $[q_0, q_M]$ be a bounded interval for y_{ij}^k, this interval is divided into an increasing sequence of M breakpoints $\{l_0, \ldots, l_M\}$. The value of $(y_{ij}^k)^\alpha$ is then approximated by using linear interpolations over the M segments according to (3.18).

$$\begin{aligned} (y_{ij}^k)^\alpha \quad := & \Big\{ a_m + b_m y_{ij}^k, \\ & y_{ij}^k \in [l_{m-1}, l_m] \ \forall m \in \{1, \ldots, M\} \end{aligned} \tag{3.18}$$

where $a_m \in R$, $b_m \in R$ are the intercepts and the slopes of the linear functions, respectively, and $l_0 < l_1 < \cdots < l_M$. Two different kinds of piecewise linear approximations are performed: first looks for define a straight line joining two points on the function ([l_{m-1},l_m]) and the second one looks for the tangent line to one point (tp_m) on the curve, see Figure 3.5.

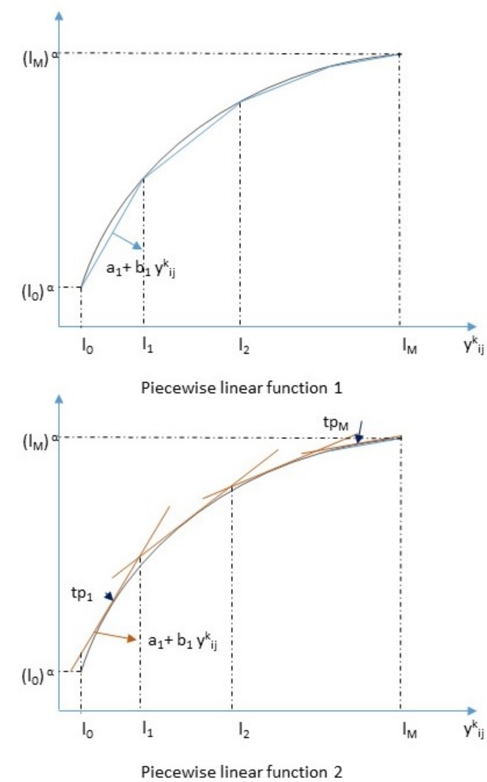


Figure 3.5: Piecewise linear approximation functions

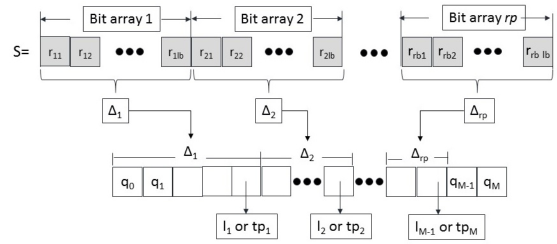


Figure 3.6: Genetic Algorithm Solution Encoding

3.4.3 Genetic Algorithm for Piecewise Linear Approximation Parameters

Using a genetic algorithm (GA) the values of the limits of each interval are established. In both piecewise linear approaches, a GA is used for finding the solution that minimizes the total sum of squared errors.

A solution S is represented by an array composed of rp arrays of binary numbers of the same size lb. Each rp array encodes the position of a required point on the array of integer values, $q_i \in [q_0, q_M]$, that represents the different possible values of the truck load. On the first approach, these points correspond to the intervals limits and on the second one, they correspond to the tangent points, see Figure 3.6. The chromosome for each individual of the initial population $P_{t=0}$ is randomly generated using a Bernoulli distribution with parameter $p = 0.5$.

The evaluation function is the sum of the squared errors of function approximation, see (3.19). For this, each linear function equation and the interval limits are computed. The fitness of a individual is defined as the inverse of the evaluation function value.

$$\begin{gathered}\sum_{\forall q_i \in [q_0, q_M]} [q_i^\alpha - (a_m + b_m \times q_i)]^2, \\ q_i \in [l_{m-1}, l_m] \; \forall m \in \{1, \ldots, M\}\end{gathered} \tag{3.19}$$

Next generations P_{t+1} are produced thanks to recombination and mutation processes.

3.4.4 Piecewise Linear Approximation Modeling

Let t_{ij}^k be the piecewise linear approximation value of $(y_{ij}^k)^\alpha$ and $t_0 = (l_0)^\alpha$. Then, the piecewise-linear functions of the road segment risk can be transformed into MILP model by introducing binary variables h_{ijk}^m and continuous variables λ_{ijk}^m, $m = 1, \cdots, M$. The h_{ijk}^m indicates the comparison between y_{ij}^k and l_{m-1}, and the λ_{ijk}^m variable evaluates the distance between y_{ij}^k and l_{m-1}, following Padberg (2000). The model for each $(y_{ij}^k)^\alpha$ is given as follows:

$$t_{ij}^k = t_0 + \sum_{m=1}^{M} b_m \lambda_{ijk}^m \; \forall i, j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \tag{3.20}$$

$$y_{ij}^k = l_0 + \sum_{m=1}^{M} \lambda_{ijk}^m \; \forall i, j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \tag{3.21}$$

$$\lambda_{ijk}^1 \leq l_1 - l_0 \; \forall i, j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \tag{3.22}$$

$$\lambda_{ijk}^m \geq (l_m - l_{m-1}) h_{ijk}^m \quad \begin{array}{l} \forall i, j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \\ m = 1, \cdots, M-1 \end{array} \tag{3.23}$$

$$\lambda_{ijk}^{m+1} \leq (l_{m+1} - l_m) h_{ijk}^m \quad \begin{array}{l} \forall i, j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \\ m = 1, \cdots, M-1 \end{array} \tag{3.24}$$

$$\lambda_{ijk}^m \geq 0, \; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L}, \; m = 1, \cdots, M \tag{3.25}$$

$$h_{ijk}^m \; \in \{0, 1\}, \; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L}, \; m = 1, \cdots, M \tag{3.26}$$

$$t_{ij}^k \geq 0, \; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L} \tag{3.27}$$

Total risk function for a set of routes is now defined as:

$$\begin{aligned} z = \;\; & P_{release} \times \beta \times \\ & \sum_{(i,j) \in \mathcal{L}} \sum_{k \in \mathcal{K}} TTAR^k \times al_{ij} \times PD_{ij} \times t_{ij}^k \end{aligned} \tag{3.28}$$

Equations (3.20)-(3.27) are included as constraints into the model defined in subsection 3.4.1.

3.5 Numerical Tests

3.5.1 Problem Instances

To assess the quality of the approximation risk function, we computed the total risk of best known solution routes for HVRP instances proposed by Golden et al. (1984). [1]

[1] The cost-optimal solution for instances 3, 4, 5, 14 and 15 see Gendreau et al. (1999); instances 13 and 17 see Brandão (2009); instance 16 see Penna et al. (2013); instance 18 see Prins (2009); and the best know solution for instance 20 see Subramanian et al. (2012).

In this work we assumed that the nodes demand is expressed in hundreds of gallons of gasoline, gasoline density is $2.805 Kg/Gallon$, and one unit of distance is equal of $100m$. A release probability equals to 0.02487845, from Kazantzi et al. (2011a) and Button and Reilly (2000), and values of 0.72 and 0.00027 for α and β are used, see Ronza et al. (2007). The risk objective (3.28) becomes:

$$
\begin{aligned}
&z = 0.02487845 \times 0.0027 \times \\
&\sum_{(i,j)\in\mathcal{L}} \sum_{k\in\mathcal{K}} TTAR^k \times \tfrac{al_{ij} \times PD_{ij}}{10} \times t_{ij}^k
\end{aligned}
\tag{3.29}
$$

The exposed population surrounding an arc (i, j), PD_{ij}, is represented by a quantity in the square grid (dimension 4×4 distance units) that contains the arc. A decay function from the center to the exterior is used in order to represent an urban area where the population density is decreasing towards peripheral zones. PD_{ij} value generator is shown in (3.30).

$$
PD_{ij} = 9500u(1 - \frac{maxDist - popDist}{maxDist}) + 500 \tag{3.30}
$$

where u is generated using a uniform distribution, $u \sim U(0.4, 0.6)$, $maxDist$ is the maximum between the length and the width of the rectangle that contains the squared grid, and $popDist$ is the maximum value between the difference of the abscise and ordinate coordinates of the left superior corner of the current square grid and the coordinates of left superior corner of the central square grid.

The HazMat incident rate of a vehicle on an arc is about 1×10^{-6} per $(vehicle-Km)$, see Button and Reilly (2000) and Kazantzi et al. (2011b). In this case we use $TTAR_k \sim U[0.6, 1.0]10^{-6}$ per $(vehicle - Km)$ $\forall k \in \mathcal{K}$.

The GA was code in *Java SE 8* and executed in an *Intel Core i7* Processor 2.4 GHz with 16 GB of RAM running *Windows 10*. The MILP formulation was implemented using a commercial solver (*Gurobi*) for *Python 2.7*.

For the piece-wise linear approximation of the incident probability function, the number of linear functions (M), is fixed at four corresponding to small load, medium-size load, large load and very-large load. After a parameter tuning for a truck load that goes from 1 (minimum demand) to 400 (maximum vehicle capacity), the parameters of GA were: a population size of 100 individuals, a mutation rate of 0.02, and 500 generations. The value assigned to lb is 10.

After running the algorithm, the results for the first piecewise linear approximation function are:

$$
\begin{aligned}
&b_1 = 0.07349097; \quad 280.5 \leq (280.5y_{ij}^k) \leq 9256.5 \\
&b_2 = 0.04590467; \quad 9256.5 \leq (280.5y_{ij}^k) \leq 30574.5 \\
&b_3 = 0.03555368; \quad 30574.5 \leq (280.5y_{ij}^k) \leq 64795.5 \\
&b_4 = 0.02979203; \quad 64795.5 \leq (280.5y_{ij}^k) \leq 112200.0
\end{aligned}
$$

Table 3.1: Total routing risk for optimal-cost solution using the first piecewise linear approximation

Inst.	n	BKS cost	Risk: Exact value (3.17) $\times 10^{-6}$	Approximation (3.29): Value $\times 10^{-6}$	Approximation (3.29): Gap %
3	20	961.03	307.65	296.53	3.62
4	20	6437.33	248.85	233.88	6.02
5	20	1007.05	431.69	418.69	3.01
6	20	6516.47	261.63	248.48	5.02
13	50	2406.36	768.90	754.07	1.93
14	50	9119.28	571.20	554.86	2.86
15	50	2586.37	700.91	673.84	3.86
16	50	2720.43	790.00	762.67	3.46
17	75	1734.53	1479.14	1454.42	1.67
18	75	2369.65	1229.73	1198.71	2.52
19	100	8661.81	1171.32	1131.36	3.41
20	100	4032.81	1189.73	1148.80	3.44

and for the second function are:

$$\begin{array}{ll} b_1 = 0.06835302; & 280.5 \leq (280.5y_{ij}^k) \leq 9995.2 \\ b_2 = 0.04468697; & 9995.2 \leq (280.5y_{ij}^k) \leq 31855.6 \\ b_3 = 0.03515308; & 31855.6 \leq (280.5y_{ij}^k) \leq 65838.6 \\ b_4 = 0.02964824; & 65838.6 \leq (280.5y_{ij}^k) \leq 112200.0 \end{array}$$

Given that the truck load varies according to the demand of the clients to visit, and the range of these values is the same for all the studied instances, the same piecewise linear approximation was used in all of them.

3.5.2 Results

Tables 3.1 and 3.2 show the expected consequences estimated using (3.17) and both piecewise linear functions. In these tables, *Inst.* denotes the name of the test-problem, n denotes the number of customers, *BKS* represents the best known solution (optimal solutions in some cases). The approximation and the exact value of the expected consequences for each cost-optimal solutions is presented, and the gap between both approaches and the exact value. All the possible route sequence combinations were considered in order to find the minimum risk for a solution.

Table 3.2: Total routing risk for optimal-cost solution using the second piecewise linear approximation

Inst.	n	BKS cost	Risk		
			Exact value (3.17) $\times 10^{-6}$	Approximation (3.29)	
				Value $\times 10^{-6}$	Gap %
3	20	961.03	307.65	313.03	1.75
4	20	6437.33	248.85	252.62	1.52
5	20	1007.05	431.69	437.34	1.31
6	20	6516.47	261.63	266.2	1.75
13	50	2406.36	768.90	775.78	0.89
14	50	9119.28	571.20	577.30	1.07
15	50	2586.37	700.91	710.52	1.37
16	50	2720.43	790.00	801.02	1.39
17	75	1734.53	1479.14	1491.46	0.83
18	75	2369.65	1229.73	1242.82	1.06
19	100	8661.81	1171.32	1187.28	1.36
20	100	4032.81	1189.73	1205.34	1.31

Given that the average difference in percentage between the exact value (by using (3.17)) and the piecewise linear approximation using the first function (3.4%) is greater than the average difference (1.3%) for the second function, this last approach is used as estimation of the risk function in optimization methods.

Table 3.3 shows the optimal risk for the first four instances obtained using the above presented MILP model of the risk problem optimization. For other instances the CPU time is more than 15 hours. From table 3.3, it is remarkable that for instance 5, the total cost for the optimal-risk solution is more than twice the optimal-cost solution. Also, the optimal risk value obtained for each instance is greater than the total risk value obtained when the optimal-risk solution is evaluated by using (3.17), that means the risk is slightly overestimated.

3.6 Conclusions

3.6.1 Conclusions (English)

The present chapter addresses the risk minimization problem for vehicle routing in hazardous materials (HazMat) transportation using heterogeneous fleet of vehicles. We propose a mixed integer linear programming model that incorporates

Table 3.3: Optimal risk values for some instances of HVRP with unlimited fleet

Inst.	n	Risk Optimization			
		MILP $\times 10^{-6}$	Exact value (3.17) $\times 10^{-6}$	Cost value	Time Sec.
3	20	156.82	154.08	2047.10	17
4	20	168.24	165.60	33556.06	68
5	20	251.84	248.79	1305.32	133
6	20	196.80	193.36	14541.96	1839

a piecewise linear approximation of the transportation risk objective. The objective function captures some variations in risk which are not considered in previous models in HazMat transportation. This function includes an estimation of the HazMat transportation incident probability as a function of the truck load and type. The proposed model is a more realistic approach and it can be used for reducing the risk in HazMat distribution.

Given the NP-hard nature of VRP problems, the development of heuristics and meta-heuristics techniques that can deal with problems with a greater number of clients is a promising aspect of future research in using heterogeneous fleet of trucks for HazMat transportation. In the next two chapters, important features in efficient local search based meta-heuristics is introduced, and a hybrid heuristic algorithm based on neighborhood search is proposed for solving the proposed piecewise linear model approximation.

3.6.2 Conclusions (Français)

Ce chapitre aborde le problème de la minimisation des risques pour le problème des tournées de véhicules (VRP) dans le transport de substances dangereuses (HazMat) en utilisant une flotte hétérogène de véhicules (HVRP). Un modèle de programmation linéaire en nombres entiers mixte est proposé, dans ce modèle une approximation linéaire par morceaux est utilisée pour la fonction objective du risque de transport.

Dans ce modèle, le HVRP est défini sur un graphe orienté complet $\mathcal{G}(\mathcal{N}, \mathcal{L})$*. L'ensemble de nœuds* $\mathcal{N} = \{0, 1, 2, \ldots, n\}$ *inclut le nœud de dépôt* 0*, et un ensemble de nœuds clients (stations de service),* $\mathcal{C}$*. Chaque client* $i \in \mathcal{C}$ *a une demande* d_i *et il est connecté avec un autre nœud* $j \in \mathcal{N}$ *par un arc* $(i, j) \in \mathcal{L}$*. Chaque arc est caractérisé par une longueur* al_{ij}*, un coût* c_{ij} *et un certain nombre de personnes exposées aux conséquences d'une libération de HazMat* PD_{ij}*. Pour satisfaire les demandes, il existe un ensemble de différents types de camions. Un type de camion*

$k \in \mathcal{K}$ est caractérisé par une capacité maximale Q_k, un coût fixe FC_k, et un taux d'accident $TTAR_k$.

Une solution est composée d'un ensemble de routes $\mathcal{SR}$ satisfaisant toutes les demandes des clients une fois. Chaque route $\sigma^r \in \mathcal{SR}$ commence et finit au dépôt, et respecte la capacité du véhicule Q_k. Les livraisons fractionnées ne sont pas autorisées.

Deux types de variables de décision sont définis:

$$y_{ij}^k : \begin{array}{l} \text{flux de biens du nœud } i \text{ vers le nœud } j \\ \text{dans le véhicule de type } k \end{array}$$

$$x_{ij}^k : \begin{cases} 1 & \text{si un véhicule de type } k \text{ parcourt l'arc } (i,j) \\ 0 & \text{autrement} \end{cases}$$

Le HVRP pour le transport HazMat est formulé comme suit:

$$z = \sum_{r \in \mathcal{SR}} R(\sigma^r) \tag{3.31}$$

sujet à:

$$\sum_{k \in \mathcal{K}} \sum_{i \in \mathcal{N}} x_{ij}^k = 1, \ \forall j \in \mathcal{N} \setminus \{0\} \tag{3.32}$$

$$\sum_{i \in \mathcal{N}} x_{ij}^k - \sum_{i \in \mathcal{N}} x_{ji}^k = 0, \ \forall k \in \mathcal{K}, \forall j \in \mathcal{C} \tag{3.33}$$

$$\sum_{k \in \mathcal{K}} \sum_{i \in \mathcal{N}} y_{ij}^k - \sum_{k \in \mathcal{K}} \sum_{i \in \mathcal{N}} y_{ji}^k = d_j, \ \forall j \in \mathcal{C} \tag{3.34}$$

$$d_j \sum_{k \in \mathcal{K}} x_{ij}^k \leq \sum_{k \in \mathcal{K}} y_{ij}^k \ \forall i,j \in \mathcal{N}, \ i \neq j \tag{3.35}$$

$$y_{ij}^k \leq x_{ij}^k (Q_k - d_i) \ \forall i,j \in \mathcal{N} \ \ i \neq j, \ \forall k \in \mathcal{K} \tag{3.36}$$

$$y_{ij}^k \geq 0, \ \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L} \tag{3.37}$$

$$x_{ij}^k \in \{0,1\}, \ \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L} \tag{3.38}$$

L'équation (3.31) exprime une fonction objective pour minimiser le risque total, soit $R(\sigma_r)$ le risque associé à la route σ_r. L'ensemble des contraintes (3.32) assure que chaque client est visité exactement une fois, et l'ensemble (3.33) et (3.34) représente les contraintes de conservation de flux. De plus, (3.34) garantit *la satisfaction de la demande. Les contraintes (3.35) et (3.36) indiquent que des marchandises ne seront pas transportées de i à j s'il n'y a pas de véhicule servant l'arc (i, j) et (3.36) définissent la charge du véhicule k en parcourant arc (i, j).*

La fonction objective du risque devient:

$$z = P_{release} \times \beta \times \sum_{(i,j)\in\mathcal{L}} \sum_{k\in\mathcal{K}} TTAR^k \times (y_{ij}^k)^\alpha \times al_{ij} \times PD_{ij} \quad (3.39)$$

Comme il s'agit d'une fonction non linéaire, yij^k, une approximation linéaire par morceaux est utilisée.

La fonction objectif capture certains aspects de l'évaluation des risques qui n'avaient pas été pris en compte auparavant dans les modèles du transport HazMat. Cette fonction inclut une estimation de la probabilité d'un incident dans le transport d'Hazmat en fonction de la charge et du type de camion. Le modèle proposé est une approche plus réaliste de l'évaluation du risque de transport, qui peut être utilisé pour réduire le risque de problèmes de distribution de HazMat.

Étant donné la nature NP-difficile des problèmes VRP, le développement de techniques heuristiques et méta-heuristiques qui peuvent traiter les problèmes avec un plus grand nombre de clients est un aspect prometteur dans les recherches futures quand une flotte hétérogène de camions est utilisée dans le transport HazMat. Dans les deux chapitres suivants, des caractéristiques importantes dans les méta-heuristiques basées sur des recherches locales efficaces sont introduites, et un algorithme heuristique hybride basé sur la recherche de voisinage est proposé pour résoudre le modèle, dans lequel une approximation linéaire par morceaux est utilisée pour faire une approximation de la fonction objective du risque dans le routage.

3.6.3 Conclusiones (Español)

El presente capítulo aborda el problema de minimización de riesgos para el problema de ruteo de vehículos (VRP) en el transporte de materiales peligrosos (HazMat) utilizando una flota heterogénea de vehculos. Un modelo de programación lineal entero mixto es propuesto, en este modelo se utiliza una aproximación lineal por partes para función objetivo de riesgo de transporte. La función objetivo captura algunos aspectos en la evaluación del riesgo que antes no se habían considerado en modelos para el transporte de HazMat. Esta función incluye una estimación de la probabilidad de un incidente en el transporte de Hazmat en dependiente de la carga y el tipo de camión. El modelo propuesto es un enfoque más realista para la evaluación del riesgo del transporte, el cual puede ser utilizado en la reducción del riesgo en los problemas de distribucin de HazMat.

Dada la naturaleza NP-hard de los problemas de VRP, el desarrollo de técnicas heurísticas y meta-heurísticas para el manejo de problemas con un gran número de clientes es un aspecto prometedor en la investigación futura cuando una flota heterogénea de camiones es usada en el transporte de HazMat. En los siguientes dos capítulos, se introducen características importantes de las meta-heurísticas basadas en eficientes búsquedas locales, y se propone un algoritmo heurístico híbrido basado en la búsqueda de vecindarios para resolver el modelo formulado, en el que una aproximación lineal por partes es utilizada para la función objetivo de riesgo en el ruteo.

> This work has lead to a conference paper and an online publication: Mixed Integer Linear Programming Model for Vehicle Routing Problem for Hazardous Materials Transportation. *8th IFAC Conference on Manufacturing Modeling, Management and Control MIM 2016, Troyes, France*. IFAC-PapersOnLine. Volume 49, Issue 12, 2016, Pages 538-543.

Chapter 4

Neighborhood Structures in Local Search Algorithms (LSA) for Heterogeneous Vehicle Routing Problem (HVRP)

Abstract (English)

The success of heuristic local search algorithms depends on an appropriated definition of the considered neighborhoods. Once the neighborhood structures are defined, efficient neighborhood search techniques, the search strategy, and the candidate selection mechanism can be proposed. The objective of this chapter is to progress on the understanding and implementation of meta-heuristics based on local search or neighborhood search for the vehicle routing problem with heterogeneous fleet. Neighborhood structures for the considered problem are studied in order to determined how much they contribute to improve the value of the initial solution value, and to have an idea on which combination of them provide better results. In section 4.1, the local search algorithms are presented. Section 4.2 introduces some aspects related with this kind of algorithms when used on combinatorial problem. Section 4.3 of this chapter provides a brief outline of some of hybrid heuristic local search algorithms. Finally, some neighborhood structures for the studied problem are presented, and computational experiments are conducted for this structures.

Résumé (Français)

Le succès des algorithmes heuristiques de recherche locale dépend d'une définition appropriée des voisinages considérés. Une fois les structures voisinage sont définies, des techniques efficaces de recherche de voisinage, la stratégie de recherche et le mécanisme de sélection des candidats peuvent être proposés. L'objectif de ce chapitre est de progresser dans la compréhension et la mise en œuvre de méta-heuristiques basées sur la recherche locale ou la recherche de voisinage pour le problème des tournées de véhicules avec une flotte hétérogène. Les structures de voisinage pour le problème considéré sont étudiées afin de déterminer dans quelle mesure elles contribuent à améliorer la valeur de la solution initiale, et d'avoir une idée de la combinaison de celles-ci qui donne de meilleurs résultats. Dans la section 4.1, les algorithmes de recherche locale sont présentés. La section 4.2 présente certains aspects liés à ce type d'algorithmes lorsqu'ils son utilisés sur des problèmes combinatoires. La section 4.3 de ce chapitre fournit un bref résumé de certains algorithmes hybrides de recherche locale heuristiques. Enfin, certaines structures de voisinage pour le problème étudié sont présentées, et des expérimentations de calcul sont menées pour ces structures.

Resumen (Español)

El éxito de los algoritmos heurísticos de búsqueda local depende de una definición apropiada de los vecindarios. Una vez que se definen los vecindarios, se pueden proponer técnicas eficientes de búsqueda usándolos, la estrategia de búsqueda a utilizar y el mecanismo de selección de los candidatos. El objetivo de este capítulo es avanzar en la comprensión e implementación de meta-heurísticas basadas en búsqueda local para el problema de ruteo de vehículos con flota heterogénea. Estructuras de vecindarios son estudiadas para determinar cuanto contribuyen a mejorar el valor de la solución inicial y cuál combinación de ellas provee el mejor resultado. En la sección 4.1, se presenta una introducción a los algoritmos de búsqueda local. La Sección 4.2 introduce algunos aspectos relacionados con este tipo de algoritmos cuando se usan en problemas combinatorios. La Sección 4.3 de este capítulo proporciona una breve descripción de algunos algoritmos de búsqueda local heurísticos híbridos. Finalmente, se presentan algunas estructuras de vecindario para los problemas de ruteo de vehículos y se realizan experimentos computacionales para estas estructuras.

4.1 Introduction

Local search algorithms (LSAs) also known as neighborhood search algorithms (NSAs) are attractive because they can be used for solving complex problems for which analytical models would involve a huge number of variables and constraints, or about which little theoretical knowledge is available (Crama et al., 1995). LSAs have become an efficient way to solve hard combinatorial optimization problems (COPs). This type of optimization problems arise in situations where discrete choices must be made to find optimal solutions among a finite or countable infinite number of alternatives as in network design, scheduling, vehicle routing, cutting stock. The use of LSA in COP has a long history that comes from the late 1950s and early 1960s when the first edge-exchange algorithms for the traveling salesman problem (TSP) appeared (Aarts and Lenstra, 1997). LSA can be implemented to quickly produce good solutions for large scale instances of the COP.

The local search approach can be considered as the basic principle underlying many classical optimization methods, like the gradient descent method for continuous nonlinear optimization or the simplex method for linear programming see (Crama et al., 1995). This intuitive solution approach used to solve COP starts with a known feasible solution, and then it tries to find better solutions by searching neighborhoods in order to decrease the value of an objective function.

The first main aspect to be taken into account in LSA is the selection of an initial solution, this aspect has a greatly influence in the quality of the final outcome and the algorithm efficiency. The second aspect is the neighborhood structure (perturbation moves), it has to be enough large to provide a good quality solution candidate but also easy to explore. Next, the strategy for searching the neighborhood at each iteration of the local search has to be considered. Finally, the method for determining what is the candidate solution to move within the neighborhood that the previous searching step will choose has to be defined. The local search terminates when the current candidate solution is a locally optimal solution with respect to the given neighborhood structure (Ahuja et al., 2002).

To construct an initial feasible solution is not generally a hard task, but some times a LSA for achieving its target of a solution close to the global optimal needs to re-start many times from different initial solutions that end in different local optimal solutions. The representation of this initial solution has impact on the neighborhood structures that can be selected to be explored. The choice of neighborhood structures for a given problem is conditioned by the trade-off between quality of the solution and complexity of the algorithm, and generally experimentation is used for making this selection process. LSAs need a reasonable definition of neighborhood structures, and an efficient way of searching them, in order they can be implemented to produce good solutions for large scale instances of a COP in a reasonable time. Then a candidate selection criteria is applied to chose the neighbor for continuing the search, a greedy strategy can be followed, to chose the one who provides the highest immediate improvement, or to chose other candidate solution than does not give the best improvement immediately, but can lead to a better solution when the algorithm run ends. It is necessary to experiment with various different strategies to make decision on the selection of the initial solution, the neighborhood structures and the candidate solution criterion.

Nevertheless, LSAs have also some drawbacks. The algorithms can be trapped as they encounter a local optimum, and there is usually no guarantee that the value of the objective function at an arbitrary local optimum comes close to the optimal value. In view of this difficulty, several extensions of local search have been proposed in order to escape from local optima, whether by accepting occasional degradations of the objective function, or working with a population of feasible solutions at the same time, detecting properties which distinguish good from bad solutions (Crama et al., 1995). Also different neighborhood structures can be used for performing the local search and the LSA can be run several times on the same problem instance, using different initial solutions, that means multi-start versions of the LSA also called hybrid LSAs.

4.2 Local search in combinatorial optimization problems

The local search algorithms (LSA) involve the definition of an optimization problem and a neighborhood structure (Aarts and Lenstra, 1997). Local search moves from one candidate solution to another candidate solution in the optimization problem search space by applying local changes to the current solution, until the desired optimal solution is achieved or a stopping criterion is met. In this section a description of the combinatorial optimization problems (COP) is provided alongside with the definition of the local search aspects related to this type of optimization problems.

4.2.1 Combinatorial optimization problem

These optimization problems are formulated as:

$$\min\{f(\vec{x}) = W\vec{x} : A \times \vec{x} \geq b, \vec{x} \in \mathbb{Z}^n\} \tag{4.1}$$

where in the feasible set $X = \{A \times \vec{x} \geq b, \vec{x} \in \mathbb{Z}^n\}$, $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$; although, A and b are usually integers, and they describe a combinatorial structure such e.g., number of permutations, spanning trees of a graph, paths, matchings etc. X is a finite of countably infinite set of solutions $\vec{x}$. Also, this set of feasible solutions can be represented directly as a set S of combinatorial structures s, which in turn are composed of subsets of a finite set $\mathbf{E}$. The definition starts with the definition of the set of finite elements $\mathbf{E} = \{1, \ldots, n_E\}$, which is composed of n_E combinatorial structures. The set of feasible solutions S is a combination of elements of $\mathbf{E}$, $S \subseteq 2^{\mathbf{E}}$, where the set of all the subsets of $\mathbf{E}$ is denoted by $2^{\mathbf{E}}$. S is not given explicitly by listing all its elements, but it is represented in a compact form of size polynomial in n_E. An element of the set S is represented through a combination of elements of $\mathbf{E}$, and each element in X corresponds to one of the elements in S. X is another way to accurately represent S using integer variables.

The cost function $f(\vec{x}) = W\vec{x}$ provides a quantitative measure of the quality of the solution $\vec{x}$, this function is mapping $f : X \rightarrow \mathbb{R}$ that assigns a real value to each solution of X. The problem is to find for a given problem instance (f, X) a solution $\vec{x}^* \in X$ that is *globally optimal* (Michiels et al., 2007). In the case of minimization problems this means that $f(\vec{x}^*) \leq f(\vec{x}),\ \forall \vec{x} \in X$. Without lost of generality a globally optimal solution is simply called optimal solution.

In a problem instance of vehicle routing problem (VRP) (f, X), X represents the set of routing solutions, a collection of tours or TSP solutions that starts and ends at the depot node satisfying the demand of each node once and respecting the vehicle capacity without splitting the node demand. f defines the total cost of the tours. A problem instance of a VRP problem can be defined for the distance $al_{i,j}$ of each pair of nodes (i, j) in the set of nodes $\mathcal{N} = \{0, 1, \ldots, n\}$, the demand q_i of each node $i \in \mathcal{N}$ and the capacity Q_k of each vehicle $k \in \{1, \ldots, K\}$. The size of the problem instance representation is expressed as the number of bits required for storing the instance; the size of the candidate solution is the number of bits to store the tours, the sequences of nodes to visit and the type of vehicle.

The running time of a polynomial-time algorithm is polynomial in the size of the problem instance, otherwise it is exponential (Michiels et al., 2007). Many COP are $NP-hard$ problems, it is generally believed that this kind of problems can not be solve optimally within polynomially bounded computational time (Aarts and Lenstra, 1997).

