OPTIMIZATION OF RAILWAY TRANSPORTATION

HAZMATS AND REGULAR COMMODITIES

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Abstract

Sustainable Supply Chain, Hazmat and Regular Commodities, Railroad Transportation Optimization, Tactical Planning Problem

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Transportation of dangerous goods has been receiving more attention in the realm of academic and scientific research during the last few decades as countries have been increasingly becoming industrialized throughout the world, thereby making Hazmats an integral part of our life style. However, the number of scholarly articles in this field is not as many as those of other areas in SCM. Considering the low-probability-and-high-consequence (LPHC) essence of transportation of Hazmats, on the one hand, and immense volume of shipments accounting for more than hundred tons in North America and Europe, on the other, we can safely state that the number of scholarly articles and dissertations have not been proportional to the significance of the subject of interest. On this ground, we conducted our research to contribute towards further developing the domain of Hazmats transportation, and sustainable supply chain management (SSCM), in general terms.

Transportation of Hazmats, from logistical standpoint, may include all modes of transport via air, marine, road and rail, as well as intermodal transportation systems. Although road shipment is predominant in most of the literature, railway transportation of Hazmats has proven to be a potentially significant means of transporting dangerous goods with respect to both economies of scale and risk of transportation; these factors, have not just given rise to more thoroughly investigation of intermodal transportation of Hazmats using road and rail networks, but has encouraged the competition between rail and road companies which may indeed have some inherent advantages compared to the other medium due to their infrastructural and technological backgrounds. Truck shipment has ostensibly proven to be providing more flexibility; trains, per contra, provide more reliability in terms of transport risk for conveying Hazmats in bulks.

In this thesis, in consonance with the aforementioned motivation, we provide an introduction into the hazardous commodities shipment through rail network in the first chapter of the thesis. Providing relevant statistics on the volume of Hazmat goods, number of accidents, rate of incidents, and rate of fatalities and injuries due to the incidents involving Hazmats, will shed light onto the significance of the topic under study. As well, we review the most pertinent articles while putting more emphasis on the state-of-the-art papers, in chapter two. Following the discussion in chapter 3 and looking at the problem from carrier company's perspective, a mixed integer quadratically constraint problem (MIQCP) is developed which seeks for the minimization of transportation cost under a set of constraints including those associating with Hazmats. Due to the complexity of the problem, the risk function has been piecewise linearized using a set of auxiliary variables, thereby resulting in an MIP problem. Further, considering the interests of both carrier companies and regulatory agencies, which are minimization of cost and risk, respectively, a multiobjective MINLP model is developed, which has been reduced to an MILP through piecewise linearization of the risk term in the objective function. For both single-objective and multiobjective formulations, model variants with bifurcated and nonbifurcated flows have been presented. Then, in chapter 4, we carry out experiments considering two main cases where the first case presents smaller instances of the problem and the second case focuses on a larger instance of the problem. Eventually, in chapter five, we conclude the dissertation with a summary of the overall discussion as well as presenting some comments on avenues of future work.

Preface

This thesis has been prepared in "traditional" format under co-direction of Dr. Mingyuan Chen, from Mechanical, Industrial and Aerospace Engineering Department (MIAE), Concordia University, and Dr. Satyaveer Singh Chauhan, from Supply Chain and Business Technology Management, John Molson School of Business (JMSB), Concordia University.

This thesis was authored by the principal researcher who developed the mathematical models, proposed various mathematical formulation approaches, carried out experiments, and validated the results, and submitted the draft of the dissertation; the thesis was reviewed by Dr. Mingyuan Chen and Dr. Satyaveer Singh Chauhan, prior to submission for defense.

I dedicate my thesis to my beloved wife, grandparents, parents and sister

Azadeh, Ahmad, Mahereh, Amir, Homa, Solmaz

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Abbreviations

BB	Branch and Bound
BC	Branch and Cut
b-MP	b-Matching Problem
CG	Column Generation
HTND	Hazmat Transportation Network Design
HVRP	Hazmat Vehicle Routing Problem
ILP	Integer Linear Programming
IP	Integer Programming
MCNF	Multicommodity Network Flow
MILNP	Mixed Integer Non-Linear Programming
MILP	Mixed Integer Linear Programming
MIP	Mixed Integer Programming
MIQCP	Mixed Integer Quadratically Constraint Problem
MPEC	Mathematical Program with Equilibrium Constraints
NDP	Network Design Problem
O/D	Origin / Destination
P-G	Pasquill-Gifford Stability Class
PIH	Poisonous Inhalation Hazard
SCM	Supply Chain Management
SP	Set Partitioning
TDG	Transportation of Dangerous Goods
TIH	Toxic Inhalation Hazard

Chapter 1

1. Introduction

Sustainable supply chain has gained increasing attention over the last few decades; after 1980s, the core of decisions at industry levels have been moving away from purely operations-oriented approaches towards strategy-oriented ones. One of such approaches was to incorporate environmental aspects in decision making processes about mainstream, midstream and downstream actors in supply chain at tactical and operational levels. Transportation of dangerous goods (TDG), for instance, involves governments, provincial and local authorities (strategic and tactical levels), carriers (tactical and operational levels), and retailers and consumers (operational level).

1.1. Overview

Transportation plays a crucial role in decisions made in strategical logistics; sustainability in transportation could involve environmental aspects as well as various types of risks threatening mankind. If the commodities to be conveyed from their origin to their temporal or final destinations, are all regular commodities, the least risk to the environment and human beings could be thought of as emission of pollutants which are adversely affecting both human life and nature. On the other hand, some factors like population growth, rising consumption and production levels and rapid pace of urbanization, have been giving rise to the level of transportation of dangerous goods globally. This has been a cause of concern for environmentalists and authorities throughout the world, thereby encouraging researchers at academia to launch researches to propose methods to mitigate the risk intrinsic to transportation of Hazmats.

Most of the scholarly articles in transportation of Hazmats, however, pertain to the road transportation while there is concrete evidence that railway transportation of hazardous materials may incur less transportation costs and will decrease the risk of transportation at a considerable extent; on the contrary, consequences in case of incident may be more than that of the roadway shipment hauling. This encouraged us work on railroad transportation of Hazmats to incorporate the associated risk constraint into decision making on route choices for each and every shipment and its constituent commodities. For this, we are proposing a multicommodity-based formulation at a tactical-operational level to minimize the costs of transportation, yard operational costs, train fixed costs, risk of population exposure in terms of incident area evacuation costs. Although a rigorous stream of scholarly research has been dedicated to the multicommodity network flow problems, but to the best of our knowledge, non of them has incorporated Hazmat constraints based on air pollutant dispersion models.

In the following sections, we proceed with delineating the scope of the thesis, then, we elaborate more on the objective and contribution of the study to the literature before presenting an outline of the structure and organization of this dissertation.

1.1.1. Canadian Railroad Transportation

The Canadian rail network currently has 45,199 route-kilometers (km) of track, 49.1% of which is owned by Canadian National Railway, CN, amounting to 22,186 km, and 25.6% of that is owned by Canadian Pacific, CP, constituting 11,574 km of the total length of the tracks; the rest 25.3%, amounting to 11,439 km, is owned by other railways. There are 19 intermodal terminals operated by either CN or CP; the network has 27 rail border crossings with the US. Besides CN and CP, there are various other domestic carriers and US-based carriers with freight rail operations in Canada such as BNFS Railway Company and CSX Transportation Inc., and the Union Pacific

Railroad Company. Furthermore, Short-line railways such as Québec North Shore and Labrador Railway (QNS&L), providing point-to-point services, are typically connecting shippers to Class I railways and / or to ports in order to move products across longer distances *TC* (2016). Figure 1-1 depicts the Canadian railway network *RAC* (2017).