4.2.2 Neighborhood structures

A neighborhood structure or neighborhood function $N(s)$ or $N(\vec{x})$ is defined on the search space $X \equiv S$. The neighborhood function is a main aspect of LSA, this function specifies for a current solution all the candidate solutions that are in some sense near to it, they are obtained through certain moves, stated in another way, changing the structure of the solution. A neighborhood is the set of all solutions that can be reached given a solution and a neighborhood structure (Sörensen et al. (2008)).

For a COP instance (f, S) or (f, X) a *neighborhood function* is a mapping $N : S \rightarrow 2^{\mathbf{E}}$. The neighborhood function defines for each solution $s \in S$ a set $N(s) \in S$ which is called the neighborhood of s, and it is assumed without loss of generality that $s \in N(s)$. The cardinality of $N(s)$ is the size of the neighborhood. Each feasible neighbor of s can be represented by an $\vec{x} \in X \subset \mathbb{Z}^n$, that means $\mathcal{N}(s) = N(\vec{x})$.

The LSA begins with an initial solution constructed using some heuristics. LSA searches through the solution space X using a neighborhood function to move from the current solution to a neighbor that improves the cost function. As this work deals with minimization problems, a cost function improvement implies a decreasing in the function value. Many possible definitions of neighborhoods structures are possible given a COP and many issues are involved in this definition (Ausiello et al., 1999).

The distance between two solutions is used as a criterion for defining neighborhoods structures. The *distance* between two solutions $s_1 \in S$ and $s_2 \in S$, $d(s_1; s_2)$, can be defined as the sum of the set of elements that appear in s_1 but not in s_2 and the set of elements that appear in s_2 but not in s_1, or the number of elements of $\mathbf{E}$ that appear in s_1 or s_2 but not both. A neighborhood is a distance-k neighborhood if $N(s)_k = \{o \in S, d(s, o) \leq k\}$.

When defining the neighborhood structure some aspects to be considered are:

- *the quality of the solution obtained.*
- *the order in which the neighborhood is search.*
- *the complexity of verifying that the neighborhood does not contain any better solution.*
- *the number of solutions generated before a local optimum is generated.*

The size of the neighborhood has to be enough large for providing good quality of local optimal solutions, but the task of checking if there is a better neighbor has to be done within a *reasonable* amount of time, i.e. searched in an efficient manner. The complexity of this procedure has not to be either computationally hard or generate an exponential number of neighbor solutions before the global optimum is found. That is the reason for approximation algorithms that can find near-optimal solutions within reasonable running time. The size of a neighborhood is said to be *very large* with respect to the size of the input data if $N(\vec{x})$ grows exponentially as n_E increases, also when neighborhoods are too large to search explicitly in practice. Very large neighborhoods can be searched heuristically and not extensively.

4.2.3 The search in the solution space

In local search, the decision about to move or not to a new solution depends on the information about the candidate solution in the neighborhood of the current search point. For searching the space, the most obvious strategy is the iterative improving, hill climbing, or discrete gradient descent algorithm. In each iteration of the LSA an improvement neighbor of the current solution is selected as the new search solution point by replacing the current solution. If there is not a neighbor that improve the current function value the LSA stops and returns the locally optimal solution, a solution $\vec{x}^{'} \in X$ is locally optimal with respect to a neighborhood structure N if $f(\vec{x}') \leq f(\vec{x}^{''})$, $\forall \vec{x}^{''} \in N(\vec{x})$. A neighborhood function is called exact if each local optimum is also a global optimum.

The two basic iterative improvements are the first improvement where the current solution is replaced by the first improving solution encountered, and the best improving solution where the best neighbor is selected.

A major inconvenient of the iterative improving algorithm is that it may get trapped in poor local optimal solution. Possible solutions to overcome this problem are: use a better neighborhood function, allow non-improving solution candidates, start the local search from a different solution, or working with a population of feasible solutions at the same time.

Larger neighborhoods can help to alleviate the problem of getting stuck in local optimal. But, as it was pointed out previously, in large neighborhoods, there is a trade-off between the number of search steps required for finding a local optimum and the computation time for each search step. Benefits from the advantages of large neighborhoods, without incurring a high time complexity of the search steps, are the bases of the idea of using consecutive, standard, small neighborhoods until a local optimum is encountered, at which point the search process switches to a different (typically larger) neighborhood, which might allow further search progress. The role of this last moves is to modify the current candidate solution in a way which will not be immediately undone by the subsequent local search phase and allows the search process escape effectively from local optima; in this way the subsequent local search phase has a chance to discover different local optima.

4.2.4 Algorithm performance

The performance of any LSA depends significantly on the underlying neighborhood relation and, in particular, on the size of the neighborhood. As it was mentioned before, sometimes the size of the neighborhoods to be explored grows exponentially in relation to the some problem parameters, as the numbers of nodes to be visited in the case of the travel salesman problem (TSP) and VRP, or the jobs to be scheduled in the case of the permutation flow shop problem. In neighborhoods that are exponentially large with respect to the size of the given problem instance and searching, finding an improving neighboring candidate solution may take exponential time in the worst case.

Using larger neighborhoods might increase the chance of finding (high quality) solutions of a given problem in fewer local search steps when using LSAs in general, the problem is the time complexity for determining improving search steps is much higher in larger neighborhood. *Typically, the time complexity of an individual local search step needs to be polynomial (with regard to the size of the given problem instance), where depending on problem size, even quadratic or cubic time per search step might already be prohibitively high* (Hoos and Stützle, 2004). The evaluation function values of individual neighbors of a candidate solution can be done more efficiently by recording and updating the respective values after each search step rather than computing them from scratch. This types of speedups are crucial for the success of the LSAs in solving combinatorial problems in practice by improving the algorithm performance.

The performance of the iterative improving algorithm not only depends on the quality of the local optima but also on the time required for finding it. This time is a function of two aspects: the time needed to explore the neighborhood and move to the new candidate solution, and the number of executed moves before arriving to the local optimum. Larger neighborhoods contain more and potentially better candidate solutions, and hence they typically offer better chances of facilitating locally improving search steps but they take longer to be explored. However, in practice, as previous stated, small neighborhoods can provide similar or superior solution quality if embedded in a metaheuristic framework because they typically can be searched more quickly (Pisinger and Ropke, 2010).

4.3 Local search methods

In a basic local search, once a new improvement of the current solution is not possible using the current neighborhood (local optimal solution) the search process terminates, but, it is possible to restart it from a randomly chosen initial position based on standard termination conditions. Depending on how the local search process and the restarting process is combined some hybrid LSAs have emerged. In this section are presented some of the most prominent heuristic LSA techniques based on neighborhoods, and an illustration of their application to VRP is given.

Heuristic search refers to techniques with the aim of finding *good* solutions for a very hard optimization problems within a reasonable amount of computation time what implies generally to use some simple rules. The heuristic local search is a technique that works with complete solutions and seeks to find better solutions by making small local changes, move or perturbations to the initial solution. Concepts such as search space, feasible or infeasible solution, neighborhoods or move, acceptance criteria, stopping criteria, restarting strategy among other are shared by the heuristic local search algorithms.

4.3.1 Greedy randomized adaptive search procedures GRASP

GRASP is an iterative process, each algorithm iteration consisting of two phases. First, a greedy construction search method is applied starting from an empty candidate solution, at each construction step adds the best ranked solution component based on a heuristic selection function. Second, a perturbation local search algorithm is used to improve the candidate solution thus obtained. The best overall solution is kept as the result. A generic GRASP pseudo-code is given in Algorithm 1.

Algorithm 1 Greedy randomized adaptive search procedures GRASP

while Stopping criterion is not meeting **do**
  $s^{'} \leftarrow$ Greedy Randomized Solution$()$
  $s^{'*} \leftarrow$ Local Search $(s^{'})$
  if $f(s^{'*}) < f(s^*)$ **then**
    $s^* = s^{'*}$
  end if
end while
Return S^*

The procedure to construct a greedy randomized solution

Algorithm 2 Greedy Randomized Solution

$s = \{\}$
while solution construction is not done **do**
  List of the restricted candidate $\mathcal{L}$
  $e_s \sim \mathcal{L}$
  $s \leftarrow s \cup e_s$
  Adapt greedy function
end while
Return S^*

The list of the restricted candidate $\mathcal{L}$ is either the list of best element candidates, and an element e_s is randomly chosen from $\mathcal{L}$, or $\mathcal{L}$ is is made of random element candidates and the best one is chosen. The benefits associated with every element (determine the probability of selecting the corresponding element) are updated at each iteration of the construction phase to reflect the changes brought on by the selection of the previous element. This choice technique allows for different solutions to be obtained at each GRASP iteration. The solutions generated by a GRASP construction are not guaranteed to be locally optimal with respect to simple neighborhood definitions. Hence, it is almost always beneficial to apply a local search to attempt to improve each constructed solution. The use of customized data structures and its careful implementation, can create an efficient construction phase which produces good initial solutions for efficient local search.

Greedy construction search methods can typically only generate one or a very limited number of different candidate solutions. GRASPs, (Feo and Resende, 1995), try to avoid this disadvantage by randomizing the construction method, such that it can generate a large number of different good starting points for a perturbation local search method.

4.3.2 Iterated local search (ILS)

A simple modification of a LSA consists of iterating calls to the local search routine, each time starting from a different initial configuration. The implicit assumption is that of a clustered distribution of local minima: when minimizing a function, determining good local minima is easier when starting from a local minimum with a low value than when starting from a random point. Iterated Local Search is based on building a sequence of locally optimal solutions by:

- perturbing the current local minimum;
- applying local search after starting from the modified solution.

The perturbation strength has to be sufficient to lead the trajectory to a different attraction basin leading to a different local optimum.

Algorithm 3 Iterated Local Search Procedure

1: $s_0 \leftarrow$ Generate an initial solution
2: $s^* \leftarrow$ Local Search(s_0)
3: **while** Stopping criterion is not meeting **do**
4: $\quad s^{'} \leftarrow$ Perturbation$(s^*, history)$
5: $\quad s^{'*} \leftarrow$ Local Search$(s^{'})$
6: $\quad s^* \leftarrow$ Acceptance Criterion$(s^*, s^{'*}, history)$
7: **end while**
8: Return s^*

The potential power of ILS lies in its biased sampling of the set of local optima. The efficiency of this sampling depends both on the kinds of perturbations and on the acceptance criteria (Lourenço et al., 2003). ILS is much better than random restart but some experimentation have to be carried out in order to optimize the iterated local search modules, the acceptance criteria, the perturbation routine, and the local search. According to Lourenço et al. (2003), ILS can perform k local searches embedded within it much faster than if the k local searches are run within random restart.

4.3.3 Variable neighborhood search (VNS)

VNS was introduced by Mladenović and Hansen (1997). The general idea is to change the neighborhood during the local search by using standard, small neighborhoods until a local optimum is encountered, at which point the search process switches to a different neighborhood, which might allow further search progress based on the fact that the notion of a local optimum is defined relative to a neighborhood relation. The neighborhoods are typically ordered in a nested way, i.e. the first (last) neighborhoods result in a comparatively small (large) modification respectively. Following is shown in the Algorithm the general version of the VNS in which both the shaking phase and the local search phase uses neighborhood structures.

Algorithm 4 Steps of the general VNS

1: INPUT $N_l = \{1, \cdots, n_{N_l}\}$ shaking phase neighborhood structures, $N_k = \{1, \cdots, n_{N_k}\}$, local searching phase neighborhood structures, stopping criterion
2: Generate initial solution s
3: **while** Stopping criterion is not meeting **do**
4:     $l \leftarrow 1$
5:     **while** $l \leq n_{N_l}$ **do**
6:         $s^{'} \leftarrow \ shake \ N_l(s)$
7:         $k \leftarrow 1$
8:         **while** $k \leq n_{N_k}$ **do**
9:             $s^{''} \leftarrow BestImprovementN_k(s')$
10:             **if** $f(s^{''}) < f(s^{'})$ **then**
11:                 $s^{'} \leftarrow s^{''}$
12:                 $k \leftarrow 1$
13:             **else**
14:                 $k \leftarrow k + 1$
15:             **end if**
16:         **end while**
17:         **if** $f(s^{'}) < f(s)$ **then**
18:             $s \leftarrow s^{'}$
19:             $l \leftarrow 1$
20:         **else**
21:             $l \leftarrow l + 1$
22:         **end if**
23:     **end while**
24: **end while**
25: Return s

Within the shaking phase an incumbent solution is modified using a neighborhood structure N_l, a solution selected at random within the neighborhood of the incumbent solution s, $N_l(s)$. The resulting solution is further improved using local search, in this case a variable neighborhood descent algorithm (VND) (lines 8-16) (Mladenović and Hansen, 1997). The VND is used and leads to a local optimum $s^{'}$. If the local optimal improves the incumbent solution it replaces the incumbent solution and the procedure starts over again with the first neighborhood $N_l, \ l = 1$. Otherwise the current solution is discarded and the procedure continues with the next neighborhood. If the last shaking phase neighborhood is reached without a solution better than the incumbent being found, the search begins again at the first neighborhood $l \leftarrow 1$ until a stopping condition.

Several questions are proposed by the authors about selection of neighborhood structures:

- *What properties of the neighborhoods are mandatory for the resulting scheme to be able to find a globally optimal or near-optimal solution?*
- *What properties of the neighborhoods will favor finding a near-optimal solution?*
- *Should neighborhoods be nested? Otherwise how should they be ordered?*
- *What are desirable properties of the sizes of neighborhoods?*

4.3.4 Adaptive large neighborhood search (ALNS)

Large neighborhood search (LNS) was presented by Shaw (1998). LNS methods explore a complex neighborhood by use of heuristics (Pisinger and Ropke, 2010). It has a simple principle: in each iteration the incumbent solution is partially destroyed and then it is repaired again; that is, first a given number of elements are removed and then they are reinserted. Every time these operations lead to an improved solution, the new solution replaces the incumbent solution, otherwise it is discarded. It is intended to limit the search in large neighborhood giving this is a time consuming process but searching a large neighborhood results in high quality local optima. Ropke and Pisinger (2006) extend Shaw's idea where a large collection of variables are modified in each iteration. In Adaptive large neighborhood search (ALNS), the neighborhoods are searched by simple and fast heuristics. ALNS is also based on the *ruin* and *recreate* paradigm. Contrary to VNS, ALNS operates on a predefined set of large neighborhoods corresponding to heuristic algorithms, destroy and repair, but they call them fix and optimize operation.

The destroy method which destructs part of the current solution typically contains an element of stochasticity such that different parts of the solution are destroyed in every invocation of the method. The neighborhood $N(s)$ of a solution s is then defined as the set of solutions that can be reached by first applying the destroy method and then the repair method.

Pseudo-code for the basic LNS is shown in Algorithm 5. Given an acceptance criterion the heuristic determines whether the candidate solution should become the new current search solution (line 6) or whether it should be rejected. The best solution is updated in line 9 when the objective function evaluated on the candidate solution is improved. In general the termination criterion can be a limit on the number of iterations or a time limit. From the pseudo-code it can be noticed that the LNS metaheuristic does not search the entire neighborhood of a solution, but merely samples this neighborhood Pisinger and Ropke (2010).

Algorithm 5 Large neighborhood search

Input: a feasible solution s
$s^b \leftarrow s$
while Stopping criterion is not meeting **do**
    $s_t = repare(dstroy(s))$
    if $accept(s_t, s)$ **then**
        $s \leftarrow s_t$
    end if
    if $f(s_t) < f(s_b)$ **then**
        $s^b = s_t$
    end if
end while
Return s^b

The degree of destruction of the destroy method is an important part of the LNS heuristic. If only a small part of the solution is destroyed then the heuristic may have trouble exploring the search space as the effect of a large neighborhood is lost. If a very large part of the solution is destroyed then the LNS heuristic almost degrades into repeated re-optimization. This can be time consuming or yield poor quality solutions dependent on how the partial solution is repaired. The destroy method must also be chosen such that the entire search space can be reached, or at least the interesting part of the search space where the global optimum is expected to be found. In the implementation of this heuristic there is some freedom in choosing the repair method. The repair method should be optimal in the sense that the best possible full solution is constructed from the partial solution, or whether it should be a heuristic assuming that one is satisfied with a good solution constructed from the partial solution. Alternately the destroy and repair operations can be viewed as fix/optimize operations: the fix method (corresponding to the destroy method) fixes part of the solution at its current value while the rest remains free, the optimize method (corresponding to the repair method) attempts to improve the current solution while respecting the fixed values.

4.4 Neighborhood structures in heterogeneous fleet VRP problems

Starting from the problem definition given in Section 3.1. A route is defined as the pair (σ^r, k), where $\sigma^r = (\sigma^r_1, \sigma^r_2, \ldots, \sigma^r_{|\sigma^r|})$, with $\sigma^r_1 = \sigma^r_{|\sigma^r|} = 0$ and $\{\sigma^r_2, \ldots, \sigma^r_{|\sigma^r|-1}\} \in \mathcal{C}$, is a simple circuit in $\mathcal{G}(\mathcal{N}, \mathcal{L})$ containing the depot, and k is the type of vehicle associated with the route. A route (σ^r, k) is feasible if the total demand of the customers visited by the route does not exceed the vehicle capacity Q_k. A solution s is represented as a collection of routes. Using three-index binary variables previously introduce in Chapter 3., x^k_{ij} take value 1 if a vehicle of type k travels directly from customer i to customer j, and 0 otherwise. y_{ij} specify the quantity of goods that a vehicle carries when it leaves customer i to service customer j.

A perturbation or move on solution s defines a transition from this to solution to a solution $s' \in N(s)$. This generation mechanisms describe how to generate the neighborhood from a given solution s.

4.4.1 Common neighborhood structures in VRP problems

Several neighborhoods structures have been defined in the VRP literature, Vidal et al. (2013) describe those structures frequently used. Two of the most commonly used neighborhoods are the insert or shift neighborhood, and the swap or interchange neighborhood. This two neighborhood structures are constructed by moving one or more customers from one route to another one. In Figure 4.1 shows the shift of one customer and the swap of two customers, one from each route. Osman (1993) calls this moves as λ-interchanges scheme. Given these moves consist of exchanging up to λ customers between two routes, it is defined on the number of nodes involved in the movement. The 1-interchange generation mechanism invokes two processes to generate neighboring solutions: a shift process which is represented by the shift(1,0) operator, and an interchange or swapping process which is represented by the $swap(1, 1)$ operator.

Other common used neighborhood is the $2 - Opt$ moves or route crossover which involves the deletion and creation of a pair of arcs. This type of move are called $k - exchange$ move given it involves the deletion of up to k arcs of the current solution and the generation of k new ones to obtain the neighbor solution. The cross exchange presented by Éric Taillard et al. (1997) are edge exchange heuristics generalizing $2 - Opt$ and $Or - Opt$ moves, and it itself is an special case of λ-interchanges scheme. A neighborhood of the type $\lambda - Opt$ contains the set of solutions obtained by deleting and reinserting k arcs. In this case the

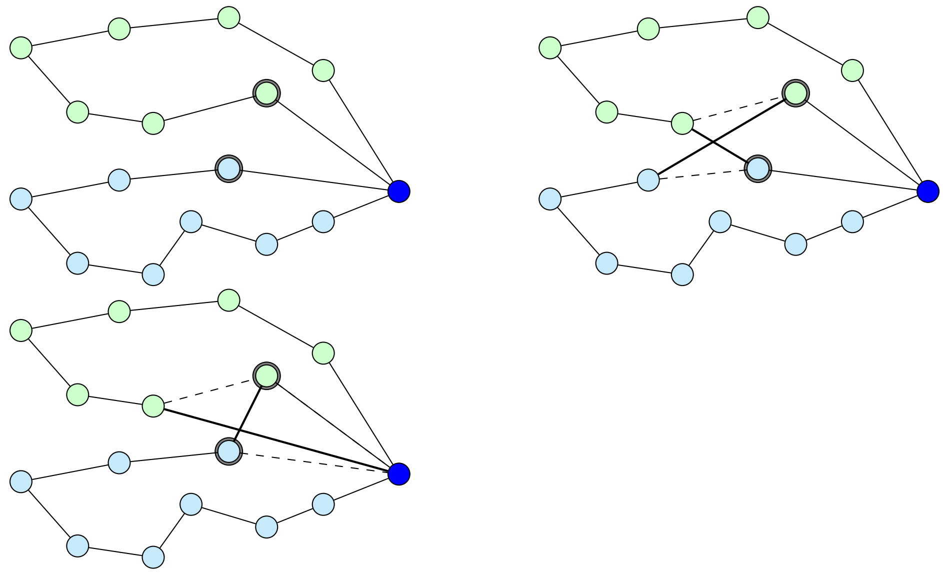


Figure 4.1: Shift (below) and swap (right) illustration. The deleted/inserted arcs are indicated with dotted/bold lines

neighborhood size is $|N_{\lambda-opt}| = O(n^{\lambda})$.

Others common neighborhood structures involve the merge of two routes into one or split a route into two different routes. In order to enhance the neighborhood search, some auxiliary data structures are adopted that allows to reduce the computational complexity when evaluating a new route (neighbor).

Neighborhood search structures that normally are used as perturbation mechanism are large neighborhood than the one utilized in the local search, or a move that the local search cannot undo in just one step.

4.4.2 Local search algorithm for solving the HVRP

Salhi and Rand (1993) incorporate local search as a perturbation procedure within constructed routes to reduce the total cost of routing in vehicle fleet composition problem. Different neighborhood structures are considered in their work. A type of destroy and repair procedure that drops the customer from a route and insert them into other routes through the cheapest cost insertion rule. Combination of routes by merging two routes. Split routes, and swapping customers between the routes. Also they use combined structures, combining and shifting for using the smaller possible vehicle, and split and shifting for reducing the number of vehicles. They apply the neighborhood structures almost in a linear way but starting the local

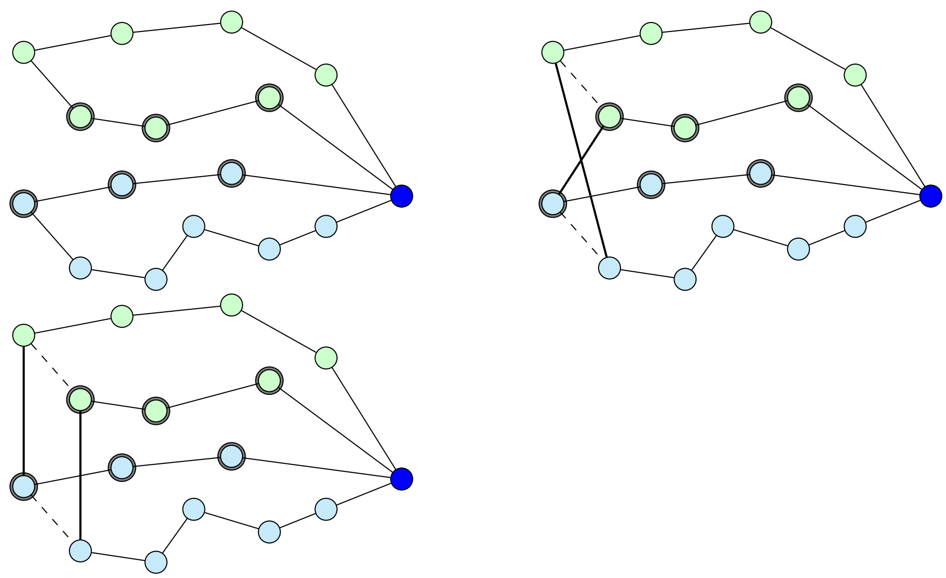


Figure 4.2: $2 - opt$ option 1 (below) and option 2 (right) illustration. The deleted/inserted arcs are indicated with dotted/bold lines

search process several times. Using the algorithm that incorporates this solution refining they found the best known solution for the instance problem 6 from the set of instance proposed by Golden et al. (1984) for the fleet size and mix vehicle routing problem (FSMVRP).

Prins (2009) presents a memetic algorithm, a genetic algorithm in which new solutions obtained by crossover and mutation are improved using a local search, for solving the FSMVRP. The chromosome encondes giant tours and then an optimal evaluation procedure splits these tours into feasible trips and assigns vehicles to them. The local search procedure works on complete solutions computed by split algorithm. The moves include the relocation of one customer (shift), the exchange of two customers (swap) and 2-OPT moves (cross and parallel). Each local search iteration scans the proposed moves and performs the first improving move. The process is repeated until no improvement is found.

Penna et al. (2013) proposed the first algorithm based on the ILS for solving the HVRP. The algorithm uses a VND procedure with a random neighborhood ordering (RVND) in the local search phase. The neighborhood structures are divided in two inter-routes and intra-route. Five of the neighborhood structures are based on the λ-interchanges schemes proposed by Osman (1993), Osman and Salhi (1996). Also a Cross-exchange operator which consists of exchanging two segments of different routes is implemented. Finally, a neighborhood structure called, $K-Shift$, which consists of transferring a set of K consecutive customers from a route to another one. The solution spaces of the seven neighborhoods are explored exhaustively, that means the computational complexity of each one of these moves is $O(n^2)$. They also implemented intra-route neighborhood structures, reinsertion, $Or-opt2$, $Or-opt3$, $2-opt$, and exchange. For starting the local search three perturbation mechanisms were adopted. First, multiple random Swap(1,1) moves are performed in sequence. Second, multiple Shift(1,1) moves are performed in sequence randomly. Finally, divided into smaller routes a random selected one.

The improvement technique as LSA maintains feasible the solution while reducing the value of the cost function. For doing this a search strategy for exploring the set of solutions induced by the move or neighborhood structure, acceptance criteria have to be established, and a selection strategy is followed. When not further improvement of the current solution is possible, a local optimum is reached, the iterative local improvement finishes. In this process a sequence of solution is visited, this is the search trajectory. The best suitable LSA for a given problem instance uses the smallest size search trajectory which provides the best improvement of a given initial solution. If a perturbation mechanisms is incorporating in order to re-start the local search, hybrid LSA, the search trajectory will be composed of an exploration or diversification path and the intensification paths. This combination of moves allows to explore intensively a promising part of the search space and to go forward new interesting areas to explore.

As mentioned by Vidal et al. (2013) one of the critical aspects in LSA is the efficient serial evaluation of moves, route feasibility and costs. Variables associated to a sequence of nodes of a route can improve the efficiency of move evaluations. Selecting the appropriated data structures for storing the values of this variables and routes characteristics is also a key aspect when designing a LSA. Care should be taken in the evaluation of a solution candidate, it is preferred to do it in constant time $O(1)$.

4.5 Experiments and results

Some computational experiments are conducted in order to measure the individual contribution of proposed neighborhood structures in improving the cost value of the initial solution. In this work it is considered neighborhood structures for FSMVRP. Given the hybrid local search algorithms are based on the combination of these neighborhoods, experiments are conducted to explore the impact of the different neighborhoods combinations within a VND framework.

4.5.1 Methodology

An initial solution is first generated via a procedure based on random split of a big Hamiltonian tour. Then, the routes are constructed by randomly selecting an available vehicle and assigning, respecting tour sequence and vehicle capacity, the non assigned nodes. The four common neighborhood structures above mentioned selected for experimentation are:

- $Shift(1,0)$: A customer k is transferred from a route to another route.
- $Swap(1,1)$: interchange a customer k from a route and a customer l, from an another route.
- $Split$: A route is divided into smaller routes.
- $2 - Opt$: Swap a nodes sequence from one route and to another involving the extremities of two distinct routes.

Also $swap(2,1)$, $swap(2,2)$, and $shift(m,0)$ moves are considered in order to determine if more complex neighborhoods or moves involving multiple route nodes contribute to improve the performance of the local search. When exploring one neighborhood the best improving move is applied, and the local search terminates when no improving move can be found.

As the computational efficiency of the move evaluations is of critical importance, some data structure are used in order to have $\mathcal{O}(1)$ move evaluations, intending to perform efficiently move evaluations.

Twelve sample problem instances taken from (Golden et al., 1984) considering the cases where the fleet is unlimited with fixed costs but without variable costs are used for experimentation. These instances go from 20 to 100 nodes, and as example of the problem structure the instance 3, that has twenty nodes and five different types of vehicles,is shown in Figure 4.3.

4.5.2 Performance Evaluations

The first experiment aims to measure the performance of each neighborhood structure when it is applying repeatedly to improve the cost function of an initial solution generated using the procedure given before (random split of a big Hamiltonian tour). The number of possible moves, the number of feasible moves, the average percentage of the objective function value improvement, and the total percentage of the objective function value improvement are registered. The proposed method was then run 100 times for each instance and using the seven previously defined moves.

Figure 4.3: Heterogeneous fleet VRP with 20 nodes and unlimited fleet using 5 different vehicle types.

Nodes Information

i	x	y	q_i
1	37	52	7
2	49	49	30
3	52	64	16
4	20	26	9
5	40	30	21
6	21	47	15
7	17	63	19
8	31	62	23
9	52	33	11
10	51	21	5
11	42	41	19
12	31	32	29
13	5	25	23
14	12	42	21
15	36	16	10
16	52	41	15
17	27	23	3
18	17	33	41
19	13	13	9
20	57	58	28

Vehicle Types

Vehicle	Capacity	Cost
A	20	20
B	30	35
C	40	50
D	70	120
E	120	225

According to the results shown in the Table 4.1, the neighborhood structures that provides the greater number of iterations is the $2-opt$; while $split$ and $swap(2,2)$ the less number of iterations. In the Table 4.2 it is shown that the size of the neighborhood to be explore increase with the size of the instance. The average number of neighbors explored remains almost the same across the instances having the same number of nodes. The average percentage of feasible moves for the neighborhood structures $Shift(1,0)$, $Swap(1,1)$, $Split$, $Swap(2,1)$, $Swap(2,2)$, $Shift(m,0)$, $2-opt$ are respectively 71.4%, 81.4%6, 100%, 67.41%, 73.13%, 42.7%, 67.68%. Excepting the moves $Shift(m,0)$, more than the 60% of the neighbors must be evaluated and compared in an exhaustive neighborhood search.

Table 4.1: Average number of iteration for proposed neighborhoods for the FSVRP

Instance number	Number of nodes	Move (neighborhood structures) $Shift(1,0)$	$Swap(1,1)$	$Split$	$Swap(2,1)$	$Swap(2,2)$	$Shift(m,0)$	$2-opt$
3	20	3.39	3.76	1.52	3.57	2.04	2.68	4.00
4	20	2.42	3.35	1.63	2.79	2.35	2.98	4.12
5	20	7.40	5.28	1.46	5.49	2.8	2.82	4.75
6	20	6.45	4.18	1.66	3.65	3.16	3.18	5.25
13	50	4.41	8.36	2.70	7.10	3.63	5.70	6.91
14	50	3.31	4.62	2.75	3.11	2.93	4.72	5.39
15	50	5.03	6.28	3.74	6.08	4.32	6.64	9.43
16	50	7.52	7.64	1.52	8.16	4.76	6.51	10.22
17	75	13.4	6.76	2.73	6.36	5.23	7.47	10.70
18	75	4.03	7.28	8.85	6.2	5.01	6.62	11.03
19	100	7.45	7.23	7.74	7.22	4.61	10.61	13.08
20	100	14.07	9.83	5.38	10.41	6.6	14.21	17.79

Table 4.2: Average size of neighbors for proposed neighborhoods for the FSVRP

Instance number	Number of nodes	Move (neighborhood structures) $Shift(1,0)$	$Swap(1,1)$	$Split$	$Swap(2,1)$	$Swap(2,2)$	$Shift(m,0)$	$2-opt$
3	20	418.31	158.25	12.72	166.58	59.34	215.84	137.49
4	20	357.11	144.15	22.33	175.85	80.39	370.45	176.18
5	20	407.57	158.78	12.34	171.67	59.24	204	137.84
6	20	351.34	143.8	22.72	176.53	80.82	367.76	176.79
13	50	2710.7	1088.02	85.65	1458.05	572.52	4611.55	1048.02
14	50	2216.51	986.25	158.97	1510.17	757.44	8275.04	1173.94
15	50	2508.38	1065.47	98.86	1586.09	711.71	4944.22	1319.34
16	50	2612.56	1089.3	88.93	1580.01	669.05	3898.1	1308.77
17	75	5196.35	2327.8	364.99	3673.8	1789.3	25295.27	2770.36
18	75	5145.8	2293.96	229.44	3570.23	1741.46	26772.85	2702.54
19	100	9196.95	4239.92	429	7160.96	3548.7	53788.59	4914.67
20	100	10061.4	4483.88	324.11	7385.98	3418.89	37863.3	5317.52

Also there was not observed a significant difference between the percentage of feasible movement across the different instances. Not matter the cost solution for a VRP with heterogeneous fleet an efficient way for evaluating a move must be defined given the perturbation of feasible neighbors generated for the moves, in the work of Vidal et al. (2014) and Penna et al. (2013) are described some operators for proving the feasibility and evaluation of moves for different types of cost functions in VRP problem.

In the Table 4.3 the average of the total improvement of the cost value function is presented. The neighborhood structures $Shift(m,0)$, $2-opt$ and $Shift(1,0)$ have the greater values. In Friedman test applied to the results shows a significant statistic evidence that not all the neighborhood structures provide the same improvement, with a $p-value \leq 3.921 \times 10^{-09}$. The large neighborhoods as $Shift(m,0)$, $2-opt$ and $Shift(1,0)$ have a positive impact on solution quality but not in the case of $swap(2,1)$.

With this information it is possible to decide which neighborhood structures are more appropriated for performing the local search and which one more appropriated for the exploration of the search space (perturbations). These last movements that are used for escaping from a local optimal solution consist of larger neighborhood than those utilized in the local search, or a move that the local search cannot

Table 4.3: Average total improvement in percentage of the initial cost value function for proposed neighborhoods for the FSVRP

Instance number	Number of nodes	Move (neighborhood structures)						
		$Shift(1,0)$	$Swap(1,1)$	$Split$	$Swap(2,1)$	$Swap(2,2)$	$Shift(m,0)$	$2-opt$
3	20	8.77	2.47	1.35	2.34	0.83	5.95	7.94
4	20	2.49	0.28	4.25	0.23	0.18	12.85	11.44
5	20	17.81	5.14	1	6.26	2.24	6.69	8.83
6	20	12.9	0.44	4.01	0.39	0.37	12.07	11.27
13	50	5.84	2.33	1.89	2.3	0.88	7.12	6.67
14	50	0.93	0.2	9.63	0.15	0.13	11.12	9.08
15	50	2.3	1.32	3.84	1.59	1.12	9.39	8.25
16	50	7	1.62	0.99	2.27	1.16	9.48	7.88
17	75	8.2	1.76	3.23	2.12	1.69	9.4	9.23
18	75	1.29	1.36	18.93	1.38	1	11.62	14.12
19	100	1.27	0.31	14.6	0.34	0.21	11.44	9.82
20	100	5.01	0.94	5.91	1.35	0.84	9.05	7.04

Table 4.4: Average percentage gap to BKS for proposed neighborhoods for the FSVRP

Instance number	Number of nodes	Move (neighborhood structures)						
		$Shift(1,0)$	$Swap(1,1)$	$Split$	$Swap(2,1)$	$Swap(2,2)$	$Shift(m,0)$	$2-opt$
3	20	17.21	25.59	27.03	25.57	27.74	20.82	18.15
4	20	33.99	37.92	32.49	37.99	38.08	19.51	22.03
5	20	11.03	27.57	33.58	26	31.9	26.29	23.29
6	20	17.72	37.83	32.45	37.89	37.94	18.71	20.96
13	50	16.7	21.51	22.01	21.54	23.35	15.17	15.76
14	50	33.91	34.96	21.53	35.03	35.06	19.26	21.92
15	50	20.47	21.73	18.82	21.41	21.94	11.43	12.78
16	50	15.49	22.03	23	21.37	22.72	12.43	14.36
17	75	18.16	26.75	24.85	26.2	26.77	16.47	16.8
18	75	45.33	45.42	18.84	45.35	45.92	29.35	25.29
19	100	31.95	33.18	14.11	33.12	33.31	17.88	20.17
20	100	17.63	22.89	16.64	22.39	23.01	12.57	15.11

undo in just one step.

Finally in the Table 4.4 is presented the average gap in percentage between the average solution obtained using the neighborhood structure in the local search and the best know solution (BKS) for each instance. For all 12 instances the average gap in percentage is 30.81%.

The purpose of the following experiments is to measure the performance of each possible combination of the proposed neighborhoods, relatively to the performance (finding a good local optimum) of the local search. The VND algorithm is used, and the order of the neighborhood structures applied follows the 5040 possible combinations of 7 previously proposed neighborhoods. The suggested method was then run 100 times for each instance. In order to measure the average performance of the combinations different initial solutions, constructed using the heuristic based on random split of a big Hamiltonian tour, are used. The best solution for a given pair initial solution-neighborhood combination and the best average result for a neighborhood combination are extracted. The results are presented in Table 4.5. The best solution found by applying the neighborhood combinations presents a maximum gap in percentage of 2.814%. The average deviation of the minimum value and the average value taking over all the instances from the BKS are 1.19%

Table 4.5: Neighborhood structures experiment results for the FSVRP

Instance	Number	BKS	Best Sol.	Average Sol.	Gap Best Avg.	Gap Best Sol.
3	20	961.03	961.92	1051.53	0.09	9.42
4	20	6437.33	6438.26	7282.53	0.01	13.13
5	20	1007.05	1007.05	1071.48	0	6.40
6	20	6516.47	6516.47	7286.36	0	11.82
13	50	2406.36	2468.35	2613.86	2.58	8.62
14	50	9119.03	9140.41	9706.07	0.23	6.44
15	50	2586.37	2603.87	2752.00	0.68	6.40
16	50	2720.43	2767.66	2948.11	1.74	8.37
17	**75**	**1734.53**	**1783.34**	**1902.34**	**2.81**	**9.68**
18	75	2369.65	2430.48	2533.00	2.57	6.89
19	100	8661.81	8733.21	9145.73	0.82	5.59
20	100	4037.90	4148.51	4318.78	2.74	6.96
Average					1.19	8.31

and 8.31% respectively. That means that using the appropriated neighborhood combination it is possible to find a near optimal solution and the diversification part (different starting point) can provide near a 7.5% of improvement.

The combinations of neighborhood structures in a VND framework reduce the average gap between the BKS and the average of the final cost value obtained across all instances, from 30.81% to 8.31%. A perturbations mechanism can provide a further improvement by providing a good starting solution that can lead the local search to a good local optimum.

Following the work of Subramanian et al. (2012) a further improvement of the initial solution is implemented. A set partitioning (SP) model is built using routes generated by the iterations of the VND algorithm; a Mixed Integer Programming (MIP) is formulated for choosing the best combination of these routes. The model is solve by means of Gurobi 6.0 solver and the results are presented in the Table 4.6. The algorithm implemented in Java using a computer with ubuntu 16.04 having an Intel Core i5-4590 CPU 3.30GHz and it was run 100 times.

As it is presented in the previous table, the average gap between the average solution and the BKS solutions goes from 8.31% to 0.88%. The greatest gaps are those for the instances 16, 17 and 20. These results agree with those find in the literature in the sense these are the hardest to solve instances. But also these results are a prove that the recombination of routes of the solutions found by the local search provide a better solution, what reinforces the need of the perturbation

Table 4.6: Neighborhood structures experiment results for the FSVRP

Instance	Number of nodes	BKS Sol.	Average Sol.	Gap Average Sol.	Best Sol.	Gap Best Sol.	Average Time(s)
3	20	961.03	961.08	0.01	961.03	0	3.6
4	20	6437.33	6441.28	0.06	6437.33	0	3.07
5	20	1007.05	1008.37	0.13	1007.05	0	2.31
6	20	6516.47	6531.7	0.23	6516.47	0	2.68
13	50	2406.36	2433.4	1.12	2415.23	0.37	18.52
14	50	9119.03	9129.76	0.12	9119.03	0	21.54
15	50	2586.37	2597.09	0.41	2586.84	0.02	22.06
16	**50**	**2720.43**	**2778.03**	**2.12**	**2745.04**	**0.9**	**20.52**
17	**75**	**1734.53**	**1768.61**	**1.96**	**1750.1**	**0.9**	**67.13**
18	75	2369.65	2409.08	1.66	2379.37	0.41	62.6
19	100	8661.81	8707.89	0.53	8687.95	0.3	111.9
20	**100**	**4037.9**	**4127.4**	**2.22**	**4093.14**	**1.37**	**117.28**
				0.88		0.36	

mechanism.

4.6 Conclusions

4.6.1 Conclusions (English)

The combination of neighborhood structures provides an enhance to the local search heuristic algorithms compare to individual use of them. The sequence order of the neighborhood structures when they are applied to an initial solution seems not to be significant. The diversification part becomes an important element when solving different instances of a vehicle routing problem with heterogeneous fleet given there is not an unique combination that fits all the instances. Near optimal results can be obtain if the appropriated initial solution is provided. The impact on the search performance of neighborhood structure combination to be used in the intensification part depends on the perturbation provided by the those used as diversification strategy. A good perturbation mechanism in local search based algorithm can explore an efficient and effective way the solution search space.

The number of required moves in LSA ranges from hundreds to thousands in instances with 50 or more nodes. In order to achieve an efficient implementation of LSA, constant time evaluation of a candidate solution is more than advisable.

Two of most important aspect of any local search-based heuristics are the feasibility check of a neighbor and the move evaluation. Any significant reduction in the time needed to determine if a neighbor is feasible or to evaluate a move increase the number of moves or size of a neighborhood structure which can be evaluated during one run of the algorithm. And, how it is shown in the results, it allows to combine different neighborhood structure in order to enhance the solution quality.

4.6.2 Conclusions (Français)

La combinaison des structures de voisinage fournit une amélioration aux algorithmes heuristiques de recherche locale par rapport à l'utilisation individuelle de ceux-ci. L'ordre d'utilisation des structures de voisinage lorsqu'elles sont appliquées à une solution initiale ne semble pas significatif. La partie de diversification devient un élément important lors de la résolution de différentes instances d'un problème de tournées de véhicules à flotte hétérogène étant donné qu'il n'y a pas une combinaison unique qui convienne à toutes les instances. Des résultats presque optimaux peuvent être obtenus si une solution initiale appropriée est fournie.

L'impact sur la performance de recherche de la combinaison de structures de voisinage à utiliser dans la partie intensification dépend de la perturbation fournie par ceux utilisés comme stratégie de diversification. Un bon mécanisme de perturbation dans l'algorithme de recherche locale peut explorer de manière efficace et efficiente l'espace de recherche de solution.

Le nombre de mouvements requis dans l'algorithme de recherche local varie d'une centaine à des milliers pour les instances avec 50 nœuds ou plus. Afin d'obtenir une mise en œuvre efficace du l'algorithme, l'évaluation en temps constant d'une solution candidate est donc plus que souhaitable.

Deux des aspects les plus importants de toute heuristique basée sur la recherche locale sont la faisabilité d'un voisin et l'évaluation du déplacement. Toute réduction significative du temps nécessaire pour déterminer si un voisin est réalisable ou pour évaluer un déplacement permet d'augmenter le nombre de mouvements ou la taille d'une structure de voisinage qui peut être évaluée pendant une exécution de l'algorithme global.

4.6.3 Conclusiones (Español)

La combinación de estructuras de vecindario proporciona una mejora para los algoritmos heurísticos de búsqueda local en comparación con el uso individual de los mismos. El orden de secuencia de las estructuras de vecindario cuando son aplicados a una solución inicial parece no ser significativo. La parte de diversificación se convierte en un elemento importante a la hora de resolver diferentes in-

stancias de un problema de ruteo de vehículos con una flota heterogénea, dado que no existe una combinación única que se ajuste a todas las instancias. Se pueden obtener resultados casi óptimos si se proporciona la solución inicial apropiada. El impacto en el rendimiento de búsqueda obtenido por la combinación de estructuras de vecindarios que se utiliza en la parte de intensificación depende de la perturbación lograda por los vecindarios utilizados como estrategia de diversificación. Un buen mecanismo de perturbación en el algoritmo basado en búsquedas locales permite explorar de manera más eficiente y eficaz el espacio de búsqueda de soluciones.

El número de movimientos requeridos por un algoritmo de búsqueda local varía de centenas a millares para las instancias con 50 o más nodos. Para lograr una implementación eficiente de un algoritmo de búsqueda local, la evaluación en tiempo constante de una solución candidata es más que recomendable

Dos de los aspectos más importantes de toda heurísticas basadas en búsqueda local es la evaluación de la factibilidad de un vecino y de un movimiento. Cualquier reducción significativa en el tiempo necesario para determinar si un vecino es factible o para evaluar un movimiento aumenta el número de movimientos o el tamaño de una estructura del vecindario que puede evaluarse durante una ejecución del algoritmo. Y, como se muestra en los resultados, permite combinar diferentes estructuras de vecindario para mejorar la calidad de la solución.

Chapter 5

Variable Neighborhood Search (VNS) to solve the Vehicle Routing Problem (VRP) for Hazardous Materials (HazMat) Transportation

Abstract (English)

This chapter focuses on the Heterogeneous Fleet Vehicle Routing problem (HFVRP) in the context of hazardous materials (HazMat) transportation. The objective is to determine a set of routes that minimizes the total expected routing risk. This is a nonlinear function, and it depends on the vehicle load and the population exposed when an incident occurs. Thus, a piecewise linear approximation is used to estimate it. For solving the problem, a variant of the Variable Neighborhood Search (VNS) algorithm is employed. To improve its performance, a post-optimization procedure is implemented via a Set Partitioning (SP) problem. The SP is solved on a pool of routes obtained from executions of the local search procedure embedded on the VNS. The algorithm is tested on two sets of HFVRP instances based on literature with up to 100 nodes, these instances are modified to include vehicle and arc risk parameters. The results are competitive in terms of computational efficiency and quality attested by a comparison with a Mixed Integer Linear Programming (MILP) previously proposed. This chapter is organized as follows. Section 5.1 gives an introduction in HazMat transportation problems and HFVRP. Section 5.2 provides a problem definition and presents the risk evaluation for HFVRP in Haz-

Mat transportation. Section 5.3. presents the solution method. In Section 5.4. the experiments and computational results are shown. The final section concludes the chapter and discusses future research directions.

Résumé (Français)

Ce chapitre se concentre sur le problème des tournées des véhicules à flotte hétérogène (HFVRP heterogeneous fleet vehicle routing problem) dans le contexte du transport de substances dangereuses (HazMat hazardous materials). L'objectif est de déterminer un ensemble de routes qui minimisent le risque total de routage. Il s'agit d'une fonction non linaire, dépendante de la charge du véhicule et de la population exposée, lorsqu'un incident se produit. Dans ce cas, une approximation linéaire par morceaux est utilisée pour estimer la valeur de cette fonction de risque. Pour résoudre le problème, une variante de l'algorithme de recherche à voisinage variable (VNS variable neighborhood search) est utilisée. Pour améliorer la performance de l'algorithme, une procédure de post-optimisation est utilisé en formulant un problème de partition d'ensemble (SP set partitioning). Le SP est résolu sur la base d'un ensemble de routes obtenues dans l'exécution de la procédure de recherche locale intégrée dans le VNS. L'algorithme est testé sur deux ensembles d'instances HFVRP basés sur la littérature de jusqu'à 100 nœuds, modifié pour inclure paramètres de risque associés au véhicule et à l'arc. Les résultats obtenus sont compétitifs en termes d'efficacité et de qualité du calcul, comparés à ceux de la programmation linéaire en nombres entiers (PLNE) précédemment proposée. Ce chapitre est organisé comme suit. La section 5.1 présente une introduction aux problèmes de transport de substances dangereuses et de HFVRP. La section 5.2 donne une définition du problème et présente l'évaluation des risques du HFVRP transportant de substances dangereuses. Section 5.3. Présente la méthode de solution. Dans la section 5.4. les expériences réalisées et les résultats de calcul obtenus sont montrés. La dernière section conclut le Chapitre et discute des futures directions de recherche

Resumen (Español)

Este capítulo se centra en el problema de ruteo de vehículos con flota heterogénea (HFVRP heterogeneous fleet vehicle routing problem) en el contexto del transporte de materiales peligrosos (HazMat hazardous materials). El objetivo es determinar un conjunto de rutas que minimicen el riesgo total de ruteo. Esta es una función no lineal, dependiente de la carga del vehículo y la población expuesta, cuando un incidente acontece. En este caso, se utiliza una aproximación lineal por partes para estimar el valor de esta función de riesgo. Para resolver el problema se utiliza

una variante del algoritmo de búsqueda con vecindarios variables (VNS variable neighborhood search). Para mejorar el rendimiento del algoritmo, se implementa un procedimiento de post-optimización a través del planteamiento de un problema partición de conjuntos (SP set partitioning). El SP se resuelve sobre la base de un conjunto de rutas obtenidas en la ejecución del procedimiento búsqueda local embebido en el VNS. El algoritmo se prueba en dos conjuntos de instancias de HFVRP basadas en la literatura de hasta 100 nodos, modificadas para incluir los parámetros de riesgo asociados al vehículo y al arco. Los resultados obtenidos son competitivos en términos de eficiencia y calidad computacional, en comparación con aquellos provenientes de la programación lineal mixta (PLEM) previamente propuesta. Este capítulo está organizado de la siguiente manera. La Sección 5.1 brinda una introducción a los problemas de transporte de materiales peligrosos y HFVRP. La Sección 5.2 proporciona una definición del problema y presenta la evaluación de riesgos para HFVRP en el transporte de materiales peligrosos. Sección 5.3. presentar el método de solución. En la Sección 5.4. se muestran los experimentos realizados y resultados computacionales obtenidos. En la sección final se dan las conclusiones del Capítulo y se analizan las direcciones futuras de investigación

5.1 Introduction

Hazardous Materials (HazMat) transportation is an integral part of our industrial life style, but there are risks associated with this activity. When a transportation accident occurs it may be followed by a HazMat release resulting in consequences such as fire, explosion, or toxic gas cloud, among others, that can affect population and the environment close to the accident site. Such HazMat transportation incidents can lead to fatalities, injuries, evacuation, property damages, environmental degradation, and traffic disruptions. Transportation risk management aims at diminishing HazMat transportation risks by reducing accident probability and consequences. This risk alleviation can be both proactive and reactive, and HazMat transportation routing is considered a major proactive risk mitigation measure (Zografos and Androutsopoulos (2004); Erkut et al. (2007)).

HazMat transportation routing problem has two main focuses: shortest path problems (associated with full truck load distribution) and vehicle routing problem (VRP) (associated with less than full truck load distribution). There is a significant research effort related to the first type of problems, but this is not the case with the second type (Androutsopoulos and Zografos (2012); Pradhananga et al. (2014a)). Tarantilis and Kiranoudis (2001b) present one of the first studies where a fleet of vehicles is used to service HazMat demands, HazMat VRP. In their work the objective is to minimize the population exposure by solving a Capacitated VRP using a list based variant of the threshold accepting algorithm (LBTA). Zografos and Androutsopoulos (2004) also take into account the VRP prospective of the HazMat transportation problem. In their proposal the transportation risk is defined as the expected consequences (traditional risk model), the product of the probability of an incident and the measure of its consequences. A route building (insertion) algorithm is used to solve a bi-objective problem that also includes cost minimization. Both, model and heuristic are used in Zografos and Androutsopoulos (2008) to solve a similar problem. In a posterior work Androutsopoulos and Zografos (2010) included the probability of accident and expected consequences arising in case of an accident occurring on a time dependent arc. Tanguchi et al. (2010) also consider the minimization transportation risk in HazMat distribution (traditional risk model), and a multi-objective problem is solved using an ant colony system (ACS). Androutsopoulos and Zografos (2012) present a bi-objective time-dependent vehicle routing problem with time windows. The risk measure defined in this work includes variations of accident probabilities, and the population density on impact area of a potential hazardous materials accident, throughout the day. They also studied variations on the impact area given different values of the load of the truck, type of hazardous materials carried, and weather conditions. However, when solving the problem, the effect of the load on the risk values was not taken into account and thus each link was assumed to have time-dependent load-invariant risk values. Pradhananga et al. (2014b) use a Multi-Objective Ant Colony System (MOACS) to solve a bi-objective HazMat routing problem, minimizing of the total scheduled travel time and the total risk value of the routes. Here, the probability of a HazMat accident on arc is obtained multiplying accident rate by the length of the arc, and the consequences is defined as the exposure population associated to the worst HazMat release incident.

In the best of our knowledge VRP in HazMat transportation with load-variant risk values and heterogeneous fleet is never studied. It is however to be considered that, the likelihood of occurrence of a HazMat transportation incident depends on the volume and the type of transported HazMat. Furthermore, given that HazMat routing problems belong to *rich* VRP (Hoff et al. (2010)), homogeneous fleet assumption is non-realistic in practice, and truck tank accident probability depends on the type of truck. In heterogeneous fleet problems tactical decisions can be made related to fleet composition to be acquired leading to unlimited version of the problem. Operational decisions can be also made relating to building the trips and the vehicles assigned to them, when a fleet is already acquired (often over a long period of time) and the vehicles have different characteristics (including carrying capacity), leading to the limited fleet problem.

A classification of Heterogeneous Fleet Vehicle Routing Problem (HFVRP) is given in Prins (2009). Fleet size and mix vehicle routing problem (FSMVRP) corresponds to an unlimited number of vehicles of each type. This problem was introduced by Golden et al. (1984), and it combines tactical and operational decisions. The other type, the Heterogeneous Vehicle Routing Problem (HVRP), considers a fixed fleet. It was proposed by Taillard (1999) and it is close related with operational decisions. Both type of HFVRP are NP-hard, as they include the VRP as a special case (Prins (2009)).

In the problem proposed by Golden et al. (1984), the objective is to minimize the total cost function which includes fixed vehicle costs and travel costs. In the problem presented by Taillard (1999), the author introduced new instances with variable unit costs and with and without fixed fleet. For the last case the objective is to find the best set of tours that can be performed by a given fleet.

With regard to solutions methods, hybrid algorithms including local search have proven to be efficient in solving FSMVRP and HVRP instances. For the FSMVRP with fixed cost instances proposed in Golden et al. (1984) the best known solution (BKS) for the Euclidean instances $3-6$ and $13-20$ are found using this type of algorithms. Salhi and Rand (1993) find BKS of the instance number 6, using a heuristic that includes some refinements consistent of neighborhood local search. Taillard (1999) provides the BKS of instances 3, 4, 14, 15, and 19. The author applied a heuristic column generation method which uses an embedded tabu search. Gendreau et al. (1999) find the BKS of instance 5, in this work a tabu search algorithm embedded within a search technic is used. Choi and Tcha (2007) give the BKS of instances 13 and 16 using an approach based on column generation and a branch-and-bound procedure. Brandão (2009) used a heuristic algorithm based on tabu search for obtaining the BKS of instances 17 and 18. Prins (2009) proposed a genetic algorithms hybridized with a local search obtaining the BKS of 9 instances. Subramanian et al. (2012) introduced a hybrid algorithm composed of an Iterated Local Search (ILS) based heuristic which uses a procedure supported on the Variable Neighborhood Descent with Random neighborhood ordering (RVND), and a Set Partitioning (SP). This algorithm finds the BKS of instance 20 and it equals the results of the other instances. Also Duhamel et al. (2012) present an efficient hybrid evolutionary local search algorithm for solving FSMVRP, and they obtain the BKS of instances with 20 and 50 nodes. For the fixed fleet problem, Taillard (1999) solves the 8 HVRP instances that he proposed, and he provides the BKS of instance 19. Tarantilis et al. (2004) used the back-tracking adaptive threshold accepting (BATA) for finding the BKS of instance 15. This algorithm utilizes a local search conduct by a random selection of the type of move. Li et al. (2007) used a record-to-record (RTR) travel metaheuristic a deterministic variant of simulated annealing for solving all instances, they find the BKS for 7 out of 8 instances. In their work, Prins (2009) and Duhamel et al. (2012) also solve the

HVRP instances and they find the BKS for 6 out of 8 instances. Subramanian et al. (2012) using the ISL-RVND+SP algorithm find the BKS for 7 out of 8 instances.

Koç et al. (2016) presented a review of several studies on HVRP variants and heuristic methods for solving them. They also utilized the classification of FS-MVRP and HVRP focused on two measures to compute the total cost to be minimized, one based on the en-route time and the other based on distance. Others variants as the pollution routing problem are taken into account but not the HazMat routing problem.

This chapter focuses on HFVRP in HazMat transportation. An application especially on fuel (gasoline and diesel) distribution is considered, starting from a distribution center to the different service stations. The objective is to determine the set of routes that minimizes the total expected routing risk linked to the truck load. We propose a Variable Neighborhood Search (VNS) algorithm. A Set Partitioning (SP) formulation is employed as post-optimization procedure. The nonlinear routing risk function is approximated by a piece-wise linear function described in Bula et al. (2016) and reminded in Chapter 3.

5.2 Problem definition

The vehicle routing problem for HazMat transportation using a heterogeneous fleet can be defined as the determination of the safest routes assigned to a fleet of different vehicles transporting a specific HazMat from a depot to a set of customers.

In this model the HFVRP is defined on a complete directed graph $\mathcal{G}(\mathcal{N}, \mathcal{L})$. The node set $\mathcal{N} = \{0, 1, 2, \ldots, n\}$ includes the depot node 0, and a set of customer nodes (service stations), $\mathcal{C}$. Each customer $i \in \mathcal{C}$ has a demand q_i and it is connected with other node $j \in \mathcal{N}$ by an arc $(i, j) \in \mathcal{L}$. Each arc is characterized by a length al_{ij}, and a population exposed to the consequences of a HazMat release (population residing within the impact area distance of the arc), PD_{ij}. To satisfy the demands there is a set of $\mathcal{K}$ different types of trucks. A truck type $k \in \mathcal{K}$ is characterized by a maximal capacity Q_k, a number a_k of trucks available, and an accident rate $TTAR_k$.

A solution is composed of a set of routes $\mathcal{SR}$ satisfying all customer demands once. Each route $\sigma^r \in \mathcal{SR}$ starts and ends at the depot, and respects the vehicle capacity Q_k. A route is a sequence of nodes, $\sigma^r = \{\sigma^r_1, \sigma^r_2, \ldots, \sigma^r_{|\sigma^r|}\}$, where σ^r_i is i-th client visited on the node route r. Split deliveries are not allowed.

For computing the risk associated with the transportation of flammable liquids three aspects are taken into account: the probability of occurrence of the initiating event, the impact assessment or outcomes due to the event, and the population exposure to the outcomes (Das et al. (2012); Ronza et al. (2007)). The transporting risk is measured using the expected population exposure inside the impact area of the HazMat truck incident. It is considered that each arc (i, j) consists of segments that are assumed to be homogeneous in the probability of a release event, as well as in the population density. In order to estimate the probability of a release incident (initiating event) on an arc (i, j), the corresponding truck accident rate (Chakrabarti and Parikh (2011)), the truck load, the conditional release probability given an accident, and the arc length are incorporated in Eq. 5.1 (Kazantzi et al. (2011b)). The conditional release probability given an accident on the arc (i, j) is defined as the product of the release probability of HazMat given a truck accident ($P_{release}$) and the probability of a certain outcome arising as a consequence of the initiating event (Das et al. (2012); Ronza et al. (2007)). In consequence, the route risk $R(\sigma^r)$ is computed as:

$$R(\sigma^r) = \sum_{(i,j)\in\sigma^r} [TTAR^k \times al_{ij}] \times P_{release} \times [\beta(y_{ij}^k)^\alpha] \times PD_{ij} \tag{5.1}$$

Where α and β are constant values that depend on the type of material transported , and y_{ij}^k is the total load of a truck type k traversing the arc (i, j) of the route σ^r (Ronza et al. (2007)). y_{ij}^k is equal to the total demand of the customers to be satisfied after the customer σ_i^r:

$$y_{ij}^k = \sum_{w=j}^{|\sigma^r|} q_w \tag{5.2}$$

ρ_{ij} regroups arc dependent parameters.

$$\rho_{ij} = (al_{ij} \times PD_{ij}) \tag{5.3}$$

And the route risk becomes:

$$R(\sigma^r) = TTAR^k \times P_{release} \times \beta \times \sum_{(i,j)\in\sigma^r} (y_{ij}^k)^\alpha \times \rho_{ij} \tag{5.4}$$

As this is a nonlinear function on y_{ij}^k, a piecewise linear approximation for $(y_{ij}^k)^\alpha$ is used as proposed by Bula et al. (2016). Let $[q_0, q_M]$ be a bounded interval for y_{ij}^k, this interval is divided into an increasing sequence of M breakpoints $\{l_0, \dots, l_M\}$. The value of $(y_{ij}^k)^\alpha$ is then approximated by using linear interpolations over the M segments according to Eq. 5.5.

$$(y_{ij}^k)^\alpha := \Big\{ a_{ij}^m + b_{ij}^m y_{ij}^k, \ y_{ij}^k \in [l_{m-1}, l_m] \ \forall m \in \{1, \dots, M\} \tag{5.5}$$

where $a_m \in R, b_m \in R$ are the intercepts and the slopes of the linear functions, respectively, and $l_0 < l_1 < \cdots < l_M$. The value M is fixed at four, for the purpose of dividing the truck load in four categories; small , medium-size, large, and very-large load, see Fig. 5.1.

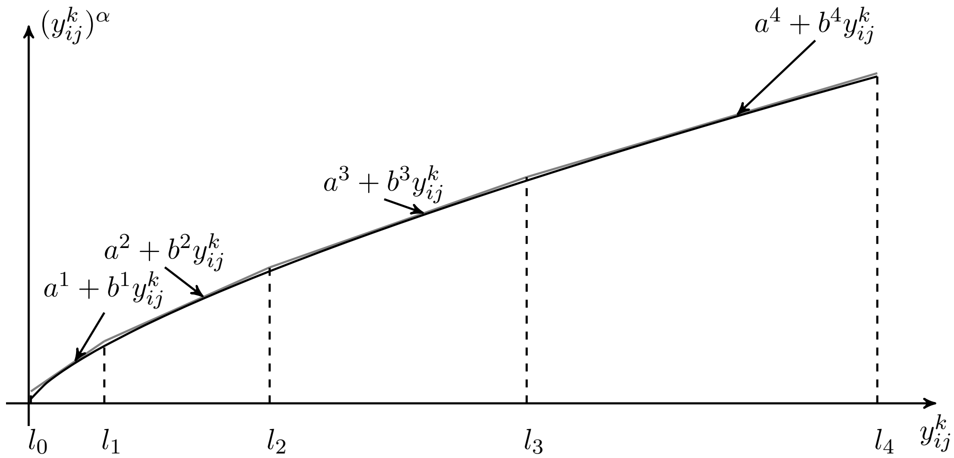


Figure 5.1: Piecewise Linear Approximation Functions

Given a set of routes $\mathcal{SR} = \{\sigma^1, \sigma^2, \cdots, \sigma^{|S|}\}$, and considering that all routes are independents, the total routing risk for this set is computed as:

$$R(\mathcal{SR}) = TTAR^k \times P_{release} \times \beta \times \sum_{r \in S} \sum_{i=2}^{|\sigma^r|} \left(a^m_{(\sigma^r_{i-1}\ \sigma^r_i)} + \left(\sum_{j=i}^{|\sigma^r|} q_{\sigma^r_i} \right) b^m_{(\sigma^r_{i-1}\ \sigma^r_i)} \right) \rho_{\sigma^r_{i-1}\sigma^r_i} \tag{5.6}$$

Where the value of $(y^k_{(\sigma^r_{i-1}\ \sigma^r_i)})^\alpha = \left(\sum_{j=i}^{|\sigma^r|} q_{\sigma^r_i} \right)$ is approximated by the appropriated linear function $a^m_{(\sigma^r_{i-1}\ \sigma^r_i)} + y^k_{(\sigma^r_{i-1}\ \sigma^r_i)} b^m_{(\sigma^r_{i-1}\ \sigma^r_i)}$ defined over the range $l_{m-1} \le y^k_{(\sigma^r_{i-1}\ \sigma^r_i)} \le l_m$.

5.3 Solution method

An implementation of the general version of Variable Neighborhood Search (VNS) is used to solve the problem of HFVRP in HazMat distribution (Hansen and Mladenović (2014)). It integrates a Variable Neighborhood Descent (VND) algorithm for local search, and a perturbation mechanism (shaking neighborhoods). Additionally, a post-optimization procedure is applied in order to improve the quality of the solution.

In the following, a description of the VNS algorithm components is given.

5.3.1 Initial Solution s_0

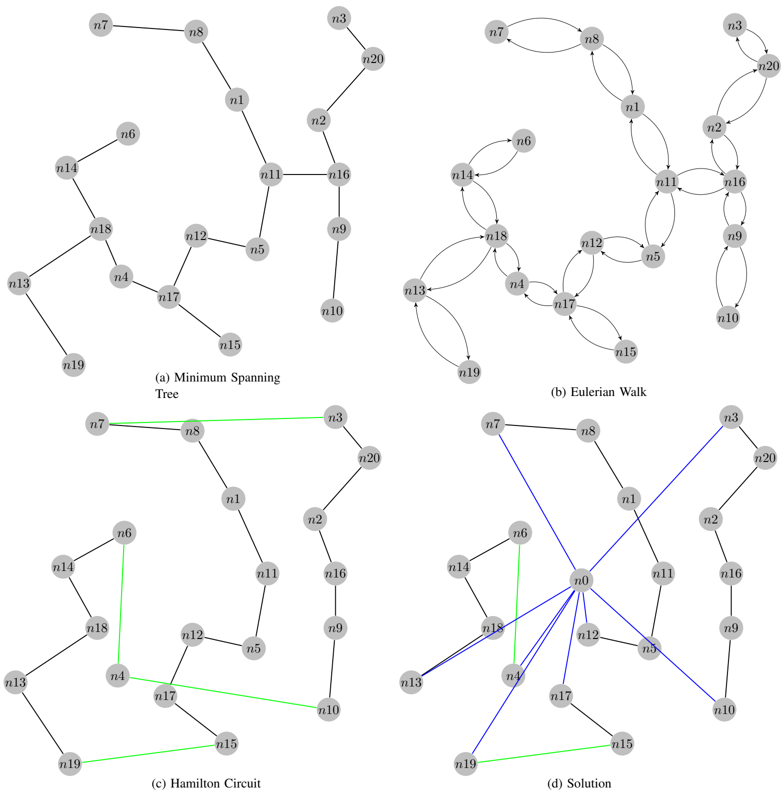
In order to construct an initial solution for the FSMVRP instances first, a minimum weight spanning tree algorithm (Papadimitriou and Steiglitz (1998)) is used.

- Find the minimum spanning tree (MST) T under the *risk measure* (the product of ρ_{ij} and q_j) between nodes.
- Create a multi-graph G by using two copies of each edge of T in order to construct an Eulerian walk.
- Find an Eulerian walk of G and an embedded tour starting for a node with degree 1 in T.

In the part (a) of Fig. 5.2 an example of a MST for 20 nodes instance is shown. In this graph the set of nodes with degree 1 is $\{3, 6, 7, 10, 15, 19\}$. The Eulerian walk is shown in the part (b). For obtaining the initial solution, the initial node (a node with degree 1 in the MST graph) of the Eulerian walk is selected (node 7 in the Fig. 2) and a Hamiltonian circuit is constructed in part (c), then a random splitting is performed as explained next. A truck type is selected at random and it starts from the first node of the Hamiltonian circuit. The route is built, following the circuit adding nodes until the truck is full. The principle is repeated starting from the next node in the Hamiltonian circuit until all nodes have been included in a route, part (d).

Given that the number of nodes with degree 1 in MST T is greater than one, there are different nodes that can be selected as the initial node for constructing the Hamiltonian circuit. This gives the opportunity to have multiple initial solutions for the same instance to begin the VNS. Let n_1 be the number of nodes that has a degree equal to 1 in T. Every time the VNS algorithm is executed a new Hamiltonian circuit is created starting from a different node from T with a degree equal to one. The previous does not imply that the n_1 Hamiltonian circuits are different of each other, but, the initial solutions can be different between them given the random split.

For generating the initial solution of the HVRP instances, first, a set of random selected nodes are fixed as seed nodes, and then, one available truck is assigned to each of them at random. The remaining nodes are assigned using a single source



(a) Minimum Spanning Tree

(b) Eulerian Walk

(c) Hamilton Circuit

(d) Solution

Figure 5.2: Construction of Initial Solution

transportation heuristic (Nagelhout and Thompson (1980)). For this purpose, the *risk measure* is used as the cost of supplying a customer node from source node (truck) rather than use the distance between them. As the initial seed nodes selection is random, multiple initial solutions can be created. The number of the initial solutions is defined as a percentage γ of the number of instance nodes, $n_1 = \gamma|\mathcal{N}|$.

5.3.2 Basic moves

To perform the shaking neighborhoods and the local search neighborhoods of the VNS algorithm, three basic operators are used: split, reverse and joint.

- ***Split***: A route $\sigma^r = \{\sigma_1^r, \ldots, \sigma_{|\sigma^r|}^r\}$ is divided in two routes $\sigma^{r_1} = \{\sigma_1^r, \ldots, \sigma_i^r\}$ and $\sigma^{r_2} = \{\sigma_{i+1}^r, \ldots, \sigma_{|\sigma^r|}^r\}$.
- ***Reverse***: A route $\sigma^r = \{\sigma_1^r, \ldots, \sigma_{|\sigma^r|}^r\}$ is reversed $(\sigma^r)^T = \{\sigma_{|\sigma^r|}^r, \ldots, \sigma_1^r\}$.

- ***Joint***: Two sub-routes $\sigma^r = \{\sigma_1^r, \cdots, \sigma_{|\sigma^r|}^r\}$ and $\sigma^t = \{\sigma_1^t, \ldots, \sigma_{|\sigma^t|}^t\}$ are merged into a single route $(\sigma^t \oplus \sigma^r) = \{\sigma_1^t, \ldots, \sigma_{|\sigma^t|}^t, \sigma_1^r, \cdots, \sigma_{|\sigma^r|}^r\}$

For evaluating in an efficient way the new route resulting from the operators, the route risk $R(\sigma^r)$ is computed as shown in the Fig. 5.3. It starts from the last node of a route going backwards until the first node which correspond to the depot in a feasible route. The load from the last customer in a route to the depot is considered zero (0).

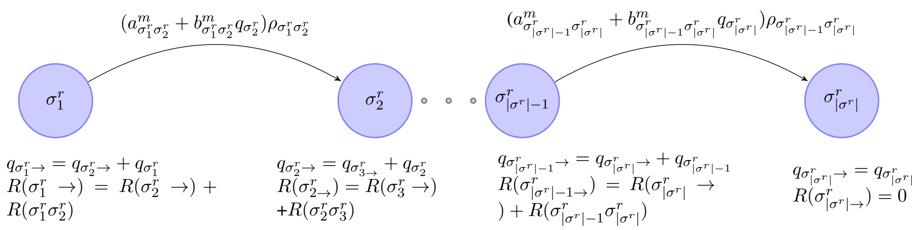


Figure 5.3: Route Risk Evaluation

Auxiliary data or preprocessing information, displayed under the nodes and over the arcs in the Fig. 3, is also recorded:

- $R(\sigma^r_{i\rightarrow})$, the cumulative risk for the path going from σ_i^r to $\sigma^r_{|\sigma^r|}$.

$$R(\sigma^r_{i\rightarrow}) = R\left(\{\sigma_i^r, \sigma_{i+1}^r, \ldots, \sigma^r_{|\sigma^r|}\}\right) = \sum_{i=2}^{|\sigma^r|} R(\sigma^r_{i-1}\sigma^r_i)$$

  $R(\sigma^r) = R(\sigma^r_{1\rightarrow})$

- $q_{\sigma^r_{i\rightarrow}}$, the cumulative demand for the path going from σ_i^r to $\sigma^r_{|\sigma^r|}$.

$$q_{\sigma^r_{i\rightarrow}} = \sum_{j=i}^{|\sigma^r|} q_{\sigma^r_j}$$

- The linear function m, the values of its parameters $a^m_{\sigma_i^r\sigma_j^r}$,$b^m_{\sigma_i^r\sigma_j^r}$, and the value of $\rho_{\sigma_i^r\sigma_j^r}$ parameter (Equation 6.11).

The auxiliary data above mentioned is also computed for the reverse route $(\sigma^r)^T = \{\sigma^r_{|\sigma^r|}, \ldots, \sigma^r_1\}$. Regarding the joint of two routes and defining $\sigma^t_{|\sigma^t|} = w$ and $\sigma^r_1 = u$ the risk of the route $(\sigma^t \oplus \sigma^r)$ is computed as:

$$
\begin{aligned}
R(\sigma^t \oplus \sigma^r) \quad & = TTAR^k \times P_{release} \times \beta \times \Big(\Gamma(\sigma^t) + \Gamma(\sigma^r) + \\
& (a^m_{wu} + b^m_{wu} q_{\sigma^r})\rho^k_{wu} + \\
& \sum_{i=2}^{|\sigma^t|} (a'^m_{\sigma^t_{i-1}\sigma^t_i} - a^m_{\sigma^t_{i-1}\sigma^t_i})\rho^k_{\sigma^t_{i-1}\sigma^t_i} + \\
& \sum_{i=2}^{|\sigma^t|} (b'^m_{\sigma^t_{i-1}\sigma^t_i} - b^m_{\sigma^t_{i-1}\sigma^t_i})\rho^k_{\sigma^t_{i-1}\sigma^t_i} \left(\sum_{j=i}^{|\sigma^t|} q_{\sigma^t_i}\right) + \\
& q_{\sigma^r} \sum_{i=2}^{|\sigma^t|} b'^m_{\sigma^t_{i-1}\sigma^t_i} \rho^k_{\sigma^t_{i-1}\sigma^t_i} \Big)
\end{aligned}
\tag{5.7}
$$

where

$$
\Gamma(\sigma^r) = \sum_{r\in S} \sum_{i=2}^{|\sigma^r|} \left(a^m_{(\sigma^r_{i-1}\ \sigma^r_i)} + \left(\sum_{j=i}^{|\sigma^r|} q_{\sigma^r_i} \right) b^m_{(\sigma^r_{i-1}\ \sigma^r_i)} \right) \rho_{\sigma^r_{i-1}\sigma^r_i}
$$

and $a^m_{\sigma^t_{i-1}\sigma^t_i}$, $b^m_{\sigma^t_{i-1}\sigma^t_i}$, $a'^m_{\sigma^t_{i-1}\sigma^t_i}$, and $b'^m_{\sigma^t_{i-1}\sigma^t_i}$ are the parameters of the appropriated linear functions for approximating the value of $y^\alpha_{\sigma^t_{i-1}\sigma^t_i}$ and $y^\alpha_{(\sigma^t\oplus\sigma^r)_{i-1}(\sigma^t\oplus\sigma^r)_i}$ respectively. The values $a^{m'}_{\sigma^t_{i-1}\sigma^t_i}$ and $b'^m_{\sigma^t_{i-1}\sigma^t_i}$ depend on the value of q_{σ^r}. While the truck load remains unaltered in all the arcs of σ_r, the load on all the arc belonging route σ_t is increased by a quantity equal to q_{σ^r}. The computation of the values $a'^m_{\sigma^t_{i-1}\sigma^t_i}$ and $b'^m_{\sigma^t_{i-1}\sigma^t_i}$ makes it difficult to assess the exact value of risk for the merged route.

The exact risk value of the new route is obtained when:

- $q_{\sigma^r} \leq min\ quantity\ value$ then $a^{m'}_{\sigma^t_{i-1}\sigma^t_i} = a^m_{\sigma^t_{i-1}\sigma^t_i}$, and $b'^m_{\sigma^t_{i-1}\sigma^t_i} = b^m_{\sigma^t_{i-1}\sigma^t_i}$
- $q_{\sigma^r} \geq max\ quantity\ value$ then all the values of $a'^m_{\sigma^t_{i-1}\sigma^t_i}$ and $b'^m_{\sigma^t_{i-1}\sigma^t_i}$ change to the highest possible m.

Additional preprocessing information is needed for computing the exact risk value for a route σ^r and the reverse route$(\sigma^r)^T$. This information makes it possible to calculate the risk when q_{σ^r} is less than $min\ quantity\ value$ or q_{σ^r} is greater than $max\ quantity\ value$. A computation procedure of all the $min\ quantity\ value$ and $max\ quantity\ value$ for each node is implemented. In other cases a linear interpolation approximation is used between the value of the last three terms of the Eq. (5.7) when q_{σ^r} is equal $min\ quantity\ value$, or when q_{σ^r} is equal $max\ quantity\ value$. The exact and approximate risk value is determined in constant time. This procedure is performed in time proportional to $O(|\sigma^r|)$. Let

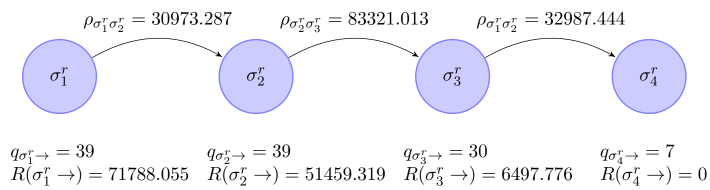


Figure 5.4: Risk Route Computation Example

us illustrate with a simple example how to compute each node values. Given the route and some of the node values shown in Fig. 5.4.

Let us assume that for this sub-route the capacity of the truck is 120.0. The maximum quantity that can be added at the end of the route is 81.0. Let $[0, 400]$ be the bounded interval for y_{ij}^k, this interval is divided into a sequence of 4 segments $\{l_0 = 1, l_1 = 36, l_2 = 114, l_3 = 235, l_4 = 400\}$. The value of $(y_{ij}^k)^\alpha$ is then approximated by using linear interpolations over the 4 segments according to Eq. (5.5).

For the arc (σ_1^r, σ_2^r) the segment $\{l_1 = 36, l_2 = 114\}$ is used for approximating the value of $(y_{ij}^k)^\alpha$, for the arcs (σ_2^r, σ_3^r) and (σ_3^r, σ_4^r) the segment $\{l_0 = 1, l_1 = 36\}$. If a quantity superior or equal to 75 is added to the arc (σ_1^r, σ_2^r) the segment $\{l_2 = 114, l_3 = 235\}$ has to be used. In the case of the arcs (σ_2^r, σ_3^r) and (σ_3^r, σ_4^r), if a quantity superior or equal to 6 and 29 is added respectively, the segment $\{l_1 = 36, l_2 = 114\}$ has to be used. If a quantity between 75 and 81 is added all the linear functions will change. This means that the value of $min\ quantity\ value$ is 5, and the value of $max\ quantity\ value$ is 75. If the value of the added quantity falls between the $min\ quantity\ value$ and the $max\ quantity\ value$ the linear interpolation is used.

5.3.3 Perturbation mechanism

The perturbation mechanism adopted consists in selecting at random a shaking neighborhood from the set of neighborhood structures N_K, for $k = 1, \cdots, n_k$ and applying it on the search solution x_{search}. At the beginning x_{search} is equal to the initial solution, x_0. Two shaking neighborhoods ($n_k = 2$) are defined: best split of a random route (Split move), and best re-insertion of a node σ_l^t from a random selected route σ^t to another route σ^r (Shift(1,0) move). These two moves are explained in the subsection 5.3.4. In each iteration of VNS main cycle one of the shaking neighborhood is selected and the current x_{search} is perturbed. This procedure is carried out while the stopping criterion is not meeting, the number of consecutive perturbations without any improvement of the incumbent solution ($n_{updates}$) is less than a fixed value ($maxUpdateNumber$).

5.3.4 Local search heuristic

The VND procedure utilizes a fixed neighborhood ordering. The neighborhoods are ordered according to the number of feasible candidate solutions that can be reached from a given a search solution. Six VRP neighborhood structures N_l, for $l = 1, \cdots, n_l,\ n_l = 6$, involving inter-route moves are employed (Vidal et al. (2013)). They are described in the utilization order:

- **Concatenation:** Two routes σ^r and σ^t are merged into a single route.
- **Swap(1,1):** permutation between a customer σ^r_k from a route σ^r and a customer σ^t_l, from a route σ^t.
- **Inter route 2-opt:** deletion of an arc $(\sigma^r_k, \sigma^r_{k+1})$ from a route σ^r and an arc $(\sigma^t_l, \sigma^t_{l+1})$ from a route σ^t and addition of arcs $(\sigma^r_k, \sigma^t_{l+1})$ and $(\sigma^t_l, \sigma^r_{k+1})$.
- **Shift(2,0):** two nodes σ^t_l and σ^t_{l+1} is transferred from a route σ^t to a route σ^r.
- **Shift(1,0):** a node σ^t_l is transferred from a route σ^t to a route σ^r.
- **Split:** a route σ^r is divided in two smaller routes $\sigma^{r'}$ and $\sigma^{r''}$ from the node σ^r_k.

Generating candidate solutions resulting from neighborhood structures is done by combining the basic move explained in the subsection 5.3.2. Given two routes $\sigma^r = \{\sigma^r_1, \sigma^r_2, \ldots, \sigma^r_{|\sigma^r|}\}$ and $\sigma^t = \{\sigma^t_1, \sigma^t_2, \ldots, \sigma^t_{|\sigma^r|}\}$, the moves of the six employed neighborhood are described next in terms of the basic move utilized:

- **Concatenation**: $\{\sigma^r \oplus \sigma^t\}$, $\{(\sigma^r)^T \oplus \sigma^t\}$, $\{\sigma^r \oplus (\sigma^t)^T\}$, $\{(\sigma^r)^T \oplus (\sigma^t)^T\}$
- **Swap(1,1)** $\{\sigma^r_1, \ldots, \sigma^r_{k-1}\} \oplus \sigma^t_l \oplus \{\sigma^r_{k+1}, \ldots, \sigma^r_{|\sigma^r|}\}$ and $\{\sigma^t_1, \ldots, \sigma^t_{l-1}\} \oplus \sigma^r_k \oplus \{\sigma^t_{l+1}, \ldots, \sigma^t_{|\sigma^t|}\}$
- **Inter route 2-opt** $\{\sigma^r_1, \ldots, \sigma^r_k\} \oplus \{\sigma^t_{l+1}, \ldots, \sigma^t_{|\sigma^t|}\}$ and $\{\sigma^t_1, \ldots, \sigma^t_l\} \oplus \{\sigma^r_{k+1}, \ldots, \sigma^r_{|\sigma^r|}\}$, $(\{\sigma^r_1, \ldots, \sigma^r_k\})^T \oplus (\{\sigma^t_{l+1}, \ldots, \sigma^t_{|\sigma^t|}\})^T$ and $(\{\sigma^t_1, \ldots, \sigma^t_l\})^T \oplus (\{\sigma^r_{k+1}, \ldots, \sigma^r_{|\sigma^r|}\})^T$
- **Shift(2,0)** $\{\sigma^r_1, \ldots, \sigma^r_{k-1}\} \oplus \{\sigma^t_l, \sigma^t_{l+1}\} \oplus \{\sigma^r_k, \ldots, \sigma^r_{|\sigma^r|}\}$ and $\sigma^{t'} = \{\sigma^t_1, \ldots, \sigma^t_{l-1}\} \oplus \{\sigma^t_{l+2}, \ldots, \sigma^t_{|\sigma^t|}\}$

- **Shift(1,0)** $\sigma^{r'} = \{\sigma^r_1, \ldots, \sigma^r_{k-1}\} \oplus \{\sigma^t_l\} \oplus \{\sigma^r_k, \ldots, \sigma^r_{|\sigma^r|}\}$ and $\sigma^{t'} = \{\sigma^t_1, \ldots, \sigma^t_{l-1}\} \oplus \{\sigma^t_{l+1}, \ldots, \sigma^t_{|\sigma^t|}\}$

- **Split** $\{\sigma^r_1, \ldots, \sigma^r_k\} \oplus \sigma_0$ and $\sigma_0 \oplus \{\sigma^r_{k+1}, \ldots, \sigma^r_{|\sigma^r|}\}$, $(\{\sigma^r_1, \ldots, \sigma^r_k\})^T \oplus \sigma_0$ and $\sigma_0 \oplus \{\sigma^r_{k+1}, \ldots, \sigma^r_{|\sigma^r|}\}$,
  $\{\sigma^r_1, \ldots, \sigma^r_k\} \oplus \sigma_0$ and $\sigma_0 \oplus (\{\sigma^r_{k+1}, \ldots, \sigma^r_{|\sigma^r|}\})^T$,
  $(\{\sigma^r_1, \ldots, \sigma^r_k\})^T \oplus \sigma_0$ and $\sigma_0 \oplus (\{\sigma^r_{k+1}, \ldots, \sigma^r_{|\sigma^r|}\})^T$

The best improvement strategy is considered. A move is accepted if it does not deteriorate the local solution more than a threshold value defined by the maximum deterioration of the function in percentage ($det.\_per.$), because in the candidate evaluation procedure an estimation (linear interpolation) of the expected routing risk is sometimes computed as explained in subsection 5.3.2. While the estimate candidate solution risk value is greater than the current solution value, the evaluation of the exact risk value could be less and the move is applied. Only feasible solutions are accepted. Whenever a given neighborhood is not able to improve the local solution, $Local\ Best$, the VND continues with next neighborhood in the list. If the current neighborhood improve the $Local\ Best$ the local search restarts with the first neighborhood structure in N_l.

In Algorithm 6 is shown the structure of the VND. The ordered neighborhoods sequence N_K, for $k = 1, \cdots, n_k$ is called on x' in order to find a new search point x'' leading to an improving local solution (lines $4 - 17$).

5.3.5 Intra-route improvement

At the end of the VND algorithm two intra-route moves are used to improve the routes of the local solution x': $2 - opt$, two nonadjacent arcs are deleted and another two are added, and $node\ exchange$, route position permutation between two customer nodes. These two moves are applied one after the other before making a decision about updating the current search point x_{search}. If the risk value of the improved local solution is less than the risk value of x_{search}, the last one is replace by the former one and the value of $n_{updates}$ is reset to zero, otherwise $n_{updates}$ is incremented by one. The $det.\_perc.$ value is updated after every VND iteration, $det.\_perc. = det.\_perc.(1 - \delta)$ with $0 < \delta < 1$.

5.3.6 Post-optimization

Every time the VND algorithm finds a new local solution (different total routing risk) the routes of the solution are added to a pool $\mathcal{SR}_{SP}$ (line 11 VND algorithm).

Algorithm 6 Local search. $VND\ algorithm(x', det.\_per., \mathcal{SR}_{SP})$

Define the ordered set of neighborhood structures N_l, for $l = 1, \cdots, n_l$
$Local\ Best \leftarrow R(x')$
$l \leftarrow 1$
while $l <= n_l$ **do**
  Select de $N_l[i]$ neighborhood from ordered list.
  Find the best neighbor x'' of $x' \in N_l[i](x', det.\_per.)$
  if $R(x'') < Local\ Best$ **then**
    $Local\ Best \leftarrow R(x'')$
    $x^{'} \leftarrow x''$
    for $\sigma^r \in x'$ **do**
      $\mathcal{SR}_{SP} \leftarrow \mathcal{SR}_{SP} \cup \sigma^r$
    end for
    $l \leftarrow 1$
  else
    $l \leftarrow (l + 1)$
  end if
end while
Return x' and $\mathcal{SR}_{SP}$

At the end of the VNS algorithm, a Set Partitioning (SP) model is solved to find the best combination of routes that minimizes the risk. Let x_{σ^r} be a binary variable taking 1 if the route σ^r is in the optimal solution and $R(\sigma^r)$ the risk function, the SP formulation for the HFVRP can be expressed as follows (Subramanian et al. (2012)):

$$\min \sum_{\sigma^r \in \mathcal{SR}_{SP}} R(\sigma^r) x_{\sigma^r} \tag{5.8}$$

subject to:

$$\sum_{\sigma^r \in \mathcal{SR}_{SP(i)}} x_{\sigma^r} = 1 \; \forall i \in \mathcal{C} \tag{5.9}$$

$$\sum_{\sigma^r \in \mathcal{SR}_{SP(k)}} x_{\sigma^r} \leq a_k \; \forall k \in \mathcal{K} \tag{5.10}$$

$$x_{\sigma^r} \in \{0,1\} \forall \sigma^r \in \mathcal{SR}_{SP} \tag{5.11}$$

$\mathcal{SR}_{SP(i)} \subseteq \mathcal{SR}_{SP}$ is the subset of routes that contain customer i. And $\mathcal{SR}_{SP(k)} \subseteq \mathcal{SR}_{SP}$ is the set of routes that utilizes a k truck type, $k \in \mathcal{K}$. Equation 5.8 expresses objective function for minimizing the routing risk. Constraints 5.9 ensures that each customer is visited exactly once. Constraints 5.10 are limits on the fleet composition. The problem is given to the linear programming solver.

5.3.7 Algorithm structure

The multi-start VNS algorithm is shown in the Algorithm 7. First, the neighborhood structure for the incumbent perturbation (N_k, for $k = 1, \cdots, n_k$) is defined (line 1). In every restart i of the algorithm an initial solution x_0 is generated (line 5) according to the procedure explained in Subsection 5.3.1. The VNS iterates while $n_{updates} < maxUpdateNumber$. To do so, first the perturbation or shaking move of the current search solution x_{search} is performed by selecting at random a neighborhood N_K (lines 10). Then a local search is carried out through the VND algorithm (line 11). Three different parameters control the performance of the VNS algorithm: the maximum deterioration of the function in percentage $det.\_per.$ (Subsection 5.3.4), the deterioration percentage ($det.\_per.$) update rate δ, and the maximum number of updates ($maxUpdateNumber$). $\mathcal{SR}_{SP}$, the set of routes that is used in the post-optimization part is an empty set at the beginning (line 3), and it is filled with new solutions found in the local search (VND algorithm).

Still on the VNS description, at the end of each VND run, two intra route moves are used for improving the local solution x', $node\ exchange$ and $2-Opt$

(line 12). Next, the $det.\_per.$, $maxUpdateNumber$, and the x_{search} are updated (lines $13 - 20$).

Finally a post-optimization procedure is undertaken (line 22) (Subsection 5.3.6) using Mixed Integer Linear Programming (MILP) formulation as input and a MILP solver as optimization problem solving tool.

Algorithm 7 Steps of the Multi-Start VNS Algorithm plus SP

1: Define the ordered set of neighborhood structures N_K, for $k = 1, \cdots, n_k$;
2: set the value of $det.\_per.$, δ, and $maxUpdateNumber$
3: $\mathcal{SR}_{SP} \leftarrow \{\}$
4: **for** $i \in \{1, \ldots, n_1\}$ **do**
5:     Generate an initial solution x_0
6:     $x_{search} \leftarrow x_0$
7:     $Global\ Best \leftarrow R(x_{search})$
8:     $n_{updates} \leftarrow 0$
9:     **while** $n_{updates} < maxUpdateNumber$ **do**
10:         Find a random neighbor x' of $x_{search} \in N_k[i](x_{search})$
11:         Local search by VND, $(x', \mathcal{SR}_{SP}) \leftarrow VND(x', det.\_per., \mathcal{SR}_{SP})$
12:         $Intra\ Route\ Improvement(x')$
13:         $det.\_per. \leftarrow det.\_per.(1 - \delta)$
14:         **if** $R(x') < Global\ Best$ **then**
15:             $Global\ Best \leftarrow R(x')$,
16:             $x_{search} \leftarrow x'$
17:             $n_{updates} \leftarrow 0$
18:         **else**
19:             $n_{updates} \leftarrow n_{updates} + 1$
20:         **end if**
21:     **end while**
22:     $x^{**} \leftarrow$ Solve SP over $\mathcal{SR}_{SP}$
23:     Return the best found solution x^{**}
24: **end for**

5.4 Experiments and results

The algorithm was coded in Java JDK 8.0 using NetBeans 8.1 and executed in an Intel Core i7 Processor 2.93 GHz with 8 GB of RAM running Windows 10. The SP is solved with Gurobi 6.0.

In the tables presented hereafter, Inst. denotes the test-instance, n denotes the number of customers of the test-instance. Sol. represents the best incumbent solution found using the MILP formulation. Avg. Sol. and Time indicate, respectively, the average solution and the average computational time associated to the correspondent problem instance of the 10 runs. Best Sol., Avg. Sol., and Stand. Dev. represents the best solution, the average solution and the standard deviation of the 10 runs. Avg. gap denotes the on average gap in percentage between the best solution found by VNS+SP algorithm and the best incumbent in MILP. Time Rel. is the relationship between the average time of SP post optimization and the average time of the multi-start VNS part.

The value of $det.\_per.$ is fixed at 0.25 after making experimentations using values of 0.0, 0.25, and 0.5. The percentage of the number of instance nodes used for the multiple starting for HVRP instances is set at 50%. The value of δ is fixed at 0.1. The maximum number of consecutive perturbations allowed without any improvement of VND is fixed at 10.

The risk is expressed in 10^{-6}. It could be interpreted as the expected population exposure resulting from an accident related to the HazMat transportation every one million times the set of routes in the solution is used. It is assumed that each individual in the affected population will incur the same risk.

5.4.1 Problem instances

The algorithm is tested on two set of instances based on the ones presented by Golden et al. (1984) and Taillard (1999). Both set were modified according Bula et al. (2016) to include the risk parameters

5.4.2 Results for FSMVRP instances

In Table 5.1 a comparison is performed between the results found by the multi-start VNS algorithm plus SP post-optimization and the best result found using the MILP formulation for the FSMVRP instances, unlimited fleet.

The VNS algorithm is capable of finding the optimal solutions for the first 4 instances but much faster than MILP. For the following 8 instances, the MILP formulation computational time is limited to 3600 seconds and the best integer solution and the lower bound are registered. VNS finds a better solution than MILP in 21.7 s on average. The average rate of standard deviation over the 10 runs is less than 0.01% for all 12 instances, which shows that VNS is very stable.

Table 5.1: Results for FSMVRP instances using multi-start VNS + SP algorithm.

		MILP*			MS VNS + SP Algorithm			
Inst.	n	Sol.	Lower Bound	Time (s)	Avg. Sol.	Best Sol.	Avg. gap (%)	Time (s)
3	20	156.82	⋆	17	156.82	156.82	0	0.86
4	20	168.24	⋆	68	168.24	168.24	0	0.62
5	20	251.84	⋆	133	251.84	251.84	0	0.5
6	20	196.8	⋆	1839	196.8	196.8	0	0.56
13	50	383.03	327.35	3600	380.44	380.44	-0.68	7.79
14	50	345.21	266.06	3600	344.57	344.57	-0.18	5.83
15	50	349.28	303.28	3600	347.71	347.71	-0.45	12.91
16	50	401.74	400.17	3600	399.43	399.42	-0.58	10.2
17	75	636.89	521.86	3600	620.02	620.02	-2.65	29.79
18	75	527.22	322.81	3600	508.06	508.06	-3.63	26.24
19	100	749.15	494.88	3600	746.71	746.66	-0.33	72.84
20	100	775.74	559.69	3600	706.44	705.26	-8.93	92.16
Avg.				2571.42			-1.45	21.69

∗Optimal solution or best solution after 3600 s. ⋆ Optimal solution

5.4.3 Results for HVRP instances

In Table 5.2 the results found by multi-start VNS + SP algorithm for the instances with limited fleet, HVRP, are shown.

Table 5.2: Results for HVRP instances using multi-start VNS+SP algorithm.

		MS VNS + SP Algorithm			
Inst	n	Avg. Sol.	Best Sol.	Stand Dev.	Time (s)
13	50	589.84	566.73	13.91	8.91
14	50	493.34	486.13	6.59	18.04
15	50	538.46	513.75	12.29	21.64
16	50	622.26	601.08	14.38	20.41
17	75	1123.79	1068.99	30.42	138.36
18	75	1065.3	983.1	38.61	118.49
19	100	1006.09	987.12	10.98	249.49
20	100	1057.3	1023.26	18.21	1473.69

The computational time for the last two instances has an important increase compare to the unlimited fleet instances. The average rate of standard deviation is 2.2% over the 10 runs, showing that the instances are more difficult to solve than FSMVRP. However, the stability remains good.

5.4.4 Impact of set partitioning

The different elements of VNS algorithm have a different contribution to the performance. Table 5.3 shows the contribution in terms of computing time and solution cost of the multi-start VNS algorithm and the SP post-optimization part.

Table 5.3: Performance evaluation of VNS-SP.

Inst.	FSMVRP			HVRP		
	Risk	SP		Risk	SP	
	Avg. gap (%) VNS+SP vs VNS	Avg. Time (s)	Time Rel. SP/VNS	Avg. gap (%) VNS+SP vs VNS	Avg. Time (s)	Time Rel. SP/VNS
3	0	0.06	0.07	0	0	0
4	0	0.04	0.08	0	0	0
5	-0.02	0.02	0.05	0	0	0
6	-0.03	0.02	0.03	0	0	0
13	0	0.23	0.03	-7.3	0.44	0.05
14	0	0.22	0.04	-0.51	0.48	0.03
15	-0.01	0.3	0.02	-2.77	1.89	0.1
16	-0.15	0.4	0.04	-3.2	1.75	0.09
17	-0.01	0.88	0.03	-0.03	39.66	0.4
18	0	0.86	0.03	-1.24	7.06	0.06
19	-0.22	1.52	0.02	-0.45	10.12	0.04
20	-1.36	1.78	0.02	-0.18	1231.73	0.84
Avg.	-0.15	0.53	0.04	-1.96	161.64	0.73

Except for the last instance of HVRP, there is not a significant increment in the computational time when adding the SP post-optimization procedure. However, adding this part to the multi-start VNS algorithm improves the average value of the risk function in 1.96% for the HVRP instances. In the case of the unlimited fleet the contribution of SP is not significant but it provides some improvements. In both versions, unlimited fleet and limited fleet, of the instance 20, the time required to solve the SP problem has an important increment.

5.5 Conclusions

5.5.1 Conclusions (English)

Heterogeneous Fleet Vehicle Routing Problem (HFVRP) arises in practical applications when transporting Hazardous Materials (HazMat). Two HFVRP variants involving limited and unlimited fleet and minimization of routing risk were considered. These variants are solved by a hybrid algorithm based on a Multi Start

Variable Neighborhood Search (VNS) metaheuristic. This algorithm uses Variable Neighborhood Descent (VND) in the local search phase and Set Partitioning (SP) formulation in a post optimization stage.

The proposed hybrid algorithm (Multi Start VNS + SP) is tested in 20 benchmark instances with up to 100 customers. The results are compared with those obtained by a Mixed Integer Linear Programming (MILP) formulation with a time limit of 3600 seconds. Multi start VNS + SP finds either the optimal solution (when MILP can prove the optimally) or a better solution.

Given the multi-objective nature of HazMat transportation problem, the study of algorithms for solving this HVRP variant including cost and risk minimization is a promising aspect of future research.

5.5.2 Conclusions (Français)

Le problème de tournées de véhicules à flotte hétérogène (HFVRP) se pose dans des applications pratiques lors du transport de substances dangereuses (HazMat). Deux variantes HFVRP impliquant une flotte limitée et illimitée et une minimisation du risque d'acheminement ont été considérées. Ces variantes sont résolues par un algorithme hybride basé sur une méta-heuristique VNS (Multi Start Variable Neighborhood Search), dont la structure est donnée dans l'Algorithme 7. Cet algorithme utilise la VND (Variable Neighbourhood Descent) dans la phase de recherche locale et une formulation de type Set Partitioning (SP) dans une étape de post-optimisation.

Algorithme 7. Étapes de l'algorithme VNS Multi-Start plus SP

Définir l'ensemble des structures de voisinage ordonnées N_K, for $k = 1, \cdots, n_k$;
Définir la valeur de $det.\_per.$, δ, and $maxUpdateNumber$
$\mathcal{SR}_{SP} \leftarrow \{\}$
for $i \in \{1, \ldots, n_1\}$ **do**
    Générer une solution initiale x_0
    $x_{search} \leftarrow x_0$
    $Global\ Best \leftarrow R(x_{search})$
    $n_{updates} \leftarrow 0$
    while $n_{updates} < maxUpdateNumber$ **do**
        Trouver un voisin aléatoire x' of $x_{search} \in N_k[i](x_{search})$
        Recherche locale VND, $(x', \mathcal{SR}_{SP}) \leftarrow VND(x', det.\_per., \mathcal{SR}_{SP})$
        $Intra\ Route\ Improvement(x')$
        $det.\_per. \leftarrow det.\_per.(1 - \delta)$

if $R(x') < Global\ Best$ **then**
$Global\ Best \leftarrow R(x')$,
$x_{search} \leftarrow x'$
$n_{updates} \leftarrow 0$
else
$n_{updates} \leftarrow n_{updates} + 1$
end if
end while
$x^{**} \leftarrow$ Résoudre le problème SP sur $\mathcal{SR}_{SP}$
Retourner la meilleure solution trouvée x^{**}
end for

L'algorithme hybride proposé (Multi Start VNS + SP) est testé sur 20 instances de référence ayant jusqu'à 100 clients. Les résultats sont comparés à ceux obtenus avec une formulation de programmation linéaire mixte (MILP) avec une limite de temps de 3600 secondes. Le multi start VNS + SP trouve soit la solution optimale (quand MILP peut prouver l'optimalité) ou une meilleure solution.

Compte tenu de la nature multi-objective du problème de transport de HazMat, l'étude d'algorithmes pour résoudre cette variante HVRP, y compris la minimisation des coûts et des risques, est un aspect prometteur de la recherche future.

5.5.3 Conclusiones (Español)

El problema de ruteo de vehículos con flota heterogénea (HFVRP) surge de aplicaciones prácticas cuando se transportan materiales peligrosos (HazMat). Se consideraron dos variantes de HFVRP, con flota limitada e ilimitada, y la minimización del riesgo de ruteo. Estas dos variantes se resuelven usando un algoritmo híbrido basado en una meta-heurística de búsqueda de vecindad variable (VNS) multi-inicio, la estructura del procedimiento se muestra en el Algoritmo 7. Este algoritmo utiliza el algoritmo de descenso con vecindad variables (VND) en la fase de búsqueda local y la formulación de un problema de partición de conjuntos (SP) en una etapa de post-optimización.

El algoritmo híbrido propuesto (Multi Start VNS + SP) se prueba en 20 instancias de referencia con hasta 100 clientes. Los resultados se comparan con los obtenidos mediante una formulación de programación lineal mixta (MILP) con un límite de tiempo de 3600 segundos. Multi start VNS + SP encuentra la solucin óptima (cuando con el MILP se puede demostrar que es óptima) o una mejor solución.

This work has lead to a journal publication: Variable neighborhood search to solve the vehicle routing problem for hazardous materials transportation. *Journal of Hazardous Materials*. Volume 324, Part B, 15 February 2017, Pages 472-480.

Chapter 6

Bi-objective Vehicle Routing Problem (VRP) for Hazardous Materials (HazMat) Transportation

Abstract (English)

True multi-objective optimization in vehicle routing problem (VRP) for hazardous materials transportation (HazMat) transportation requires in several cases to avoid inappropriate aggregation of other objectives than risk. The objective of this chapter is to present a solution framework for determining a set of routes that minimizes simultaneously two conflicting objectives, the total routing risk, and the total transportation cost. Two different solution approaches, a multi-objective neighborhood dominance-based algorithm and a meta-heuristic ϵ-constraint method, are employed for addressing HazMat routing problems using heterogeneous fleet. The remainder of this chapter is organized as follows. First, the introduction presents a overview of multi-objective optimization solution approaches uses for the multi-objective combinatorial optimization problem here considered. In section 6.2, the bi-objective heterogeneous vehicle routing problem (HVRP) in HazMat transportation problem is introduced, along with a mathematical programming formulation. In section 6.3, a description of the multi-objective neighborhood dominance-based algorithm is given. Section 6.4 presents the meta-heuristic ϵ-constraint method. Section 6.5 shows the results of the computational experiments. Finally, Section 6.6 discusses the conclusions and directions for future research.

Résumé (Français)

Une véritable optimisation multi-objectif dans le problème de tournées des véhicules (VRP) pour le transport de substances dangereuses nécessite dans plusieurs cas d'éviter l'agrégation inappropriée d'autres objectifs que le risque. L'objectif de ce Chapitre est de présenter un cadre de solution pour déterminer un ensemble de tournées qui minimise simultanément deux objectifs contradictoires, le risque total des tours et le coût total de transport. Deux approches de solution différentes, un algorithme multi-objectif basé sur la dominance et la recherche à voisinage et une méthode ϵ-contraint méta-heuristique sont utilisées pour résoudre les problèmes de routage HazMat en utilisant une flotte hétérogène. Le Chapitre est organisée comme suit. L'introduction présente un résumé des approches de solution d'optimisation multi-objectif utilisés pour le problème d'optimisation combinatoire ici considéré. Dans la Section 6.2, le problème bi-objectif des tournées de véhicules hétérogènes (HVRP) dans le problème de transport HazMat est introduit, avec une formulation de programmation mathématique. Dans la section 6.3, une description est donnée pour l'algorithme basé sur la dominance et la recherche à voisinage variable multi-objectif. La section 6.4 présente la méthode méta-heuristique ϵ-contraint. La section 6.5 montre les résultats et des expériences du calcul. La section 6.6 présente les conclusions et les orientations de la recherche future.

Resumen (Español)

Una verdadera optimización multi-objetivo en el problema de ruteo de vehículos (VRP) para el transporte de materiales peligrosos requiere en varios casos evitar la agregación inapropiada de otros objetivos distintos al riesgo. El objetivo de este Capítulo es presentar un marco de solución para determinar un conjunto de rutas que minimiza simultáneamente dos objetivos en conflicto, el riesgo total de ruteo y el costo total de transporte. Se emplean dos enfoques de solución diferentes, un algoritmo multi-objetivo basado en búsqueda en vecindarios y en el concepto de dominancia y un método meta-heurístico ϵ-restringido, para abordar los problemas de ruteo de vehículos en el transporte de materiales peligrosos utilizando una flota heterogénea. El resto de este Capítulo está organizado de la siguiente manera. En primer lugar, en la introducción se presenta una visión general de los enfoques de solución de optimización multi-objetivo usados para el problema de optimización combinatoria aquí considerado. En la Sección 6.2, se presenta el problema de ruteo de vehículos con flota heterogénea bi-objetivo (HVRP) en el transporte de materiales peligrosos, junto con una formulación de programación matemática. En la Sección 6.3, se da una descripción del algoritmo multi-objetivo basado en búsqueda en vecindarios y en dominancia. La Sección 6.4 presenta el

método meta-heurístico ϵ-restringido. La Sección 6.5 muestra los resultados de los experimentos computacionales. Finalmente, en la Sección 6.6 se discute las conclusiones y las direcciones de futuras investigaciones.

6.1 Introduction

As remarked by Androutsopoulos and Zografos (2012), most of research in hazardous materials (HazMat) transportation focuses on selecting the routes of minimum risk. However, since more than 25 years ago authors as List et al. (1991) have pointed out the need of multi-objective models in HazMat routing. HazMat transportation decisions are multi-objective in nature, and they comprise different and sometimes conflicting objectives among different stakeholders as shippers, freight carriers, administrators, customers and residents (Taniguchi et al., 2010). It is important, in addition to the minimization of the risks, to consider other cost functions including economic, social, and environmental aspects associated with the transportation of this type of goods. The objectives in a vehicle routing problem (VRP) can be also multiple, diverse and conflicting with each other (Jozefowiez et al., 2008).

When solving a multi-objective problem two different method approaches can be employed, approximate the Pareto efficient set or the Pareto front without any prior input from a decision maker (generating methods), or to use information from a decision maker as part of the solution process (preference methods). In the first case no-preference methods or a vector optimization (Pareto) approach could be used, and scalarization approaches in the second case. (Rangaiah, 2009).

This part deals with the HazMat transportation problem where a fleet of different type of vehicles (trucks) are used for distributing a single HazMat utilizing a road network traversing population centers. The risk values are considered to vary with the type and load of the trucks, and the size of the neighboring population. The objective is to present solution methods for determining a set of routes that minimizes simultaneously two conflicting objectives, the total routing risk and the total transportation cost. Two different solution approaches based on a neighborhood search algorithm are used for addressing these kind of problems, a multi-objective neighborhood dominance-based algorithm and a meta-heuristic ϵ-constraint method.

6.1.1 Multi-objective based neighborhood search (local search) algorithms

The goal when solving a multi-objective optimization problem is to optimize simultaneously the various objective functions. But, these objectives are often contradictory or conflicting, that means, an improvement in one objective leads to a detriment in other(s) objective(s). A huge number of solutions can be found when solving a multi-objective optimization problem. These solutions will not be optimal, in the sense that they will not optimize all the objectives of the problem, instead, they are trade-off solutions. It is said that $\vec{x}^*$ is globally optimal in **Pareto sense**, if there does not exists any vector $\vec{x}' \in X$, such that $\vec{x}'$ dominates the vector $\vec{x}^*$. Unfortunately, this concept almost gives not a single solution but a set of solutions called **Pareto optimal set** or **Pareto efficient set**. The vectors $\vec{f}(\vec{x}^*)$ corresponding to the solutions include in the Pareto optimal set are called **non-dominated solutions**. The plot of the objective functions whose non-dominated vectors are in the Pareto optimal set is called the **Pareto front**, $\mathcal{PF}$.

Multi-objective meta-heuristics based on *neighborhood search algorithms* (NSA) are extensions of well-known local search meta-heuristics that deal with the notion of non-dominated points, but they require more effort in diversification (Ehrgott and Gandibleux, 2008). In the case of the dominance-based multi-objective local search algorithms are defined by a neighborhood structure and a dominance relation that iteratively improve an archive of non-dominated solutions (Liefooghe et al., 2012). These algorithms are composed of a dominance relation, a solution selection, a neighborhood exploration, an archiving of the Pareto optimal set approximation, and stopping condition.

In NSAs generation relies upon one individual, a current solution x_s, and its neighbors $\{x\} \subseteq N(x_s)$. NSAs methods are good in local converge to the non-dominated frontier, but as Ehrgott and Gandibleux (2008) emphasized that NSAs require more effort in diversification (cover the whole non-dominated front) compare to *evolutionary algorithms* (EA) given their rapid convergence because of the less dispersed search. For covering the Pareto front completely a diversification strategy has to be implemented, that is why multi-objective meta-heuristics are often hybridized.

Not so many methods have been proposed for NSAs.Schaus and Hartert (2013) introduce an extension of large neighborhood search (LNS), called multi-objective LNS (MO-LNS). They use this algorithm to solve some multi-objective combinatorial optimization problems, the multi-objective quadratic assignment problem, the multi-objective binary knapsack, and a bi-objective tank allocation problem. Instead of the unique best-so-far solution in mono-objective optimization, the MO-LNS keeps a best-so-far approximation of the Pareto efficient set in an archive. In

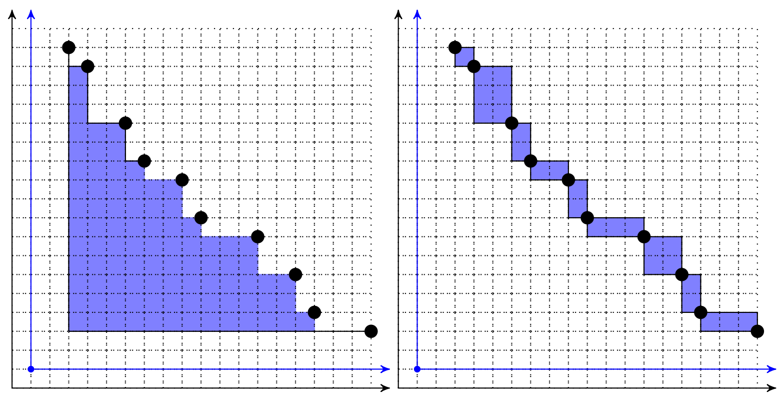


Figure 6.1: The intensification subspace and the diversification subspace

order to achieve the two types of improvements of the archive, diversification and intensification, they use a dynamic change of the filtering behavior of the different objectives. Three different filtering modes are applied during the search: no-filtering, weak-filtering, and strong-filtering, depending on how the upper bound of the objective is taking into account for accepting a new candidate solution. They use the nearest neighbor strategy for the selection of the restarting solution. Each time they select the nearest solution from a random point on the hyperplane formed by the extremities of the archive. Duarte et al. (2015) introduce an adaptation of the Variable Neighborhood Search (VNS) metaheuristic to solve multi-objective combinatorial optimization problems. They use a reduced set of efficient points (with the desired size) as the incumbent solution. To defined wether to change or not the current neighborhood two approximations of the Pareto front are compared, the incumbent solution and the new Pareto front. For the shaking step each element of the current approximation of the Pareto front is perturbed attending to one of the considered objective functions.

In order to have a a good trade-off between the diversification and intensification part required by multi-objective meta-heuristics based on NSAs when considering new candidate solution, both alternatives must be considered, either a contribution to diversify the potential efficient set, or an improvement to existing solutions in the potential efficient set (Schaus and Hartert, 2013). In the first case, it is a solution that neither dominate nor is dominated by any solution in the actual approximation of the Pareto front. In the second case, it consists of a solution that dominates at least one solution in the approximation of the Pareto front (see Figure 6.1).

The aim of intensification, starting from a solution, it is to discover new solutions dominating the starting solution, while the diversification mode attempts to find new non-dominated solutions without necessarily trying to dominate existing ones. Which results, starting from a single point a local search based algorithm is possible to obtain a subset of potential efficient solutions. A decision has to be also made about the size of the output set and which type of strategy applied in the search.

The selection of a solution from which starts the local search have a strong impact on the quality of Pareto set. Clusters of solutions in this set appearing in the objective space have high chances to be reinforced (Schaus and Hartert, 2013), that is why the diversification strategy has a great importance in the multi-objective adaptation of local search algorithms. The local search should not lead to a particular region of the objective space. Finally a stopping criterion has to be defined, in general this criterion depends on a multi-objective algorithm performance metric.

6.1.2 ϵ-constraint approach

ϵ-constraint is *a posteriori* scalarization method where one of the objective functions is optimized, while all the others objective functions are converted into constraints functions and incorporating them in the constraint part of the model.

$$\min f_1(\vec{x}) \tag{6.1}$$

subject to:

$$f_2(\vec{x}) \leq e_1$$
$$\dots$$
$$f_p(\vec{x}) \leq e_{p-1}$$
$$\vec{x} \in X,$$

by changing the value of e_i parameters of the right hand side of the constrained objective functions the efficient solutions of the problem are obtained. Contrary to the weighting method, ϵ-constraint method can produce unsupported efficient solutions in multi-objective integer and mixed integer programming problems (Mavrotas, 2009). However this method has some disadvantages: (a) the calculation of the range of the objective functions over the efficient set, (b) the guarantee of efficiency of the obtained solution and (c) the increased solution time for problems with several (more than two) objective functions (Mavrotas, 2009).

The number of generated Pareto optimal solutions are specified by adjusting the number of the grid points in each of the objective function ranges. In order to properly apply the ϵ-constraint method the ranges of at least $p - 1$ objective functions are needed, they will be used as the additional objective function constraints. The range of each objective function is obtained from a payoff table that is determined based on utopia and pseudo nadir points. For constructing the payoff table the individual optima of the objective functions $f_i^*(\vec{x}_i^*)$ are calculated. Where $\vec{x}_i^*$ is the optimal solution to objective function f_i. the value of the other objective functions $f_1, f_2, \ldots, f_{i-1}, f_{i+1}, \ldots, f_p$ is calculated, which are represented by$f_1(\vec{x}_i^*), f_2(\vec{x}_i^*), \ldots, f_{i-1}(\vec{x}_i^*), f_{i+1}(\vec{x}_i^*), \ldots, f_p(\vec{x}_i^*)$ and correspond to the $i-th$ row of the $p \times p$ payoff table

$$\begin{pmatrix} f_1(\vec{x}_1^*) & \cdots & f_i(\vec{x}_1^*) & \cdots f_p(\vec{x}_1^*) \\ \vdots & \ddots & & \vdots \\ f_1(\vec{x}_i^*) & \cdots & f_i(\vec{x}_i^*) & \cdots f_p(\vec{x}_i^*) \\ \vdots & & & \ddots \\ f_1(\vec{x}_p^*) & \cdots & f_i(\vec{x}_p^*) & \cdots f_p(\vec{x}_p^*) \end{pmatrix} \tag{6.2}$$

One of the disadvantages of the ϵ-constraint method is that the range of the objective functions constructed based on the payoff table may not be optimized.

Then the ϵ-constraint method divides the range of $p-1$ objective functions $f_2, \ldots, f_p$ in $p-1$ equal intervals using $p-2$ intermediate equidistant grid points, respectively. In a bi-objective optimization problem there are two possibility for selecting the objective function to be optimized. Two different parameters have to be decided in this stage, the number of grid points in the objective function to be transformed into constraints, and which function is going to be selected to be optimized.

Another point of attention is that the obtained optimal solutions of the ϵ-constraint method may be inefficient. When solving the the optimization problem,

$$\min f_j(\vec{x}) \tag{6.3}$$

subject to:

$$\begin{array}{ccc} f_2(\vec{x}) & \leq & e_1 \\ & \cdots & \\ f_p(\vec{x}) & \leq & e_{p-1} \\ & \vec{x} \in X & \end{array} \tag{6.4}$$

can be multiple optimal solutions to the problem 6.3 and the interesting solution are those where the objectives function constraints are satisfied as equalities. Mavrotas (2009) proposed a method in which the optimal solution of problem 6.3 is guaranteed to be an efficient solution. They proposed the transformation of objective function constraints to equalities by explicitly incorporating the appropriate slack or surplus variables.

$$\min f_j(\vec{x}) - eps(s_2 + \ldots + s_p) \tag{6.5}$$

subject to:

$$\begin{array}{rcl} f_2(\vec{x}) + s_2 & = & e_1 \\ & \cdots & \\ f_p(\vec{x}) + s_p & = & e_{p-1} \\ & \vec{x} \in X & \end{array} \tag{6.6}$$

where eps is an adequately small number.

6.1.3 Performance metrics in multi-objective optimization

The performance metrics are comparison methods for measuring the quality of the solution sets obtained by different algorithms. They consider mainly three aspects of an approximation to the Pareto optimal front (Riquelme et al., 2015):

- ***the convergence***: how distant is the Pareto front approximation from the theoretical Pareto optimal front.
- ***the diversity***: the relative distance among solutions in the Pareto front approximation (distribution); and range of values covered by the solutions in this set (spread or extent).
- ***the number of optimal solutions***: the cardinality of the solutions that are Pareto optimal (the real set containing all the solutions that are non-dominated).

That means that in a good multi-objective algorithm the distance of resulting non-dominated set from the Pareto-optimal front should be minimized, and the solutions should be distributed and a wide range of values should be present (Zitzler et al., 2000).

As remarked by Riquelme et al. (2015) the vast majority of existing metrics are unary, they receive as parameter only one approximation of the Pareto Front for the evaluation, and considering one or multiples aspect, a real value is computed. The most used performance metric is the hypervolume indicator (Riquelme et al., 2015) and (Cheng et al., 2010). The preference for this metric is mainly due to the fact it is the only unary metric with the capability of considering all three aspects: accuracy, diversity and cardinality. Also, the hypervolume indicator is the only strictly monotonic unary indicator known (Zitzler et al., 2008). The other metric used here is the Δ metric; an unary indicator that measures the distribution and extent of spread achieved among the solutions in the Pareto front approximation. Following is given the definition of these metrics:

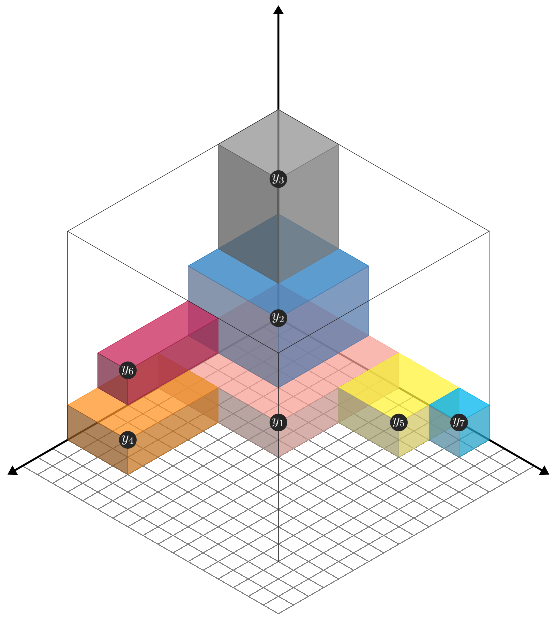


Figure 6.2: Hypercube given three different conflicting objectives

Hypervolume indicator

$I_{hv}(\mathcal{PF})$ measures the area dominated by the potential Pareto-optimal solutions $\mathcal{E}$ in the objective space $\mathcal{PF}$. This metric reflects the dominance of this last set, and in bi-objective optimization is a good measure of the convergence of a given approximation to the Pareto-front. It must be taken into account that the hypervolume not only reflects dominance, but also promotes diverse Pareto front sets.

$$I_{hv}(\mathcal{PF}) = \bigcup_{i=1}^{|\mathcal{PF}|-1} v_i \tag{6.7}$$

the hypercube v_i is constructed with respect to a reference point (see Figure 6.2).

Δ metric

measures the extent of spread achieved among the obtained solutions. In multi-objective optimization is important to get a set of solutions that spans the entire Pareto-optimal solutions, the most widely and uniformly spread out set of non-

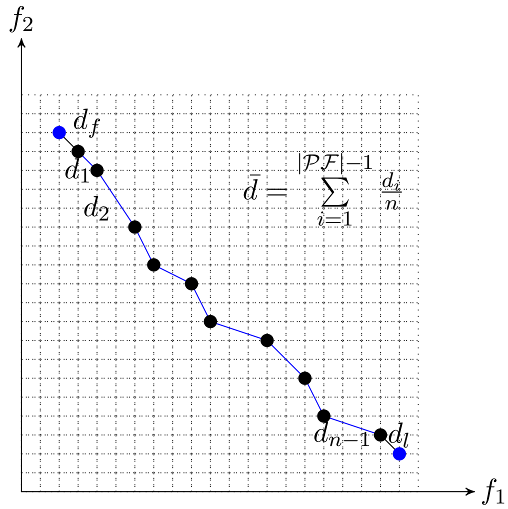


Figure 6.3: The Δ metric in a two-objectives space

dominated solutions the closer to zero the value of this metric. Given an approximation to the Pareto-front $\mathcal{PF}$, Δ metric is derived as follows:

$$\Delta(\mathcal{PF}) = \frac{d_f + d_l + \sum_{i=1}^{|\mathcal{PF}|-1} |d_i - \bar{d}|}{d_f + d_l + (|\mathcal{PF}| - 1)\bar{d}} \tag{6.8}$$

where d_i is the Euclidean distance between consecutive solutions and $\bar{d}$ is the average of d_i. The terms d_f and d_l are the minimum Euclidean distances from solutions in $\mathcal{PF}$ to the extreme solutions of the optimal Pareto front (see Figure 6.3).

6.2 The bi-objective heterogeneous fleet vehicle routing HazMat transportation problem

The HFVRP is defined on a complete directed graph $\mathcal{G}(\mathcal{N}, \mathcal{L})$. The node set $\mathcal{N} = \{0, 1, 2, \ldots, n\}$ includes the depot node 0, and a set of client nodes, $\mathcal{C}$. Each client $i \in \mathcal{C}$ has a demand q_i, and it is connected with other node $j \in \mathcal{N}$ by an arc $(i, j) \in \mathcal{L}$. Each arc is characterized by a length al_{ij}, and a population exposed to the consequences of a HazMat release (population residing within the arc impact area), PD_{ij}. To serve the client nodes there is a set of $\mathcal{K}$ different types of trucks.

A truck type $k \in \mathcal{K}$ is characterized by a maximal capacity Q_k and an accident rate $TTAR_k$.

In the HazMat transportation problem, each routing solution is composed of a set of routes $\mathcal{SR}$ satisfying all client demands once. Each route $\sigma^r \in \mathcal{SR}$ starts and ends at the depot, and respects the associated vehicle capacity Q_k. A route σ^r is a sequence of nodes, $\{\sigma_1^r, \sigma_2^r, \ldots, \sigma_{|\sigma^r|}^r\}$, where σ_d^r is d-th client visited on the route. Two conflicting objective functions are simultaneously minimized, see Bula et al. (2016), the total transportation cost and the total routing risk. These objectives are described in greater detail below, beginning with the the total transportation cost $(C(\mathcal{SR}))$, which is defined by Equation 6.7.

$$C(\mathcal{SR}) = \sum_{\sigma^r \in \mathcal{SR}} \sum_{d=2}^{|\sigma^r|} al_{(\sigma_{d-1}^r\ \sigma_d^r)} + \sum_{r \in \mathcal{SR}} FC_{Truck(\sigma^r)} \tag{6.9}$$

where the variable transportation cost is considered proportional to $al_{(\sigma_{d-1}^r\ \sigma_d^r)}$, one length unit is equivalent to one monetary unit. The $Truck(\sigma^r)$ function returns the truck type k of the route σ^r, and FC_k is the fixed cost for using the truck type k. Regarding the total routing risk $R(\mathcal{SR})$, it is computed as defined by Bula et al. (2016):

$$\begin{aligned} & R(\mathcal{SR}) = TTAR^k \times P_{release} \times \beta \times \\ & \sum_{\sigma^r \in S} \sum_{d=2}^{|\sigma^r|} \left(a^m_{(\sigma_{d-1}^r\ \sigma_d^r)} + \left(\sum_{e=d}^{|\sigma^r|} q_{\sigma_e^r} \right) b^m_{(\sigma_{d-1}^r\ \sigma_d^r)} \right) \rho_{(\sigma_{d-1}^r \sigma_d^r)} \end{aligned} \tag{6.10}$$

$P_{release}$ is the release probability of HazMat given a truck accident. $a^m_{(\sigma_{d-1}^r\ \sigma_d^r)}$ and $b^m_{(\sigma_{d-1}^r\ \sigma_d^r)}$ are the value of the piecewise linear function parameters defined over the range $l_{m-1} \leq \sum_{e=d}^{|\sigma^r|} q_{\sigma_e^r} \leq l_m$, used for approximating the value of $(\sum_{e=d}^{|\sigma^r|} q_{\sigma_e^r})^\alpha$ (see Figure 6.4). α and β are constant values that depends on the type of material transported, see Ronza et al. (2007). $q_{\sigma_e^r}$ is the demand of the σ_e^r client. $\rho_{(\sigma_{d-1}^r \sigma_d^r)}$ regroups arc $(\sigma_{d-1}^r \sigma_d^r)$ dependent parameters, $al_{(\sigma_{d-1}^r \sigma_d^r)}$ and $PD_{(\sigma_{d-1}^r \sigma_d^r)}$.

$$\rho_{(\sigma_{d-1}^r \sigma_d^r)} = al_{(\sigma_{d-1}^r \sigma_d^r)} \times PD_{(\sigma_{d-1}^r \sigma_d^r)} \tag{6.11}$$

In order to formulate the transportation problem as a mixed integer linear program, the following decision variables are used:

$$x_{ij}^k : \begin{cases} 1 & \text{if a vehicle of type } k \text{ travels the link } (i,j) \\ 0 & \text{otherwise} \end{cases} \tag{6.12}$$

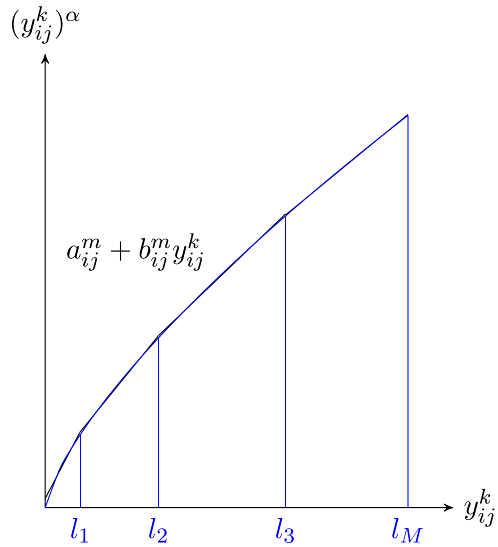


Figure 6.4: Piecewise linear approximation of $y_{ij}^k = (\sum_{e=d}^{|\sigma^r|} q_{\sigma_e^r})^\alpha$

and the the quantity to be transported from node i to node j in a vehicle of type k, y_{ij}^k:

$$y_{ij}^k = y_{(\sigma_{d-1}^r \sigma_d^r)}^k = \sum_{e=d}^{|\sigma^r|} q_{\sigma_e^r} \tag{6.13}$$

given a route σ^r, $d = 2, \cdots, |\sigma^r|$, $i = \sigma_{d-1}^r$ and $j = \sigma_d^r$.

To obtain the linear approximation of the risk consequences by M piecewise-linear functions when the interval of quantity flow, y_{ij}^k, is partitioned into M small segments $[l_{m-1}, l_m],\ m = 1, \cdots M$, the variable $t_{ij}^k = (a_{ij}^m + b_{ij}^m y_{ij}^k)$ is defined. Thus, it is necessary to introduce two other set of variables: binary variable h_{ijk}^m that indicates the comparison between y_{ij}^k and l_{m-1}, and the continuous variable λ_{ijk}^m that evaluates the distance between y_{ij}^k and l_{m-1}.

The full mixed integer linear programming (MILP) formulation of the problem is shown next, and it is based on the mono objective version presented by Bula et al. (2016) for the routing risk minimization.

$$\min z_1 = C(\mathcal{SR}) = \sum_{(i,j)\in\mathcal{L}} \sum_{k\in\mathcal{K}} x_{ij}^k a l_{ij} + \sum_{j\in\mathcal{N}\setminus\{0\}} \sum_{k\in\mathcal{K}} FC_k x_{0j}^k \tag{6.14}$$

$$\min z_2 = R(\mathcal{SR}) = \quad P_{release} \times \beta \times \sum_{(i,j)\in\mathcal{L}} \sum_{k\in\mathcal{K}} TTAR^k \times \rho_{ij} \times t_{ij}^k \tag{6.15}$$

subject to:

$$t_{ij}^k = t_0 + \sum_{m=1}^{M} b_{ij}^m \lambda_{ijk}^m \; \forall i,j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \tag{6.16}$$

$$y_{ij}^k = l_0 + \sum_{m=1}^{M} \lambda_{ijk}^m \; \forall i,j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \tag{6.17}$$

$$\lambda_{ijk}^1 \leq l_1 - l_0 \; \forall i,j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \tag{6.18}$$

$$\lambda_{ijk}^m \geq (l_m - l_{m-1}) h_{ijk}^m \quad \begin{array}{l} \forall i,j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \\ m = 1, \cdots, M-1 \end{array} \tag{6.19}$$

$$\lambda_{ijk}^{m+1} \leq (l_{m+1} - l_m) h_{ijk}^m \quad \begin{array}{l} \forall i,j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \\ m = 1, \cdots, M-1 \end{array} \tag{6.20}$$

$$\sum_{k\in\mathcal{K}} \sum_{i\in\mathcal{N}} x_{ij}^k = 1, \; \forall j \in \mathcal{N} \setminus \{0\} \tag{6.21}$$

$$\sum_{i\in\mathcal{N}} x_{ij}^k - \sum_{i\in\mathcal{N}} x_{ji}^k = 0, \; \forall k \in \mathcal{K}, \forall j \in \mathcal{C} \tag{6.22}$$

$$\sum_{k\in\mathcal{K}} \sum_{i\in\mathcal{N}} y_{ij}^k - \sum_{k\in\mathcal{K}} \sum_{i\in\mathcal{N}} y_{ji}^k = q_j, \; \forall j \in \mathcal{C} \tag{6.23}$$

$$q_j \sum_{k\in\mathcal{K}} x_{ij}^k \leq \sum_{k\in\mathcal{K}} y_{ij}^k \; \forall i,j \in \mathcal{N}, \; i \neq j \tag{6.24}$$

$$y_{ij}^k \leq x_{ij}^k (Q_k - q_i) \; \forall i,j \in \mathcal{N} \;\; i \neq j, \; \forall k \in \mathcal{K} \tag{6.25}$$

$$\lambda_{ijk}^m \geq 0, \; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L}, \; m = 1, \cdots, M \tag{6.26}$$

$$h_{ijk}^m \; \in \{0,1\}, \; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L}, \; m = 1, \cdots, M \tag{6.27}$$

$$t_{ij}^k \geq 0, \; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L} \tag{6.28}$$

$$y_{ij}^k \geq 0, \ \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L} \tag{6.29}$$

$$x_{ij}^k \in \{0,1\}, \ \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L} \tag{6.30}$$

Equations (6.14) and (6.15) express objective functions for minimizing the total routing cost and the total routing risk, respectively. The constraints (6.16)-(6.20) are used for the piecewise linear approximation value of $(y_{ij}^k)^\alpha$. The set of constraints (6.21) ensures that each customer is visited exactly once, and the set (6.22) and (6.23) represents the conservation flux constraints. Additionally, (6.23) guarantees demands satisfaction. Constraints (6.24) and (6.25) state that no goods are transported from i to j if no vehicle is serving the arc (i,j), and (6.25) define the load of the vehicle k when traversing arc (i,j).

The HVRP in HazMat transportation is *NP-hard* since it is an extension of the HVRP (Prins, 2009). Heuristic methods are proved to obtain good quality routing solutions efficiently for the mono-objective version. In the case of the multi-objective optimization, even thought the Pareto-optimal set (non-dominated solutions) may have a finite number of solutions, its computation involves solving many NP-hard combinatorial optimization problems, or its size could be exponentially large in the test instance size. Based on a hybrid neighborhood search algorithm two new solution approaches are developed for finding an approximation of the Pareto-optimal set (efficient, accurate, and well distributed points). The next section presents a detailed description of the two procedures.

6.3 Dominance-based multi-objective neighborhood search algorithm

Multi-objective meta-heuristics based on *neighborhood search algorithms* (NSA) are extensions of well-known local search meta-heuristics that deal with the notion of non-dominated solutions. Liefooghe et al. (2012) describe dominance-based multi-objective local search algorithms as methods defined by a neighborhood structure and a dominance relation that iteratively improve an archive of non-dominated solutions. NSA methods are good in local convergence to the Pareto (non-dominated) front, but as Ehrgott and Gandibleux (2008) emphasized, NSAs require more effort in diversification (to cover the whole non-dominated front) compared to *evolutionary algorithms* (EA) given their rapid convergence because of the less dispersed search. For covering the Pareto front completely, a diversification strategy has to be implemented, that is why multi-objective meta-heuristics are often hybridized. Not so many methods have been proposed for NSAs, Schaus and

Hartert (2013) introduce an extension of large neighborhood search (LNS), called multi-objective LNS (MO-LNS), and Duarte et al. (2015) introduce an adaptation of the Variable Neighborhood Search (VNS) metaheuristic to solve multi-objective combinatorial optimization problems.

This first algorithm presented in this work aims at approximating the Pareto-optimal set for a multi-objective VRP in HazMat transportation problems. It is defined by a series of neighborhood structures and a dominance relation that iteratively improve a set of potential efficient solutions. Next, the algorithm elements as the generation of initial Pareto-optimal set approximation, the selection of solutions, the neighborhood exploration and the recording of the potential efficient solutions, and the stopping condition are described. The starting point of the algorithm description is the generation of the initial Pareto set approximation, and it continues with a bottom-up description of the entire algorithm.

6.3.1 Initial Solution

Neighborhood search based algorithms improve an incumbent solution, thus, an initial solution is needed. In its turn, multi-objective optimization is a vector optimization given as a result an efficient set or Pareto-optimal set. In this case, each efficient set element corresponds to a routing solution, $\mathcal{SR}$. The size of the potentially efficient set at each iteration ni of the proposed algorithm, $PS(ni)$, could be fixed or variable, including the initial approximation, $PS(ni = 0)$. Thus, given that the output of the algorithm is a potentially efficient set, it is reasonable to have an initial incumbent solution with more than one point. Two different strategies are considered to generate this initial set:

Random splitting of a Hamiltonian circuit:

The Christofides algorithm is used for constructing a Hamiltonian circuit (Papadimitriou and Steiglitz, 1998). First, a minimum spanning tree is generated. Next, following the nodes in the appearing order at the tree, a giant tour visiting all the nodes at least once is created. Then, only the first apparition of the nodes is kept to have an Hamiltonian tour. This procedure is repeated a fixed number of times (size of the initial solution set), half of the times the arc weights correspond to the Euclidean distances and other half, to a risk measure ($\rho_{ij} \times q_j$).

For obtaining a routing solution, a random splitting of a Hamiltonian circuit is performed by selecting a truck at random and starting from the first node a route is built, following the circuit adding nodes until the truck is full. The principle is repeated starting from the next node in the Hamiltonian circuit until all nodes have been included in a route. Algorithm 8 presents this procedure.

Algorithm 8 Initial solution from random splitting of a Hamiltonian circuit

$PS(ni = 0) \leftarrow \emptyset$
$\mathcal{PF} \leftarrow \emptyset$ Initial objective vector set.
for $ol = 1, 2$ **do**
  if $(ol = 1)$ **then** $edge\ weight = al_{ij}$
  else $edge\ weight = \rho_{ij} \times q_j$
  end if
  $\mathcal{T} \leftarrow Minimum\_Spanning\_Tree(\mathcal{G}, edge\ weight)$.
  $\mathcal{EC} \leftarrow Eulerian\_Circuit(\mathcal{T})$.
  for $vi = 1, \cdots, |PS(ni)|/2$ **do**
    Select a $vertex_{vi}$ from $\mathcal{T}$ with degree 0.
    $\mathcal{HC} \leftarrow Hamiltonian\_Circuit(\mathcal{EC}, vertex_{vi})$
    $\mathcal{SR} \leftarrow \emptyset$
    while $\mathcal{HC} \neq \emptyset$ **do**
      $\sigma^r \leftarrow \{\mathcal{HC}_0\}, \mathcal{HC} \leftarrow \mathcal{HC} \setminus \mathcal{HC}_0$
      Select a truck k at random.
      $route\_load \leftarrow q_{\sigma^r_1}$
      while $route\_load \leq Q_k$ and $\mathcal{HC} \neq \emptyset$ **do**
        $next\_node \leftarrow \mathcal{HC}_0$
        if $route\_load + q_{next\_node} \leq Q_k$ **then**
          $\sigma^r \leftarrow \sigma^r \bigcup \mathcal{HC}_0, \mathcal{HC} \leftarrow \mathcal{HC} \setminus \mathcal{HC}_0$
          $route\_load \leftarrow route\_load + q_{next\_node}$
        end if
      end while
      $\mathcal{SR} \leftarrow \mathcal{SR} \bigcup (\sigma^r, k)$
    end while
    $PS(ni = 0) \leftarrow PS(ni = 0) \bigcup \mathcal{SR}$
    $\mathcal{PF} \leftarrow \mathcal{PF} \bigcup \vec{f}(\mathcal{SR})$
  end for
end for
$\mathcal{PF} \leftarrow$ keep the elements of the Pareto front approximation obtained from $\mathcal{PF}$.
$PS(ni = 0) \leftarrow$ routing solutions corresponding with $\mathcal{PF}$.

Path-Relinking:

This technique generates a path through the neighborhood space such that the minimum permutation distance (*mpd*) (Lacomme et al., 2015b) between two potential efficient solutions decreases. A routing solution is represented using an array of integers. The *mpd* of an array is usually the smallest Hamming distance between the permutation. The two potential efficient set solutions consist of the resulting best ones when minimizing the total cost and the total routing risk, respectively, using the mono-objective version of the local search algorithm. See Algorithm 9.

Algorithm 9 Initial solution from Path-Relinking

$PS(ni = 0) \leftarrow \emptyset$
$\mathcal{PF} \leftarrow \emptyset$
$\mathcal{SR}_{cost} \leftarrow$ cost minimization problem.
$\mathcal{SR}_{risk} \leftarrow$ risk minimization problem.
for $\mathcal{SR}_v \in Path - Relinking(\mathcal{SR}_{cost}, \mathcal{SR}_{risk})$ **do**
    $PS(ni = 0) \leftarrow PS(ni = 0) \bigcup \mathcal{SR}_v$
    $\mathcal{PF} \leftarrow \mathcal{PF} \bigcup \vec{f}(\mathcal{SR}_v)$
end for
$\mathcal{PF} \leftarrow$ keep the elements of the Pareto front approximation obtained from $\mathcal{PF}$.
$PS(ni = 0) \leftarrow$ routing solutions corresponding with $\mathcal{PF}$.

The post-optimization procedure described in the previous chapter is also employed here for getting the two optimal initial solutions. A Set Partitioning (SP) model is solved to find the best combination of routes that minimizes the routing risk or the routing cost after, the routes are drawn from a pool obtained through the neighborhood search based algorithm.

6.3.2 Neighborhood Exploration

The local search is implemented on the selected potential efficient set point that has been previously perturbed, $PS^{'}(ni)_u$ (see Algorithm 10), applying a local search neighborhood structure p, from $N_p,\ p = 1, \dots, P$. The local search leads to a local optimum vector consisting of two neighbors (one for each objective) of the search point obtained through a best improvement neighborhood search, and it is notated as $\{PS^{'}(ni)^1_u, PS^{'}(ni)^2_u\}$. The neighborhood exploration is done simultaneously in all objective functions. At the end, each one of the two final solutions obtained improves each one of the two objective functions separately, the total transportation cost and the total routing risk. The notion of local optimum is defined in terms of Pareto optimality, that means there does not exist any other solution in the neighborhood space dominating the solution that is being evaluated.

The local search procedure adopted is the Variable Neighborhood Descent (VND) used by Bula et al. (2017). It relies on six inter-route neighborhoods:

$shift(1,0)$, $shift(2,0)$, $swap(1,1)$, $swap(2,2)$, $2-opt$ and merging two different routes; and two intra-route neighborhoods: $Shift(1,0)$ and $2-opt$.

6.3.3 Updating the neighborhood

The local search is driven each time by one of the two objective functions being optimized. That is, the local search is performed at least two times, because when an improving neighbor is found the local search restarts from the first objective. The decision whether to change or not the neighborhood structure depends on the definition of an improving move. A neighborhood structure is kept if and only if there is an improving move, that is when it is possible to include a new potential Pareto front point into the local approximation of Pareto front. This new point can be included into the intensification subspace where a new point replaces at least one point in the local approximation of Pareto front, or into the diversification subspace where a new point is added into the front approximation without replacing any other point. Algorithm 10 shows the procedure for determining if the evaluation of a best neighbor $\{z_1(PS^{'}(ni)_u^1),\, z_2(PS^{'}(ni)_u^2)\}$ improves or not the current local approximation of the Pareto-front. As stated in Section 3, z_1 evaluates the total transportation cost and z_2 the total routing risk. $\prec$ is used for expressing the Pareto dominance relationship.

Algorithm 10 Updating the front

Define $\mathcal{PF}$, $\{z_1(PS^{'}(ni)_u^1), z_2(PS^{'}(ni)_u^2)\}$
$flag \leftarrow TRUE$
while $flag$ and $o \leq |\mathcal{PF}|$ **do**
    if $\{z_1(PS^{'}(ni)_u^1), z_2(PS^{'}(ni)_u^2)\} \prec \mathcal{PF}_o$ **then**
        $\mathcal{PF} \leftarrow \mathcal{PF} \backslash \{\mathcal{PF}_o\}$
    end if
    if $\mathcal{PF}_o \prec \{z_1(PS^{'}(ni)_u^1), z_2(PS^{'}(ni)_u^2)\}$ **then**
        $flag \leftarrow FALSE$
    end if
    $o \leftarrow o + 1$
end while
if $flag$ **then**
    $\mathcal{PF} \leftarrow \mathcal{PF} \cup \{z_1(PS^{'}(ni)_u^1), z_2(PS^{'}(ni)_u^2)\}$
end if
Return $flag$,$\mathcal{PF}$

The local search algorithm is shown in Algorithm 11, starting from a searching point $PS^{'}(ni)_u^{ol}$ the local Pareto-Front approximation $\mathcal{PF}$ is composed of one element $\{z_1(PS^{'}(ni)_u), z_2(PS^{'}(ni)_u)\}$ and the potential efficient set $PS^{''}(ni)$ only includes the point $PS^{'}(ni)_u$, Lines 2-3. The local search starts with a perturbed solution and the neighborhood exploration is carried out. If the move fails in adding at least new point to $\mathcal{PF}_{local}$ the next neighborhood structure $p,\ p = 1, \cdots, P$, is used for the local search, as show in Lines 8-27. If at least a new potential efficient point is discovered the local search goes back to the initial neighborhood, $p = 1$, Lines 15 and 23. With regard to the update of the searching point $PS(ni)^{'}_u$, this is performed only if a new best point for the filtering objective z_l is found, Line 12. Here X represents the feasible search space. $PS^{'}(ni)_v$ corresponds to a routing solution $\mathcal{SR}$, and this in turn can be also expressed in terms of the binary decision variables x^k_{ij} and the integer decision variables y^k_{ij}.

6.3.4 The general Algorithm

Algorithm 12 presents the general structure of the multi-objective neighborhood dominance-based algorithm. From the work of Liefooghe et al. (2012) the strategies for (i) selecting a proper set of points whose neighborhood is to be explored and (ii) exploring the neighborhood of this set are based on algorithm parameters to be selected experimentally. There is not a general approach to follow in a particular local search based algorithm.

The algorithm starts (lines 2-3) by generating an initial approximation of the Pareto front $\mathcal{PF}$ and the potential efficient set $PS(ni = 0)$, Subsection 6.3.1. The initial value of the hypervolume indicator is computed (line 4).

The approximation of the potential efficient set $PS(ni)$ is the incumbent solution. In order to carry out the local search, the set of points to be perturbed is initialized (line 8). A random selected mono-objective shake procedure is applied to each of these points, and then, the neighborhood exploration is performed. The number of times the perturbation of any point $PS^{'}(ni)_u\ u = 1 \cdots, |PS(ni)_{subset}|$ is executed, it is at least 2, the number of considered objectives. The starting selection have a strong impact on the quality of the approximation of the Pareto front, see Schaus and Hartert (2013). Three different approaches are explored in order to select the points to be perturbed:

- Random procedure: a simple random sample without replacement is chosen from the set $PS(ni)$; each individual $PS(ni)_v$ has the same probability of being chosen at each iteration of the Pareto-front approximation perturbation.

- Nearest neighbor objective-space: this is computed on the objectives space, where one axis is the cost and the other axis is the risk. First, points equally

Algorithm 11 Local search: updating the neighborhood

Define $\{z_1(PS^{'}(ni)_u), z_2(PS^{'}(ni)_u)\}$, X, local search neighborhood structures $N_p, p = 1, \ldots, P$, perturbed solution $PS^{'}(ni)_u \in X$, Filtering objective ol
$\vec{z}_s \leftarrow \{z_1(PS^{'}(ni)_u), z_2(PS^{'}(ni)_u)\}$
$\mathcal{PF}_{local} \leftarrow \{z_1(PS^{'}(ni)_u), z_2(PS^{'}(ni)_u)\}$
$p \leftarrow 1$
while $p \leq P$ **do**
    $PS^{''}(ni)_u \leftarrow$ Exploration of neighborhood$[N_p(PS^{'}(ni)_u)]$
    $p \leftarrow p + 1$
    for $PS^{''}(ni)_u^o \in PS^{''}(ni)_u$ **do**
        if $o = ol$ **then**
            if $z_{ol}(PS^{''}(ni)_u^{ol}) < \vec{z}_s^{\,ol}$ **then**
                $\vec{z}_s^{\,ol} \leftarrow z_{ol}(PS^{''}(ni)_u^o)$
                $PS^{'}(ni)_u \leftarrow PS^{''}(ni)_u$
                $\{\mathcal{PF}_{local}, flag\} \leftarrow$ Updating the front$(\mathcal{PF}_{local}, \vec{z}(PS^{''}(ni)_u))$
                if $flag$ **then**
                    $p \leftarrow 1$
                end if
            end if
        else
            if $z_u(PS^{'}(ni)_u^o) < \vec{z}_s^{\,u}$ **then**
                $\vec{z}_s^{\,u} \leftarrow z_u(PS^{'}(ni)_u^o)$
                $\{\mathcal{PF}_{local}, flag\} \leftarrow$ Updating the front$(\mathcal{PF}_{local}, \vec{z}(PS^{''}(ni)_u))$
                if $flag$ **then**
                    $p \leftarrow 1$
                end if
            end if
        end if
    end for
end while
Return $\mathcal{PF}_{local}, PS^{'}(ni)_u$

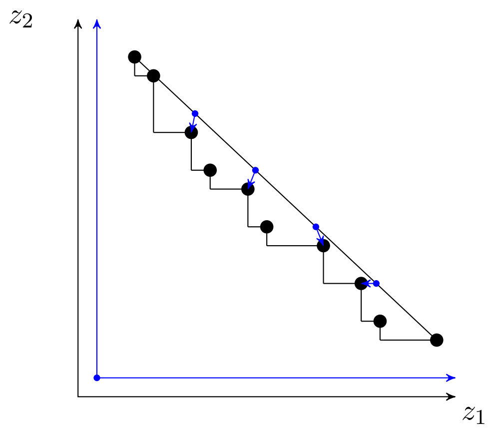


Figure 6.5: The nearest neighbor strategy. The closest solutions (pointed by arrows) to each of the equally spaced points on the line formed by two extreme solutions are showed.

spaced from each other are selected on a line formed by two extreme solutions (i.e. the best cost and the best risk solutions). Then, the closest solutions (the nearest neighbor according to an Euclidean distance metric) to each of these equally spaced points are founded. This nearest neighbor strategy is illustrated in the Figure 6.5.

- Crowding distance: also computed on the objectives space. The elements of the set $PS(ni)$ are ranked according to their crowding distance, the distance of two neighboring solutions on either side of a solution along each objective axis. This is a density estimation of solutions for the Pareto Front approximation. The smaller the value the more crowded the solution, the idea is to select from the less crowded solutions, those with the greatest values.

These three approaches are compared to the multi-objective intensified shake procedure where all the points in the solution are perturbed.

Two mechanisms can be applied during the perturbation (Line 6) of the selected points, $split$ of a route or $shift(1,0)$. During the perturbation of a point, $shift$ and $split$ of a route are randomly selected with equal probabilities.

Each selected point $PS(ni)_v$ to be perturbed is copied twice (the number of objectives) to get the set of points $\{PS(ni)^1_v, PS(ni)^2_v\}$, Line 10. The $ol - th$ perturbation of the $v - th$ solution is carried out and the local search (updating the neighborhood) procedure described in the Subsection 6.3.3 is applied (line 16). If at least one of the current local values is updated the neighborhood search is

Algorithm 12 General Dominance-based multi-objective local search algorithm

Define $\{z_1(PS(ni)_v), z_2(PS(ni)_v)\}$,$X$, Select the set of perturbation neighborhood structures N_s, for $s = 1, \cdots, S$, and $mnop$ the maximum number of permutation.
Generate an initial approximation of the potential efficient set $PS(ni = 0)$
Initial Pareto front approximation $\mathcal{PF} \leftarrow \{[z_1(PS(ni)_v), z_2(PS(ni)_v)] | v = 1, \ldots, |PS(ni)|\}$
$I_{hv} \leftarrow Hypervolume(\mathcal{PF})$
$perturbations \leftarrow 1$
while $perturbations \leq mnop$ **do**
    $PS^{'}(ni),\ \mathcal{PF}^{'} \leftarrow \emptyset,\ \emptyset$
    Select $PS(ni)_{subset} \subseteq PS(ni)$
    for $PS(ni)_v \in PS(ni)_{subset}$ **do**
        $\{PS'(ni)_v^1, PS'(ni)_v^2\} \leftarrow \{PS(ni)_v, PS(ni)_v\}$
        $ol \leftarrow 1$
        while $ol \leq 2$ **do**
            $PS(ni)_u \leftarrow PS^{'}(ni)_v^{ol}$
            $s \sim U[1, 2, \cdots, S]$
            Perturb $PS(ni)_u$, $PS'(ni)_u \leftarrow N_p(PS(ni)_u)$
            $\{PS'(ni)_u, PF_{local}\} \leftarrow$ Local Search $(PS'(ni)_u)$
            $flag \leftarrow false$
            for $p \in \{1, 2\}$ **do**
                if $z_p(PS'(ni)_u) < z_p(PS'(ni)_v^p)$ **then**
                    $PS'(ni)_v^p \leftarrow PS'(ni)_u$
                    $ol \leftarrow 1$
                    $flag \leftarrow true$
                end if
            end for
            if $flag$ **then**
                Updating the front($\mathcal{PF}^{'}(ni), \mathcal{PF}_{local\,u}$) $u = 1, \ldots, |\mathcal{PF}_{local}|$
            else
                $ol \leftarrow ol + 1$
            end if
        end while
        for $PF(ni)_u \in PF(ni)$ **do**
            $PF'(ni) \leftarrow$ Updating the front($PF^{'}(ni), \{z_1(PS(ni)_u), z_2(PS(ni)_u)\}$)
        end for
    end for
    if $Hypervolume(PF') > I_{hv}$ **then**
        $PS(ni),\ \mathcal{PF} \leftarrow PS^{'}(ni),\ \mathcal{PF}^{'}$
        $I_{hv} \leftarrow Hypervolume(PF)$
        $perturbations \leftarrow 1$
    else
        $perturbations \leftarrow perturbations + 1$
    end if
    $ni \leftarrow ni + 1$
end while

continued over the point $PS(ni)_v$, else, the next point is selected, Lines 18-27. It is considered that the local optimum is better than the incumbent solution if the hypervolume indicator of the Pareto-front approximation $\mathcal{PF}$ increases in value. The number of consecutive perturbations without improvement of the hypervolume indicator is established as the stopping criterion.

In the construction of the proposed algorithm the local search is guided by using dominance ranking approaches, and quality indicators are applied for preferences in the iterations as proposed by Zitzler et al. (2008). Also following the advice of these authors, an individual-based selection is used over a set-based selection.

6.4 ϵ-constraint multi-objective local search algorithm

In this section a description of this solution approach based on a scalarization metaheuristic algorithm is provided. An ϵ-constraint approach is applied instead of a weighting method due to its capability to produce unsupported efficient solutions in multi-objective integer and mixed integer programming problems (Mavrotas, 2009). In this case the local search is implemented in such a way that the heuristic ϵ-constraint method produces only efficient solutions (best efficient neighbor).

First, the utopia point and the pseudo nadir point are found. The utopia point, $\{f^U_{Cost}, f^U_{Risk}\}$, corresponds to the solution of each one of the two mono-optimization problems, the minimization of the total transportation cost and the total routing risk. The pseudo nadir, $\{f^{SN}_{Cost}, f^{SN}_{Risk}\}$, is composed of value obtained from the constrained optimization of each objective to the minimum value of the other objective. In ϵ-constraint method, once the objective function f_l to be minimized is selected the range $f^{SN}_s - f^U_s$ of the other objective function is divided by n_Δ points, Mavrotas (2009).

Algorithm 13 describes the solution method proposed. x represents a feasible solution point to the bi-objective problem. As the total routing cost ($z_1(x)$) and the total routing or transportation risk ($z_2(x)$) are conflicting objectives, the solution found in Line 11 would be the same or improved in Pareto sense of that one found in Line 8. That means, it will lay in the intensification space and not in the diversification space. We can replace Line 12 by the expression $z_1(x'^*_{constrained}) < z_2(x^*_{constrained})$ given that the cost will be less or equal than the constrained valued but never greater.

Algorithm 13 Bi-objective ϵ-constraint algorithm for cost and risk minimization

1: Define $\vec{z} = \{z_1(x), z_2(x)\}$, $X, n_\Delta, f^U_{Cost}, f^U_{Risk}, f^{SN}_{Cost}, f^{SN}_{Risk}$
2: $\Delta_{Cost} = \frac{f^{SN}_{Cost} - f^U_{Cost}}{n_\Delta}$
3: $\epsilon_{Cost} = f^U_{Cost}$
4: Initialize efficient set $ES \leftarrow \{\}$
5: **while** $\epsilon_{Cost} + \Delta_{Cost} < f^{SN}_{Cost}$ **do**
6: $\quad \epsilon_{Cost} = \epsilon_{Cost} + \Delta_{Cost}$
7: $\quad x^*_{constrained} \leftarrow \min z_2(x),\ s.t.\ z_1(x) \leq \epsilon_{Cost} \wedge x \in X$
8: $\quad \vec{z}_a \leftarrow (z_1(x^*_{constrained}), z_2(x^*_{constrained}))$
9: $\quad \epsilon_{Risk} = z_2(x^*_{constrained})$
10: $\quad x'^*_{constrained} \leftarrow \min z_1(x),\ s.t.\ z_2(x) \leq \epsilon_{Risk} \wedge x \in X$
11: $\quad \vec{z}_b \leftarrow (z_1(x'^*_{constrained}), z_2(x'^*_{constrained}))$
12: $\quad$ **if** $\vec{z}_a \preceq \vec{z}_b$ **then**
13: $\qquad ES \leftarrow ES \cup x^*_{constrained}$
14: $\quad$ **else**
15: $\qquad ES \leftarrow ES \cup x'^*_{constrained}$
16: $\quad$ **end if**
17: **end while**

For getting the solutions in Lines 7 and 10, the hybrid algorithm based on neighborhood search described in the previous Chapter is used. An adaptation of the post-optimization procedure is carried out in order to find the minimum constrained routing risk and the minimum constrained routing cost, the constraint described by the Equation 6.30 is added. The Set-Partitioned formulation for the ϵ-constraint problem for the case when minimizing the cost constrained routing risk is expressed as follows:

$$\min \sum_{\sigma^r \in \mathcal{SR}_{SP}} R(\sigma^r) x_{\sigma^r} \tag{6.31}$$

subject to:

$$\sum_{\sigma^r \in \mathcal{SR}_{SP}} C(\sigma^r) x_{\sigma^r} \leq \epsilon_{Cost} \tag{6.32}$$

$$\sum_{\sigma^r \in \mathcal{SR}_{SP(i)}} x_{\sigma^r} = 1\ \forall i \in \mathcal{C} \tag{6.33}$$

$$x_{\sigma^r} \in \{0, 1\} \forall \sigma^r \in \mathcal{SR}_{SP} \tag{6.34}$$

where x_{σ^r} is a binary variable taking 1 if the route σ^r is in the optimal solution. For filling the route pool the described neighborhood structures are utilized but performing the local search according to Algorithm 14.

There are different possibilities for starting the local search for the next grid point, it could be the same initial solution or to start the next iteration of the algorithm from the previous iteration solution. Once the point is selected in Line 6, a local search meta-heuristic is called for solving the objective constrained problem (for both, cost constraint and risk constraint).

6.4.1 Local Search Implementation

Algorithm 14 presents the local search implementation of the bi-objective ϵ-constraint algorithm when the cost function is selected as the objective function to serve as constraint and the risk objective is selected as objective function of the optimization problem. In lines 6 and 7 the best value of both objective functions is computed for each feasible neighbor and then the value of the no-optimized objective function is computed. The neighbor with the best risk value but respecting the cost constrained value is selected.

Algorithm 14 Exploration of a neighborhood: Cost constrained

1: Define $\vec{z} = \{z_1(x), z_2(x)\}$, X, $Cost_{Constrained}$,neighborhood structure $N_p(x)$, initial solution $x_0, x_0 \in X$
2: $\vec{x}^{'} \leftarrow x_0$
3: $\vec{z}^{'} \leftarrow \{z_1(x_0), z_2(x_0)\}$
4: **for** $x'' \in N_p(x_0)$ **do**
5:     **if** $x'' \in X$ **then**
6:         compute risk direction $\vec{z}(x'') = \{z_1(x''), z_2(x'')\}$
7:         compute cost direction $\vec{z}(x''') = \{z_1(x''), z_2(x'')\}$
8:         **if** $z_2(x'') < \vec{z}_2^{'} \wedge z_1(x'') < Cost_{Constrained}$ **then**
9:             $\vec{x}^{'} \leftarrow x^{''}$
10:             $\vec{z}_2^{'} \leftarrow z_2(x^{''})$
11:         **else if** $\mathbf{z_2(x''') < \tilde{z}_2^{'} \wedge z_1(x''') < Cost_{Constrained}}$ **then**
12:             $\vec{x}^{'} \leftarrow x^{'''}$
13:             $\vec{z}_2^{'} \leftarrow z_2(x^{'''})$
14:         **end if**
15:     **end if**
16: **end for**
17: Return $x^{'}$

Table 6.1: Results for the parameters tuning of the multi-objective neighborhood dominance-based algorithm

Initial solution generation	Criteria to select front elements	Instance	Number of local searches guided by cost obj.	Number of local searches guided by risk obj.	Number of front perturbations	Average Time	Average Hyper-volume	Average Delta
Random split Hamiltonian circuit	All elements	3	4608.5	7458.6	61.9	72.3	0.9291	0.9592
		4	7598.7	11806.6	85.1	186.3	0.8225	1.1514
		5	5490.5	9544	73.7	91.4	0.8697	0.7624
		6	7742.9	13268.1	56	176.3	0.7913	1.6576
Path Relinking	Random	3	1540.1	2416	53.5	29.4	0.9241	0.8455
		4	1250.9	2184.8	41.9	35.9	0.8123	0.5346
		5	1824.9	3081	70.2	33.2	0.8734	0.7298
		6	2451.8	4106.9	54.5	59.8	0.7878	1.6592
Path Relinking	Crowding Distance	3	1309.3	2057.1	45.8	26.1	0.9239	0.8445
		4	1275.1	2218.1	43.2	36	0.8153	0.6017
		5	1695.4	2841.9	66.6	34.3	0.8707	0.7632
		6	1708.8	2949.2	47.6	44.4	0.7866	1.6455
Path Relinking	Closest neighbor to the line	3	1418.1	2210.5	45.9	27.4	0.9222	0.8307
		4	1234.9	2163.6	40.2	35.3	0.8159	0.5867
		5	1348.7	2240.1	53.7	25.3	0.867	0.7517
		6	1886.7	3064.2	45.6	48.1	0.7843	1.627
Path Relinking	All elements	3	1657.2	2604.4	50.7	30.9	0.9242	0.8277
		4	1234.2	2144.8	40.9	36.9	0.808	0.5792
		5	1855.2	3138.5	62.1	35.9	0.8705	0.7606
		6	3321	5567	44.1	79.8	0.7881	1.658

6.5 Experiments and Results

The HVRP instances proposed by Golden et al. (1984) modified to include the risk parameters (Bula et al. (2016)) are used to assess the performance of the algorithms. Both algorithms were coded in *Java SE 8* and executed in an *Intel Core i5* Processor 3.3 GHz with 8 GB of RAM running *Ubuntu 16.04*. The version 6.0 of the (*Gurobi*) solver was used for the post-optimization part (Set Partitioning).

6.5.1 Parameters tuning

Two different categorical parameters are selected for the implementation of the multi-objective neighborhood dominance-based algorithm: the strategy for generating the initial set and the method for selecting the points to be perturbed. For the first parameter two strategies were tested: random splitting of a Hamiltonian circuit and generating solutions using path relinking. The second parameter, the selection method of the points to be changed, four categories were considered: all elements, random selection, nearest neighbor objective-space, and crowding distance ranking. In order to select the levels of these three parameters an experimental design was used for comparing the different parameters combinations or treatments. Five different treatments were considered in total, as it is shown in the two first column of Table 6.1. The first four instances were used as a blocking factor. Each treatment considered was run 30 times and the hypervolume was used as response variable.

The $p - value = 0.2758$ of a Friedman test shows that there is not significant statistical difference between the treatments. The path relinking method is selected for generating the initial solution and the crowding distances as approach for selecting the front elements to be perturbed.

The number of elements to be perturbed is another parameter to consider, smaller the number of the points selected, less the amount of time required to find a Pareto front approximation. This parameter is proposed as a function of the number of nodes of the problem instance n. Four different levels were tested: $0.75 \times n$, $1.5 \times n$, and all the front elements. Fewer the number of elements selected to be perturbed, less the value of the hypervolume indicator, however there is not a statically significance difference between the results obtained using all the elements of the current front and $1.5 \times n$, this last value is utilized for running all the experiments.

In the case of the ϵ-constraint multi-objective local search algorithm the parameters to fix are: the objective function f_i to be minimized, the number of n_Δ division points for the range of the other objective function, and the starting solution in the local search for the next grid point. After some experimentation the routing risk is selected as the objective function to be minimized, and the local search for the next grid point is always started from the best cost solution. The number of n_Δ points depends on the minimum and maximum value of the cost function, and this value was fixed to 1000 (Friedman test, $p - value = 0.01832$) after testing the values of 500, 1000 and 2000.

6.5.2 Results

The results are organized and presented by the number of nodes of the instances. Table 6.2 summarizes the results for instances with 20 demands. Figure 6.6 shows some examples of the Pareto front approximations for the twenty node instances obtained using the dominance-based multi-objective local search algorithm (○) and the ϵ-constraint multi-objective local search algorithm (△). Table 6.2 and Figure 6.4 show that indeed, the simultaneous minimization of total cost and of total risk are conflicting objectives. The multi-objective dominance-based local search algorithm performs better than the multi-objective ϵ-constraint local search algorithm except for the instance number four (4), as show the values of hypervolume and Δ metric. The Δ metric increases with the value of the hypervolume given the shape of the Pareto front approximation (see Figure 6.6), which presents some discontinuities, or unsupported efficient solutions. The value of slope is close to zero next to extreme point for the best risk and tends to increase close to the extreme point for the best cost. The different Pareto-front approximations shows that an important decreasing in risk can be achieved at the cost of a small increase in the total routing cost near the best cost solution, but it is the opposite case when we are

Table 6.2: Results for bi-objective optimization for 20 nodes instances of FSMVRP HazMat transportation problem

	Multi-objective VNS			$\epsilon-$Constraint		
Instance number	Average time (s)	Average hypervolume	Average Δ metric	Average time (s)	Average hypervolume	Average Δ metric
3	25.97	0.9238	0.8143	40.89	0.8821	0.6964
4	33.24	0.8160	0.5976	38.93	0.8861	0.6155
5	32.43	0.8716	0.7465	34.57	0.7849	0.6324
6	81.55	0.7883	1.6555	44.89	0.7712	1.4729

close to the best risk solution.

For the 20 node instances the percentage of cost ranges from 18% to 50% in order to be located in the first 10% of the risk value range for the 20 nodes instances.

The dominance-based multi-objective local search algorithm behaves better in terms of the convergence to the real Pareto front based on the observed hypervolume values. As the number of the elements to be perturbed taken from the approximation of the Pareto front depends on the number of nodes of the problem instance, the time for the instances with a large number of nodes is increasing, given the apparently large number of members of the real Pareto front. In the case of the ϵ-constraint multi-objective algorithm based on local search, it seems the quality of the constrained solutions have to be improved somehow to improve its convergence.

The results for fifty node instances are presented in Table 6.3 and Figure 6.7. Also for these instances, the dominance-based local search algorithm performs better than the $\epsilon-$constraint algorithm. The number of non-dominated solutions found by the first algorithm is higher. As in the case of instance 4, for instance 14, the second algorithm presents a better hypervolume value thanks to a closer approximation of the middle part of the front as it is portrayed in Figure 6.7. For the 50 nodes instances, the percentage of cost ranges from 12% to 40% in order to be located in the first 10% of the risk value range.

Table 6.4 and Figure 6.8 present the results for the 75 and 100 node instances. In this case the dominance-based algorithm performs better than the ϵ-constraint algorithm. For the 100 nodes, instances where more discontinuities are portrayed in the Pareto-front approximation by the dominance-based algorithm, the ϵ-constraint algorithm underperforms in the Pareto-front approximation. The percentage of cost range goes from 18% to 38% in order to be located in the first 10% of the risk value range for the 100 nodes instances.

The computation time for the the multi-objective neighborhood dominance-

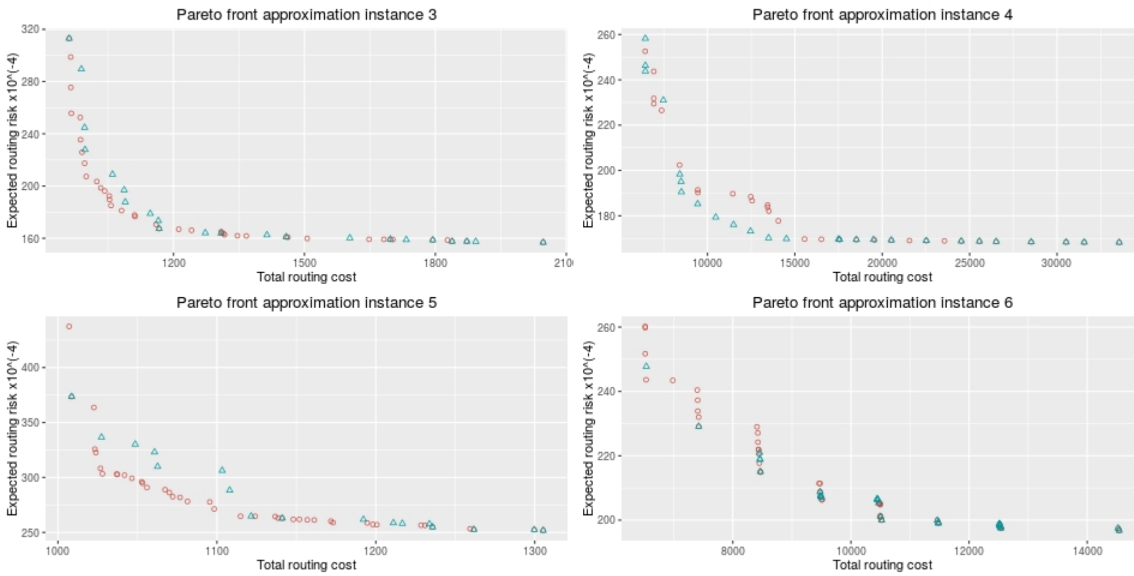


Figure 6.6: Pareto front approximation. Dominance-based multi-objective local search algorithm ○ and ϵ-constraint multi-objective local search algorithm △ 20 node instance

Table 6.3: Results for bi-objective optimization for 50 nodes instances of FSMVRP HazMat transportation problem

	Multi-objective VNS			$\epsilon-$Constraint		
Instance number	Average time (s)	Average hypervolume	Average Δ metric	Average time (s)	Average hypervolume	Average Δ metric
13	1393.24	0.7793	0.8807	199.26	0.7019	0.7374
14	840.38	0.929	1.2768	201.41	0.9239	0.7547
15	647.28	0.8951	1.2428	203.81	0.8634	0.9023
16	953.36	0.8357	0.9706	157.21	0.7257	0.7561

Table 6.4: Results for bi-objective optimization for 75 and 100 node instances of FSMVRP HazMat transportation problem

		Multi-objective VNS			$\epsilon-$Constraint		
Instance number	Number of nodes	Average time	Average hypervolume	Average Δ metric	Average time	Average hypervolume	Average Δ metric
17	75	2433.61	0.873	1.0483	560.98	0.7907	0.7446
18	75	7761.25	0.8979	1.4526	542.73	0.8344	0.9276
19	100	3945.71	0.8625	1.3429	1512.68	0.7789	0.8448
20	100	5727.85	0.831	1.3287	545.6	0.3867	0.7861

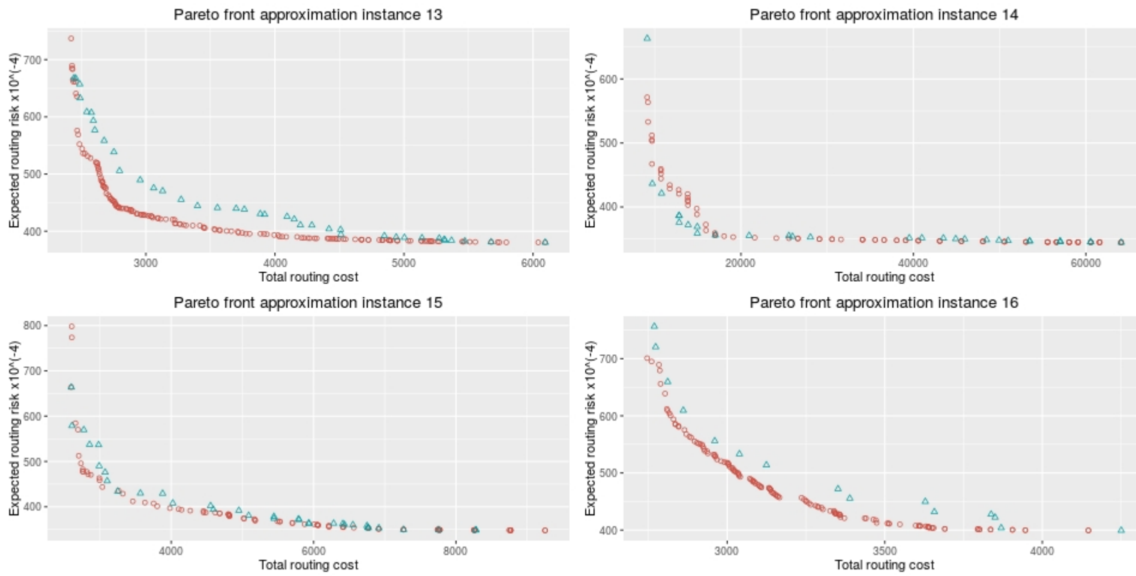


Figure 6.7: Pareto-front approximation. Dominance-based multi-objective local search algorithm ○ and ϵ-constraint multi-objective local search algorithm △ 50 node instances

based algorithm increases with the instance size, given the number of elements of the Pareto front approximation to be perturbed depends on the number of nodes. In the case of the ϵ-constraint multi-objective local search algorithm, as the number of n_Δ division points is fixed, the impact on the instance size is less.

6.6 Conclusions

6.6.1 Conclusions (English)

The bi-objective heterogeneous fleet vehicle routing (HVRP) problem for hazardous materials (HazMat) transportation problem is presented to determine a set of routes that minimizes simultaneously two conflicting objectives, the total routing risk, and the total transportation cost. Two algorithms are proposed for approximating the Pareto front, a dominance-based multi-objective local search algorithm and an ϵ-constraint multi-objective algorithm based on local search. The first algorithm is a generating or no-preference method and the second one is a scalarization method. The hypervolume indicator and the Δ metric are used to evaluate the performance of the two methods. The approximation of the Pareto front of different

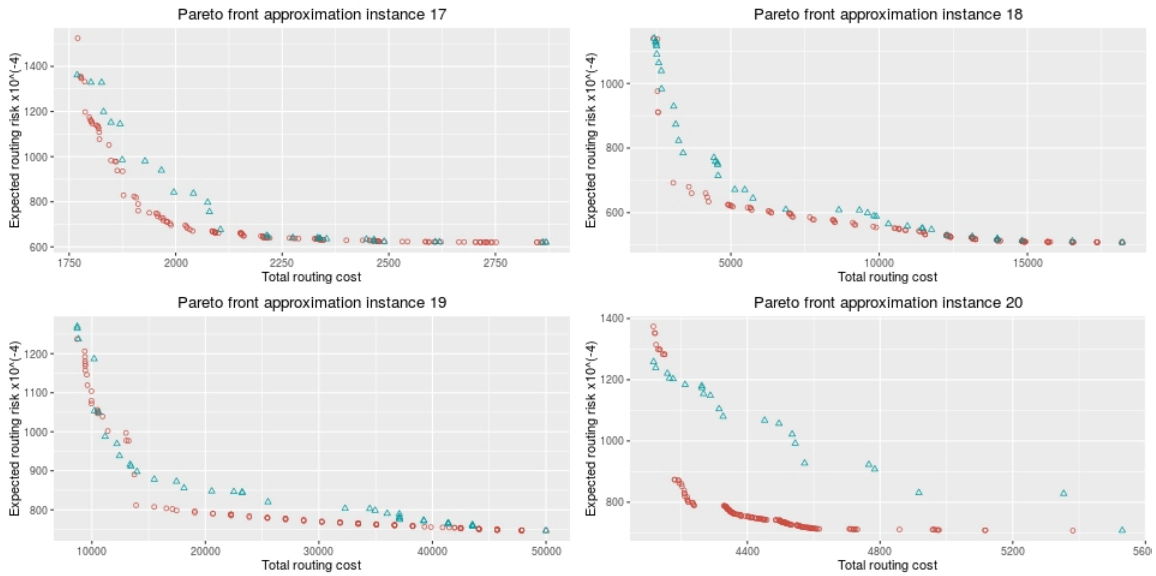


Figure 6.8: Pareto-front approximation. Dominance-based multi-objective local search algorithm ○ and ϵ-constraint multi-objective local search algorithm △ 75 and 100 node instances

studied instances of the problem presents non-supported efficient solutions.

For the studied problem, the algorithm that constructs the whole picture of the Pareto front, dominance-based local search, has a better behavior in terms of the quality of the approximation than the algorithm that uses the scalarization approach, ϵ-constraint. Both algorithms are based on a local search approach and the adaptation to the multi-objective optimization implied the management of the intensification and diversification strategies. The main disadvantage of the ϵ-constraint multi-objective algorithm based on local search is the lack of guarantee of efficiency of the obtained solutions for the constrained problem, and in the case of the dominance-based multi-objective local search algorithm, it is the rapid convergence to some local zones of the Pareto front.

The results indicate that trade-offs between the two conflicting objectives, the total transportation cost and the total expected routing risk, imply a large increment to be made with respect to the total routing cost in order to reduce the total risk routing when close to the minimum risk. However, there is a zone in the Pareto front close to the minimum risk where the total routing cost is not highly compromised in order to achieve a significant reduction in the total routing risk. Multi-objective optimization is an useful tool for providing alternative routes to HazMat shippers that represent an acceptable risk for the authorities and the people living close to the roads.

6.6.2 Conclusions (Français)

Le problème bi-objectif de tournées de véhicules à flotte hétérogène (HVRP) pour le transport de matières dangereuses (HazMat) est présenté pour déterminer un ensemble de tournées minimisant simultanément deux objectifs contradictoires, le risque total de routage et le coût total de transport. Le modèle mathématique est rappelé ici:

$$\min z_1 = C(\mathcal{SR}) = \sum_{(i,j)\in\mathcal{L}} \sum_{k\in\mathcal{K}} x_{ij}^k al_{ij} + \sum_{j\in\mathcal{N}\setminus\{0\}} \sum_{k\in\mathcal{K}} FC_k x_{0j}^k \tag{6.35}$$

$$\min z_2 = R(\mathcal{SR}) = P_{release} \times \beta \times \sum_{(i,j)\in\mathcal{L}} \sum_{k\in\mathcal{K}} TTAR^k \times \rho_{ij} \times t_{ij}^k \tag{6.36}$$

sujet à:

$$t_{ij}^k = t_0 + \sum_{m=1}^{M} b_{ij}^m \lambda_{ijk}^m \ \forall i,j \in \mathcal{N} \ \ i \neq j, \ \forall k \in \mathcal{K} \tag{6.37}$$

$$y_{ij}^k = l_0 + \sum_{m=1}^{M} \lambda_{ijk}^m \ \forall i,j \in \mathcal{N} \ \ i \neq j, \ \forall k \in \mathcal{K} \tag{6.38}$$

$$\lambda_{ijk}^1 \leq l_1 - l_0 \ \forall i,j \in \mathcal{N} \ \ i \neq j, \ \forall k \in \mathcal{K} \tag{6.39}$$

$$\lambda_{ijk}^m \geq (l_m - l_{m-1}) h_{ijk}^m \quad \begin{array}{l} \forall i,j \in \mathcal{N} \ \ i \neq j, \ \forall k \in \mathcal{K} \\ m = 1, \cdots, M-1 \end{array} \tag{6.40}$$

$$\lambda_{ijk}^{m+1} \leq (l_{m+1} - l_m) h_{ijk}^m \quad \begin{array}{l} \forall i,j \in \mathcal{N} \ \ i \neq j, \ \forall k \in \mathcal{K} \\ m = 1, \cdots, M-1 \end{array} \tag{6.41}$$

$$\sum_{k\in\mathcal{K}} \sum_{i\in\mathcal{N}} x_{ij}^k = 1, \ \forall j \in \mathcal{N} \setminus \{0\} \tag{6.42}$$

$$\sum_{i\in\mathcal{N}} x_{ij}^k - \sum_{i\in\mathcal{N}} x_{ji}^k = 0, \ \forall k \in \mathcal{K}, \forall j \in \mathcal{C} \tag{6.43}$$

$$\sum_{k\in\mathcal{K}} \sum_{i\in\mathcal{N}} y_{ij}^k - \sum_{k\in\mathcal{K}} \sum_{i\in\mathcal{N}} y_{ji}^k = q_j, \ \forall j \in \mathcal{C} \tag{6.44}$$

$$q_j \sum_{k\in\mathcal{K}} x_{ij}^k \leq \sum_{k\in\mathcal{K}} y_{ij}^k \; \forall i,j \in \mathcal{N},\; i \neq j \tag{6.45}$$

$$y_{ij}^k \leq x_{ij}^k (Q_k - q_i) \; \forall i,j \in \mathcal{N} \;\; i \neq j,\; \forall k \in \mathcal{K} \tag{6.46}$$

$$\lambda_{ijk}^m \geq 0,\; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L},\; m = 1,\cdots,M \tag{6.47}$$

$$h_{ijk}^m \; \in \{0,1\},\; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L},\; m = 1,\cdots,M \tag{6.48}$$

$$t_{ij}^k \geq 0,\; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L} \tag{6.49}$$

$$y_{ij}^k \geq 0,\; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L} \tag{6.50}$$

$$x_{ij}^k \in \{0,1\},\; \forall k \in \mathcal{K}, \forall (i,j) \in \mathcal{L} \tag{6.51}$$

Les équations (6.35) et (6.36) expriment des fonctions objectives pour minimiser le coût total et le risque total des tournées, respectivement. Les contraintes (6.37)-(6.41) sont utilisées pour la valeur d'approximation linéaire par morceaux de $(y_{ij}^k)^\alpha$. L'ensemble des contraintes (6.42) assure que chaque client est visité exactement une fois, et l'ensemble (6.43) et (6.44) représentent les contraintes de conservation de flux. De plus, (6.44) garantit la satisfaction des demandes. Les contraintes (6.45) et 6.46) indiquent qu'aucune marchandise n'est transportée de i à j si aucun véhicule ne sert l'arc (i,j), et (6.46) définit la charge du véhicule k en parcourant arc (i,j).

Deux algorithmes sont proposés pour l'approximation du front de Pareto de ce problème, un algorithme de recherche locale multi-objectif basé sur la dominance et un algorithme multi-objectif de type ϵ-contrainte basé sur la recherche locale. Le premier algorithme est une méthode de génération ou de non-préférence dont l'algorithme est rappelé ci-dessous.

Algorithme 12. Algorithme générale de recherche locale multi-objectif basé sur la dominance Pareto

---

1: Définir $\{z_1(PS(ni)_v), z_2(PS(ni)_v)\}$,$X$, Sélectionner l'ensemble des structures de voisinage de perturbation N_s, par $s = 1,\cdots,S$, et $mnop$ le nombre maximum des permutations.

Générer une approximation initiale de l'ensemble de solutions potentiellement efficaces $PS(ni = 0)$
Premire approximation de la frontière Pareto $\mathcal{PF} \leftarrow \{[z_1(PS(ni)_v), z_2(PS(ni)_v)] | v = 1, \ldots, |PS(ni)|\}$
$I_{hv} \leftarrow Hypervolume(\mathcal{PF})$
$perturbations \leftarrow 1$
while $perturbations \leq mnop$ **do**
  $PS^{'}(ni),\ \mathcal{PF}^{'} \leftarrow \emptyset,\ \emptyset$
  Sélectionner $PS(ni)_{subset} \subseteq PS(ni)$
  for $PS(ni)_v \in PS(ni)_{subset}$ **do**
    $\{PS'(ni)_v^1, PS'(ni)_v^2\} \leftarrow \{PS(ni)_v, PS(ni)_v\}$
    $ol \leftarrow 1$
    while $ol \leq 2$ **do**
      $PS(ni)_u \leftarrow PS^{'}(ni)_v^{ol}$
      $s \sim U[1, 2, \cdots, S]$
      Faire la perturbation $PS(ni)_u, PS'(ni)_u \leftarrow N_p(PS(ni)_u)$
      $\{PS'(ni)_u, PF_{local}\} \leftarrow$ Recherche locale $(PS'(ni)_u)$
      $flag \leftarrow false$
      for $p \in \{1, 2\}$ **do**
        if $z_p(PS'(ni)_u) < z_p(PS'(ni)_v^p)$ **then**
          $PS'(ni)_v^p \leftarrow PS'(ni)_u$
          $ol \leftarrow 1$
          $flag \leftarrow true$
        end if
      end for
      if $flag$ **then**
        Mise jour de la frontière $(\mathcal{PF}^{'}(ni), \mathcal{PF}_{local\,u})\ u = 1, \ldots, |\mathcal{PF}_{local}|$
      else
        $ol \leftarrow ol + 1$
      end if
    end while
    for $PF(ni)_u \in PF(ni)$ **do**
      $PF'(ni) \leftarrow$ Mise jour de la frontière$(PF^{'}(ni), \{z_1(PS(ni)_u), z_2(PS(ni)_u)\})$
    end for
  end for
  if $Hypervolume(PF') > I_{hv}$ **then**
    $PS(ni),\ \mathcal{PF} \leftarrow PS^{'}(ni),\ \mathcal{PF}^{'}$
    $I_{hv} \leftarrow Hypervolume(PF)$
    $perturbations \leftarrow 1$
  else

$perturbations \leftarrow perturbations + 1$
end if
$ni \leftarrow ni + 1$
end while

et le second est une méthode de scalarisation dont voici l'algorithme:

Algorithme 13. Algorithme ϵ-contrainte pour la minimisation des coûts et des risques des tournées

---

Définir $\vec{z} = \{z_1(x), z_2(x)\}$, $X, n_\Delta, f^U_{Cost}, f^U_{Risk}, f^{SN}_{Cost}, f^{SN}_{Risk}$
$\Delta_{Cost} = \frac{f^{SN}_{Cost} - f^U_{Cost}}{n_\Delta}$
$\epsilon_{Cost} = f^U_{Cost}$
Initialiser un ensemble de solutions efficaces $ES \leftarrow \{\}$
while $\epsilon_{Cost} + \Delta_{Cost} < f^{SN}_{Cost}$ **do**
  $\epsilon_{Cost} = \epsilon_{Cost} + \Delta_{Cost}$
  $x^*_{constrained} \leftarrow \min z_2(x),\ s.t.\ z_1(x) \leq \epsilon_{Cost} \wedge x \in X$
  $\vec{z}_a \leftarrow (z_1(x^*_{constrained}), z_2(x^*_{constrained}))$
  $\epsilon_{Risk} = z_2(x^*_{constrained})$
  $x^{'*}_{constrained} \leftarrow \min z_1(x),\ s.t.\ z_2(x) \leq \epsilon_{Risk} \wedge x \in X$
  $\vec{z}_b \leftarrow (z_1(x^{'*}_{constrained}), z_2(x^{'*}_{constrained}))$
  if $\vec{z}_a \preceq \vec{z}_b$ **then**
    $ES \leftarrow ES \cup x^*_{constrained}$
  else
    $ES \leftarrow ES \cup x^{'*}_{constrained}$
  end if
end while

Pour évaluer la performance de ces méthodes, deux indicateurs sont utilisés: l'hypervolume et métrique Delta. L'approximation du front de Pareto des différentes instances étudiées du problème présente des solutions efficaces non supportées.

Pour le problème étudié, l'algorithme de recherche locale basé sur la dominance a un meilleur comportement en termes de qualité de l'approximation que l'algorithme qui utilise l'approche ϵ-contrainte. Les deux algorithmes utilisent une approche de recherche locale et l'adaptation nécessaire à l'optimisation multi-objectif implique la gestion des stratégies d'intensification et de diversification.

Le principal inconvénient de l'algorithme multi-objectif de type ϵ-contrainte basé sur la recherche locale est le manque de garantie d'efficacité des solutions *obtenues pour le problème contraint, dans le cas de l'algorithme basé sur la dominance, c'est la convergence rapide vers certaines zones locales du front de Pareto. Les résultats indiquent que les compromis entre les deux objectifs contradictoires, le coût total du transport et le risque total d'acheminement prévu, induisent une augmentation importante du coût total de routage afin de réduire le risque total à proximité du risque minimum. Cependant, il existe une zone dans le front de Pareto proche du risque minimum où le coût total de routage n'est pas fortement compromis afin d'obtenir une réduction significative du risque de routage total. L'optimisation multi-objectif est un outil utile pour fournir des itinéraires alternatifs aux transporteurs de HazMat, en proposent un risque acceptable pour les autorités et les personnes vivant à proximité des routes.*

6.6.3 Conclusiones (Español)

Se presenta el problema bi-objetivo de transporte de materiales peligrosos (HazMat) con una flota heterogénea de vehículos (HVRP), se busca determinar un conjunto de rutas que minimice simultáneamente dos objetivos en conflicto, el riesgo total de ruteo y el costo total de transporte. Se proponen dos algoritmos para aproximar el frente de Pareto, un algoritmo de búsqueda local multi-objetivo basado en la dominancia de Pareto y un algoritmo multi-objetivo ϵ-constraint, ambos basados en la búsqueda local. El primer algoritmo es un método generativo o de no preferencia y el segundo es un método de escalarización. El indicador de hypervolumen y la métrica Δ se utilizan para evaluar el rendimiento de los dos métodos. Los resultados muestran que la aproximación del frente de Pareto para las diferentes instancias del problema estudiado presenta soluciones eficientes no soportadas.

Para el problema estudiado, el algoritmo que construye la imagen completa de el frente de Pareto, búsqueda local basada en la dominancia Pareto, tiene un mejor comportamiento en términos de la calidad de la aproximación que el algoritmo que usa el enfoque de escalarización, ϵ-constraint. Ambos algoritmos se basan en un enfoque de búsqueda local y la adaptación a la optimización multi-objetivo implica la gestión de las estrategias de intensificación y diversificación. La principal desventaja del algoritmo multi-objetivo ϵ-constraint basado en la búsqueda local es la falta de garantía de la eficiencia de las soluciones obtenidas para el problema restringido, y en el caso del algoritmo de búsqueda local multi-objetivo basado en dominancia Pareto, es la rápida convergencia a algunas zonas locales del frente de Pareto.

Los resultados indican que los trade-offs entre los dos objetivos en conflicto, el costo total de transporte y el riesgo total de ruteo, implican un gran incremento del costo total de ruteo para reducir el riesgo total ruteo cuando se está cerca del *riesgo mínimo. Sin embargo, hay una zona en el frente de Pareto cercana al riesgo mínimo donde el costo total de ruteo no está muy comprometido para lograr una reducción significativa en el riesgo total de ruteo. La optimización multi-objetivo es una herramienta útil para proporcionar rutas alternativas a los transportistas de materiales peligrosos que representen un riesgo aceptable para las autoridades y las personas que viven cerca de las redes de rutas utilizadas.*

Chapter 7

Conclusions, Recommendations and Perspectives

7.1 Conclusions, Recommendations and Perspectives (English)

This work addresses the less studied variant of routing problem in hazardous materials transportation, the vehicle routing problem. Aiming at a more realistic approach a heterogeneous fleet is considered, and at the time of the routing risk analysis, a function depending on the type of transported material, the truck type, the load size and some characteristics of the traversed arc is considered. Former studies suggest that the routing risk estimation function that includes the previously stated variables is nonlinear, and given the availability of suitable solutions methods for the mixed linear programming formulation used for modeling the heterogeneous fleet vehicle routing problem, a piecewise linear approximation of the routing risk objective function is taken into consideration. Hazardous transportation is multi-objective in nature, different stakeholders have different conflicting objectives that demand trade-off solutions. Study the hazardous material transportation problem implies to consider other objectives that the routing risk minimization problem. The leading aim of this study is to study the multi-objective vehicle routing problem in the context of hazardous material transportation using a heterogeneous fleet, and design methods for approximating the Pareto-front and Pareto-efficient set of this multi-objective combinatorial optimization problem.

To accomplish the study goal, first, a mathematical model for the bi-objective heterogeneous fleet vehicle routing optimization problem is constructed. This formulation is based on the three-index flow variables formulation for the heterogeneous fleet vehicle routing problem when total routing cost is minimized, but here the simultaneous minimization of the total routing risk is also taken into account. The mathematical formulation of the multi-objective vehicle routing problem implies to have mathematical relationships to express both objective functions, and the constraints that define the search space. The total routing cost objective function is taken from the literature review about the heterogeneous fleet vehicle routing problem; but the total routing risk objective function is constructed based on studies related to vehicle transportation accidents when transporting hazardous material using road networks, and the different possible incident outcomes. The elements considered for the risk assessment when a vehicle is traversing a path are: the estimation of the hazardous material transportation incident probability, the incident outcomes, and the consequences or impact over exposed receptor, the population. This quantification of the risk depends on the type of truck used for transporting the material, the type of material carried by the vehicle or truck, the size of the load when traversing the path, and the population neighboring the segment composing the path between two stop truck points. This risk route assessment mathematical model is nonlinear and a piecewise linear approximation is employed in order to keep as a modeling framework the mixed integer linear programing. The heterogeneous fleet vehicle routing problem test instances used in the literature were extended to include the parameters for computing total routing risk objective function, keeping the search space for the routing decision variables. Small number node instances were solve using commercial solver for mixed integer linear optimization problems with the aim at proving the conflicting nature of the two considered objective, and having a measure of the required computing time to get an exact solution of this, relatively easy to solve, instances.

Hybrid solution methods implementation based on neighborhood search are explored for solving the routing risk minimization given that they have proved to give good results when minimizing the total routing cost. These solutions algorithms are meta-heuristics based on local or neighborhood search algorithms. The hybrid method developed to solve the mono-objective problem is based on variable neighborhood search with inter and intra route moves. Efficient neighborhood exploration needs a fast evaluation of a solution neighbor or candidate solution. Following the guide lines of the researched literature auxiliary, data structures were implemented to do this type of evaluation, but paying particular attention to the variation of the transportation risk evaluation of all the path segments in a tour caused by the changes in the load size and the truck type. Also, the evaluation of the transportation risk when reversing the tour node sequence is considered. An approximation of risk transportation computation is implemented which requires the inclusion of the acceptance criteria of candidate solution when exploring a neighborhood. A pre-computation of the risk parameter that regroups arc dependent parameters, length and population density, is performed. The contribution of the main components of the local search algorithm is analyzed, generation of initial solution, local search (intensification phase), perturbation (exploration phase) and post-optimization. The algorithm is tested on the heterogeneous fleet vehicle routing problem extended instances, proving to be competitive.

An adaption of the previous mono-objective algorithm based on local search is carried out. Two different no-preference or generating multi-objective optimization approaches are implemented: scalarization, through the development of an ε-constraint method; and vector optimization, based on Pareto-dominance method. Multi-objective vehicle routing problems are multi-objective combinatorial optimization problems and solution methods based on local search applied to solve these problems have not been sufficiently studied, compared to evolutionary or trajectory algorithms. One important problem to deal is the rapid convergence of local search algorithms, thus diversification strategies of neighborhood search are developed. The main multi-objective local search algorithm elements are studied: the generation of the initial solution, the selection of the Pareto-front approximation elements to be perturbed, over which the hybrid local search is implemented, and the size of the Pareto-front set approximation. An experimental design was used for selecting the level to fix the values of the parameters related to this algorithm elements. Two guiding multi-objective performance metrics are used for comparing the algorithm variation and performance: the hypervolumen and the Δ-metric. Each one of the solution approaches for the generating multi-objective optimization presents a main inconvenient to overcome: manage the solution diversity of the elements of the Pareto-front approximation, in the case of the Pareto-dominance, and to ensure the non-dominated solution nature in the case of constrained optimization.

The total routing cost and the total routing risk objective functions are indeed conflicting when the simultaneous optimization is carried out for the instances studied. The Pareto-front approximation presents non-supported solutions that demand the implementation of a dominance-Pareto methods instead of aggregating methods. In most of the studied instances the multi-objective dominance-Pareto approach shows a better performance in approximating the Pareto-front, using as algorithm performance metric the hypervolumen. Even though the conflicting nature of the concerned objectives, the Pareto-front shows that to accept small increment in the total routing cost can produce higher reduction in percentage of the expected consequences given the probability of a hazardous material transportation incident. The implementation of multi-objective optimization methods here developed gave as result solutions dispersed all along the Pareto-front. Shippers, freight transporter, consumers and government can take advantage of this behavior for an efficient and responsible transportation of the hazardous materials using street and road networks.

There are some important byproducts of this research. In order to complement the heterogeneous fleet vehicle routing instances a method was developed for generating the population that can be affected by an hazardous material incident, and this information was preprocessed for getting the parameter for each path segment between two nodes that integrates the population and distance of a segment. Also a simulation of the route belonging to a solution was developed in order to make a comparison between the real expected risk consequences and the approximation provided by the traditional risk model. An study was conducted for determining the impact of the local search move can have in providing good solutions to the cost routing problem and how the perturbation move and the post optimization elements can improve the results. Finally, a framework for the evaluation of the multi-objective algorithms was developed.

This work can be improved by using a more a richer measure for the risk assessment, namely the FN-curve. It would be necessary to study how to perform efficient evaluation of a candidate solution considering that this measure it is graph or can be represented as a double entry matrix. The risk measure used in this work is based on computing an approximation of the expected consequences, and in order to have this value, an estimation of the truck accident rate is required. This last value is obtained having as reference the truck but not the driver or managerial aspect for shift programming and truck maintenance or the traffic conditions that can change with the time. The population is considered fixed and independent of the time when the truck is traversing the segment path. Event though the time slot can be easily incorporated to the model given this can be considered a path segment associated element and there is already good studies about efficient ways to evaluate candidate solutions in local search for travel time aspects. Even though experimentation about the characteristics of the initial solution for having a good solution when the exploitation phase is applied there was not a conclusive answer for the its appropriate structure. Determining exactly which are the appropriate elements in the Pareto-front approximation to be selected to perform, it is let to the random selection this task. It would be a good idea to use some techniques and tools taken from machine learning to explore which solutions have more potential to improve a solution in both the diversification and the intensification spaces.

The approach used in this work can be applied to study the multi-objective variant of optimization problems in green logistics, energy-efficient transportation, valuable transportation. For instance, to reduce greenhouse gas (GHG) emissions, particularly carbon dioxide (CO_2), in vehicle routing problem, speed and acceleration, which have a large impact on a vehicle fuel economy and exhaust gases expelled by the engine, has to be incorporate into the model. Vehicle fuel consumption measure is used as bypass for the greenhouse gas emissions, and this is a function of vehicle speed, load and engine type; and the arc characteristics.

This function is nonlinear and the approximation using piecewise linear functions can be implemented and hybrid methods based on neighborhood search used for finding good solutions.

Also, it is intended with this work to incentive the research in multi-objective combinatorial optimization based on neighborhood search. Efficient and effective methods that exploit the good performance of local search based algorithms when solving mono-objective problems. This work is limited to two objectives, more than two objective problem needs also to be explored.

7.2 Conclusions, recommandations et perspectives (Français)

Ce travail réalisé comportant le problème des tournées de véhicules transportant des substances dangereuses a pour but de prendre en compte une flotte hétérogène ainsi qu'une évaluation du risque en fonction du type de matière transportée, du véhicule ainsi que le chemin choisi. Des études précédentes ont supposé que la fonction du risque qui prend en compte les variables citées ci-dessus est forcément non linéaire. De ce fait, en prenant en compte l'existence des méthodes de programmation linéaire pouvant réaliser une modélisation du problème de tournée de véhicules hétérogènes, une approximation linéaire approchée de la fonction objective du risque de la tournée a été considérée. Le transport de substances dangereuses est un problème multi-objectif en nature, chaque décideur a ses propres intérêts et objectifs qui peuvent entrer en conflits avec d'autres. Il est donc nécessaire de chercher un compromis entre les différents objectifs. L'étude de ce type de problème a pour but de prendre en compte d'autres objectifs autre que la minimisation du risque associé au transport. De ce fait, l'objectif principal de ce travail est d'étudier le problème de tournée de flotte de véhicules hétérogène transportant des substances dangereuses, et de proposer ainsi les approximations de front et optimum Pareto pour ce problème combinatoire et multi-objectif.

Pour ceci, un modèle mathématique bi-objectif modélisant le problème des tournées de véhicules avec une flotte hétérogène a été construit. Il se base sur le modèle à trois indexes avec variables de flux du problème de minimisation du coût total de la tournée. On a aussi pris en compte simultanément lors de cette modélisation la minimisation du risque de la tournée. Ce type de modélisation multi-objective nécessite une relation mathématique entre les objectifs, ainsi que les différentes contraintes existantes. La fonction objective du coût de la tournée totale de véhicules hétérogènes a été prise de la littérature. Cependant, la fonction objective du risque a été construite à partir de ce travail. De ce fait, les éléments pris en compte dans la fonction du risque d'un véhicule sur une voie sont: la probabilité d'un incident impliquant les substances dangereuses, les dégâts de l'incident incluant aussi les conséquences sur la population. La quantification du risque dépend aussi du type de véhicule, de la matière transportée de son chargement et de la population avoisinante du chemin parcouru entre deux points. Ce type d'évaluation de risque est non linéaire et donc un affinage par morceaux a été utilisé pour approximer cette fonction et l'utiliser en optimisation linéaire en nombres entiers. Aussi, le nombre d'instances utilisés dans la littérature a été augmenté pour prendre en compte aussi les variables ajoutées dans notre étude. On a ensuite simulé la fonction objective du risque total de la tournée. Des instances à un nombre petit de nœuds ont été résolues en utilisant des solveurs commerciaux pour l'optimisation linéaire en nombre entiers de ce problème. Ceci a été fait pour prouver le conflit entre les deux fonctions objectives choisies, et aussi pour avoir une estimation du temps nécessaire pour avoir une solution exacte.

Quant à la minimisation du risque, des solutions de méthodes hybrides ont été explorées, en prenant en compte leur efficacité dans la minimisation du coût total de la tournée. Ces solutions se basent sur des algorithmes méta-heuristiques et sont basées sur algorithmes de recherche locale ou de recherche de voisinage. La méthode hybride proposée pour résoudre le problème mono-objectif est basée sur la recherche à voisinage variable (VNS) en prenant en compte les mouvements inters et les intra chemins. L'exploration efficace du voisinage nécessite une évaluation rapide d'une solution avoisinante ou d'une autre candidate. En se basant sur les principales méthodes de la littérature, des structures auxiliaires des données ont été implémenté dans ce type d'évaluation en prenant en compte l'évaluation de la variation du risque lié au transport dans tous les segments d'une tournée causé par le changement du type du véhicule ou de sa capacité. De plus, l'évaluation du risque dans le chemin retour a aussi été considérée. Une approximation au calcul du risque lié au transport a aussi été prise en compte, ce qui a nécessité l'inclusion des critères d'acceptation des solutions candidates quand on réalise une recherche local. De ce fait, une pré-calcul du paramètre du risque regroupant les paramètres dépendants du chemin, sa longueur ainsi que la densité de la population a été réalisée. Une analyse de la contribution des principaux composants de l'algorithme de recherche locale a été réalisée, i.e.la génération de la solution initiale, la recherche locale (phase d'intensification), la perturbation (phase d'exploration) ainsi que la post-optimisation. L'algorithme a été testé sur un problème de tournée de véhicules d'une flotte hétérogène avec de grandes instances, prouvant son efficacité.

Une adaptation de l'algorithme mono-objectif précèdent basé sur la recherche locale a été réalisé. Deux approches d'optimisation multi-objective ont été implémentées: la scalarisation à travers le développement d'une méthode à ϵ-contrainte, et une optimisation de vecteur basée sur la méthode de dominance de Pareto. Les problèmes de tournées de véhicules multi-objectifs sont des problèmes combinatoires, et leurs solutions se basant sur la recherche locale n'ont pas encore été suffisamment étudiées (comparé aux algorithmes évolutionnaires ou trajectoires). Le problème le plus important à prendre en compte est la convergence rapide de l'algorithme de recherche locale. Par conséquent, divers stratégies de recherches locales ont été développées. Les éléments d'algorithme multi-objectif de recherche locale ont été étudiés: la génération de la solution initiale, la sélection de l'approximation du front de Pareto des éléments perturbés; sur lesquels la méthode hybride a été appliquée; ainsi que la taille de l'approximation établie du front de Pareto. Pour sélectionner le niveau des valeurs des paramètres de l'algorithme, on a utilisé une méthode expérimentale. Aussi, deux indicateurs de performance de guidage multi-objectif ont été utilisé pour comparer la variation et la performance de l'algorithme: l'hyper volume ainsi que l'indicateur Δ. Chacune des solutions approchées de l'optimisation multi-objective générée présente un inconvénient majeur à surmonter: manager la diversité de solution des éléments de l'approximation front de Pareto; dans le cas d'une dominance Pareto; et assurer une solution non dominante dans le cas d'une optimisation à contrainte.

Certes, les fonctions objectives du coût total et du risque total de la tournée sont en conflits lors d'une optimisation simultanée pour les instances étudiées. L'approximation du front de Pareto présente des solutions non supportées qui demandent l'implémentation d'une méthode de dominance Pareto au lieu d'une méthode d'agrégation. Dans les exemples les plus étudiées, l'approche par approximation multi-objective de la dominance Pareto présente une meilleure performance lors de l'approximation du front de Pareto, et ceci en utilisant l'indicateur d'hyper volume. Même en cas de conflit de la nature des deux fonctions objectives, le front de Pareto démontre que l'acceptation d'une petite incrémentation du coût total de la tournée peut produire des réductions importantes des conséquences prévisionnelles en fonction de la probabilité d'incident d'un véhicule transportant des substances dangereuses. L'implémentation de la méthode multi-objective utilisée dans ce problème a générée des solutions dispersées tout au long du front Pareto. Les chargeurs, fréteurs, clients et gouvernement pourraient prendre avantage de ce comportement pour transporter de manière plus efficace et responsable tout matériel dangereux en utilisant le réseau routier.

Cette recherche a ainsi générée d'autres résultats. Une méthode de génération de la population affectée par un incident de substances dangereuses a été développée, ceci vient complémenter la tournée de flotte de véhicule hétérogène. Cette information a été utilisée pour générer le paramètre de chaque segment de chemin entre deux points qui intègre la population et la distance de ce segment. Aussi, une simulation du chemin appartenant à la solution a été développée pour réaliser une comparaison entre les conséquences réelles du risque et l'approximation proposée par le modèle de risque traditionnel. Une étude a été menée pour déterminer l'impact de la recherche locale qui pourrait générer de bonnes solutions du coût de la tournée de véhicules et comment le coup de perturbation ainsi que les éléments de la post optimisation pourraient améliorer les résultats. Finalement, un modèle d'évaluation de l'algorithme multi-objectif a été développé.

Ce travail pourrait être amélioré en utilisant une évaluation plus concise du risque, notamment la courbe-FN. Il est en effet nécessaire d'étudier comment évaluer efficacement une solution candidate en prenant en compte que cette dernière est un graphe ou représentée comme une matrice double. La mesure du risque utilisée dans ce travail est basée sur une approximation simulée des conséquences prévisionnelles, et pour avoir cette valeur, il est nécessaire de réaliser une estimation du taux d'accident d'un camion. Cette dernière valeur a été obtenue en prenant seul en compte le camion et non pas le conducteur ou l'aspect manageriel du programme de remplacement et de maintenance ou les conditions du trafic qui changent au cours du temps. Aussi, la population est considérée stable et est indépendante du temps lors d'un passage d'un camion par un segment de route. Autant que le créneau horaire pourrait être inséré facilement dans le modèle en l'associant à chaque segment de chemin. Il y a en effet plusieurs études sur comment évaluer une solution dans une recherche locale avec aspect temporel. Aussi, il n'y a pas de conclusion sur une méthode appropriée sur la phase d'exploitation même si l'expérimentation sur les caractéristiques de la solution initiale a générée de bons résultats. Il est aussi gardé aléatoire le choix de sélection d'évaluation des éléments pour l'approximation du front de Pareto. Il serait donc intéressant d'utiliser quelques techniques d'apprentissage pour explorer quelle solution aurait le plus de potentiel pour améliorer la solution dans son espace de diversification et d'intensification.

Cette approche utilisée dans ce rapport pourrait aussi être appliquée pour des études d'optimisation multi-objectives dans la logistique verte, le transport avec efficacité énergétique et le transport de valeur. Par exemple, on pourrait utiliser ce modèle pour réduire les émissions de gaz à effet de serre (GES), et plus particulièrement le CO2 dans la tournée de véhicules. On pourrait aussi l'appliquer au problème d'accélération de décélération qui a un impact majeur sur l'économie du carburant et sur les rejets du véhicule. La mesure de consommation en carburant du véhicule a été utilisée comme substitut aux émissions GES, qui est en fonction de la vitesse du véhicule, sa charge ainsi que son type de moteur, ainsi que les autres caractéristiques du chemin. Cette dernière fonction est non linéaire et donc on devrait utiliser une approximation linéaire par morceaux ainsi que d'autres méthodes hybrides basées sur la recherche de voisinage pour trouver de bons résultats.

Aussi, il est sous-entendu avec ce travail d'inciter la recherche en optimisation multi-objective combinatoire basée sur le recherche de voisinage. En effet, il existe des méthodes efficaces qui exploitent la bonne performance des algorithmes de la recherche locale utilisés pour résoudre les problèmes mono-objectifs. Ce travail est limité à deux objectifs, le problème à plus de deux objectifs devrait aussi être exploré.

7.3 Conclusiones, Recomendaciones y Perspectivas (Español)

Este trabajo aborda la variante menos estudiada del problema de ruteo el transporte de materiales peligrosos, el problema de ruteo del vehículos. Buscando un enfoque más realista se considera una flota heterogénea, y al momento del análisis de riesgo para una ruta, se considera una función que depende del tipo de material transportado, el tipo de camión, el tamaño de la carga y algunas características del segmento atravesado. Estudios anteriores sugieren que la función de estimación de riesgo de ruteo que incluye las variables previamente establecidas no es lineal. Dada la disponibilidad de métodos de soluciones adecuados para formulaciones del tipo programación lineal mixta, utilizadas para modelar el problema de ruteo de vehículos de flota heterogénea, una aproximación lineal por partes de la función objetivo de riesgo de ruteo se toma en consideración. El transporte de materiales peligrosos es multi-objetivo por naturaleza, diferentes partes interesadas tienen diferentes objetivos, muchas veces conflictivos, que exigen soluciones negociadas (*trade-offs*). Estudiar el problema del transporte de materiales peligrosos implica considerar otros objetivos además de la minimización del riesgo de ruteo. El objetivo principal de este estudio es el problema de ruteo de vehículos multi-objetivo en el contexto del transporte de materiales peligrosos utilizando una flota heterogénea, y los métodos de diseño para aproximar el conjunto del frente-Pareto y el conjunto Pareto-eficiente de este problema de optimización combinatoria multi-objetivo.

Para lograr el objetivo de estudio, primero, se construye un modelo matemático para el problema de optimización de ruteo de vehículos de la flota heterogénea bi-objetivo. Este modelo se basa en la formulación de variables de flujo con tres índices para el problema de ruteo de vehículos de flota heterogénea cuando se minimiza el costo total de ruteo, pero aquí también se tiene en cuenta la minimización simultánea del riesgo total de ruteo. La formulación matemática del problema de ruteo de vehículos multi-objetivo implica tener relaciones matemáticas para expresar, tanto las funciones objetivo, como las restricciones que definen el espacio de búsqueda. La función de objetivo de costo de ruteo total se toma de la revisión de la literatura sobre el problema de ruteo de vehículos de la flota heterogénea; pero la función objetivo de riesgo de ruteo total se construye sobre la base de estudios relacionados con accidentes de transporte de vehículos cuando se transportan materiales peligrosos utilizando redes de carreteras, y los diferentes resultados posibles de los incidentes de transporte. Los elementos considerados para la evaluación de riesgos cuando un vehículo está atravesando una ruta son: la estimación de la probabilidad de incidente de transporte de material peligroso, los resultados del incidente y las consecuencias o el impacto sobre un receptor expuesto, en este caso la población. Esta cuantificación del riesgo depende del tipo de camión utilizado para transportar el material, el tipo de material transportado por el vehículo o camión, el tamaño de la carga al atravesar el camino y la población vecina al segmento que compone el camino entre dos puntos de paradas de los camiones. Este modelo matemático de evaluación de ruta de riesgo no es lineal y se emplea una aproximación lineal por partes para mantener como marco de modelado el de programación lineal entera mixta. Las instancias de prueba del problema de ruteo de vehículo de flota heterogénea utilizadas en la literatura se ampliaron para incluir los parámetros para calcular la función objetivo de riesgo de ruteo total, manteniendo el espacio de búsqueda para las variables de decisión de ruteo. Se resolvieron instancias con un número pequeño de nodos clientes utilizando un *solver* comercial para problemas de optimización lineal de enteros mixtos; con el objetivo de probar la naturaleza conflictiva de los dos objetivos considerados, y tener una medida del tiempo de cálculo requerido para obtener una solución exacta de estas instancias relativamente fáciles de resolver.

Se explora la implementación de métodos híbridos de solución basados en la búsqueda de vecindario para resolver la minimización del riesgo de ruteo, esto dado los buenos resultados cuando se minimiza el costo total de ruteo. Estos algoritmos de soluciones son meta-heurísticos basados en algoritmos de búsqueda local o de vecindario. El método híbrido desarrollado para resolver el problema mono objetivo se basa en la búsqueda de vecindarios variables con movimientos entre y dentro de las rutas. La exploración eficiente del vecindario necesita una evaluación rápida de una solución vecina o candidata. Siguiendo las líneas guías de la literatura se implementaron estructuras de datos auxiliares para hacer este tipo de evaluación, pero prestando especial atención a la variación de la evaluación de riesgo de transporte de todos los segmentos de ruta en un recorrido causado por los cambios en el tamaño de la carga y el tipo de camión. Además, se considera la evaluación del riesgo de transporte al revertir la secuencia de nodos del recorrido. Se implementa una aproximación del cálculo del riesgo de transporte, la cual requiere la inclusión de criterios de aceptación de la solución candidata al explorar un vecindario. Se realiza un pre-cálculo del parámetro de riesgo que reagrupa los parámetros dependientes del segmento de ruta: la longitud y la densidad de población. Se analiza la contribución de los componentes principales del algoritmo de búsqueda local, la generación de la solución inicial, la búsqueda local (fase de intensificación), la perturbación (fase de exploración) y la post-optimización. El algoritmo se prueba en las instancias extendidas del problema de ruteo de vehículos de la flota heterogénea, demostrando ser competitivo.

Se lleva a cabo una adaptación del algoritmo mono-objetivo previo basado en la búsqueda local para la solución de la versión multi-objetivo. Se implementan dos enfoques diferentes de optimización multi-objetivo sin preferencia o generativos: escalarización, mediante el desarrollo de un método ε-*constraint*; y optimización vectorial, basado en el la dominancia de Pareto. Los problemas de ruteo de vehículos multi-objetivo son problemas de optimización combinatoria multi-objetivo y los métodos de solución basados en la búsqueda local aplicada para resolver estos problemas no han sido suficientemente estudiados, si se les compara con los algoritmos evolutivos o de trayectoria. Un problema importante a tratar es la rápida convergencia de los algoritmos de búsqueda locales, por lo que se desarrollan estrategias de diversificación en la búsqueda de vecinos. Se estudian los principales elementos del algoritmo multi-objetivo de búsqueda local: la generación de la solución inicial, la selección de los elementos de la aproximación del frente-Pareto para ser perturbados, sobre los cuales se implementa la búsqueda local híbrida, y el tamaño del conjunto del frente-Pareto aproximado. Se utilizó un diseño experimental para seleccionar el nivel para los valores de los parámetros relacionados con estos elementos de algoritmo. Dos métricas orientadoras del rendimiento de algoritmos multi-objetivo son utilizadas para comparar la diversidad y la convergencia: el hipervolumen y la métrica Δ. Cada uno estos dos enfoques de solución para la generación de la optimización multi-objetivo presenta un inconveniente principal a superar: gestionar la diversidad de soluciones de los elementos de la aproximación del frente-Pareto, en el caso del algoritmo basado en dominancia de Pareto, y garantizar la naturaleza no-dominada de una solución encontrada, en el caso de la optimización restringida.

Las funciones objetivo de costo total de ruteo y de riesgo total de ruteo son de hecho contradictorias cuando se lleva a cabo la optimización simultánea para las instancias estudiadas. La aproximación del frente-Pareto presenta soluciones no-soportadas que exigen la implementación de un método de dominancia-Pareto en lugar de métodos de agregación. En la mayoría de las instancias estudiadas, el enfoque de dominancia-Pareto muestra un mejor rendimiento en la aproximación del frente de Pareto, utilizando como métrica de rendimiento del algoritmo el hipervolumen. A pesar de la naturaleza conflictiva de los objetivos concernientes, el frente de Pareto muestra que aceptar un pequeño incremento en el costo total de ruteo puede producir una mayor reducción en el porcentaje de las consecuencias esperadas dada la probabilidad de un incidente de transporte de material peligroso, que estima el riesgo de ruteo. La implementación de métodos de optimización multi-objetivo aquí desarrollados dan como resultado soluciones dispersas a lo largo del frente-Pareto. Los despachadores, el transportista de carga, los consumidores y el gobierno pueden aprovechar este comportamiento para un transporte eficiente y responsable de los materiales peligrosos utilizando redes de calles y carreteras.

Hay algunos subproductos importantes de esta investigación. Para complementar las instancias de ruteo de vehículos de flota heterogénea se desarrolló un método para generar la población que puede verse afectada por un incidente de transporte de un material peligroso, y esta información se preprocesó para obtener el parámetro para cada segmento de ruta entre dos nodos que integra la población y la distancia de un segmento. También se desarrolló una simulación de la ruta perteneciente a una solución para hacer una comparación entre las consecuencias reales estimadas a través del riesgo esperado y la aproximación proporcionada por el modelo de riesgo tradicional. Se llevó a cabo un estudio para determinar el impacto del movimiento de búsqueda local en la provisión de buenas soluciones al problema de minimización de costos de ruteo, y de cómo los movimientos de perturbación y los elementos de post-optimización pueden mejorar los resultados. Finalmente, se desarrolló un marco para la evaluación de los algoritmos multi-objetivo desarrollados.

Este trabajo puede mejorarse utilizando una mejor medida para la evaluación del riesgo de transporte, como es el caso de la curva FN. Sería necesario estudiar cómo realizar una evaluación eficiente de una solución candidata, ya que esta medida es un gráfico o puede también ser representada como una matriz de doble entrada. La medida de riesgo utilizada en este trabajo parte del cálculo de una aproximación de las consecuencias esperadas, y para obtener este valor, se requiere una estimación de la tasa de accidentes de camiones. Este último valor se obtiene teniendo como referencia el camión pero no el conductor o aspectos gerenciales en la programación de turnos y el mantenimiento del camión o las condiciones del tráfico cambiantes con el tiempo. La población se considera fija e independiente del tiempo cuando el camión está atravesando la ruta del segmento. sin embargo, el impacto del intervalo de tiempo se puede incorporar fácilmente al modelo, dado que se puede considerar como un elemento asociado al segmento de ruta y que existen ya buenos estudios sobre formas eficientes de evaluar soluciones candidatas en búsqueda local considerando aspectos del tiempo de viaje. A pesar de que la experimentación sobre las características apropiadas de la solución inicial para tener una buena solución cuando se aplica la fase de explotación no hubo una respuesta concluyente. O que la selección de los elementos de la aproximación del frente-Pareto se realiza de forma aleatoria. Sería una buena idea usar algunas técnicas y herramientas del aprendizaje de máquina para explorar qué soluciones tienen mayor potencial para mejorar una solución tanto en la diversificación como en los espacios de intensificación.

El enfoque utilizado en este trabajo se puede aplicar para estudiar la variante multi-objetivo de los problemas de optimización en logística verde, el transporte energético-eficiente o en el transporte de valores. Por ejemplo, para reducir emisiones de gases de efecto invernadero, particularmente dióxido de carbono (CO_2), en el problema de ruteo de vehículos, la velocidad y aceleración, que tienen un gran impacto en la economía de combustible del vehículo y los gases de escape expulsados por el motor, deben ser incorporadas en el modelo. La medida de consumo de combustible del vehículo que se usa como una forma de estimar las emisiones de gases de efecto invernadero, es una función de la velocidad del vehículo, carga y tipo de motor, y las características del segmento de ruta a recorrer. Esta función no es lineal y la aproximación mediante funciones lineales por partes se puede implementar, al igual que los métodos híbridos basados en la búsqueda de vecindarios se pueden utilizar para encontrar buenas soluciones.

Además, se pretende con este trabajo incentivar la investigación en optimización combinatoria multi-objetivo basada en la búsqueda de vecindarios. Explorar métodos eficientes y efectivos que exploten el buen rendimiento de los algoritmos basados en búsquedas locales al resolver problemas mono-objetivo y multi-objetivo. Este trabajo está limitado a dos objetivos, también se deben explorar problemas objetivos con más de dos objetivos.

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