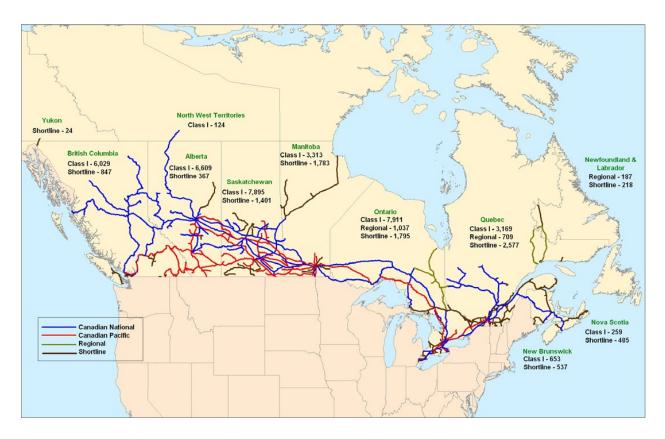


Figure 1-1: Canadian Railway Network

Transportation is playing an increasingly crucial role in our modern society. It can have a highly significant impact on economy. In Canada, transportation and warehousing accounted for 4.3% and 4.5% of Total Gross Domestic Product (GDP) in 2015 and 2016, *TC (2015)* and *TC (2016)*, respectively, making an important component of the Canadian economy. In 2015, this sector had 3.1% growth in real terms over the last year, more than triple the growth rate for all industries *TC (2015)*. In 2016, this sector had 3.0% growth in real terms over the last year, more than triple the last year, more than double the growth rate for all industries. "The compound annual growth rate for GDP in the transportation

sector over the previous five years of 2.9% also exceeds that of the economy as a whole (1.4%)", *TC* (2016).

There has been a new trend of shifting from bulk commodities towards containerized freight transportation in 2015; from 2014 to 2015 containers by rail increased by 6% while coal rail carloads and crude oil carloads dropped by 16% and 24%, respectively *TC* (2015). However, most freight traffic in 2016 were bulk commodities; the volume of the commodities carried though railroad was an estimated 297.4 million tons, down 2.5% from 2015 *TC* (201).

In terms of international transportation of commodities, international trade traffic increased by 0.7% from 2015 to 2016, amounting to \$128.3 billion, where rail export's share of the total rail international trade (\$128.3 billion) constitutes \$81.9 billion and import's share of that amount, makes up \$46.4 billion. The most significant products, on the import side, were automotive and chemical products.

1.1.2. Transportation of Dangerous Goods (TDG)

Transportation of dangerous goods (TDG) is vitally important owing to the essential role that Hazmats play in every aspect of the modern life. Weather it be in a developed country or in a developing country, Hazmats are used extensively as fuels in vehicles for transportation, as fuel in heating our homes and offices, as chemicals both in manufacturing and daily household cleaner products, paints, in farming and medicine, as lithium-ion batteries, in our smart phones and other devices. In general, "dangerous goods mean a product, substance or organism that, because of its quantity, concentration, or physical or chemical characteristics may pose a real hazard to human health or the environment" (*TC*, 2011). Dangerous goods have been classified into 9 main categories by Emergency Response Guidebook *UN2009 (2009)* and *Cloutier and Cushmac (2016)* that listed as follows:

- Explosives
- Gases
- Flammable Liquids and Combustible Liquids
- Flammable Solids; Substances liable to spontaneous combustion; substances, which in contact with water, emit flammable gases
- Oxidizing Substances and Organic Peroxides
- Toxic Substances and Infectious Substances
- Radioactive Materials
- Corrosive Substances
- Miscellaneous dangerous goods, hazardous materials and articles

Being an integral part of our industrial lifestyle, Hazmats need to be transported in considerably large volumes from their origin points to their temporal and final destinations due to their different production and consumption points. For instance, crude oil should be shipped from oil fields to refineries and then the processed oil products such as gasoline and heating oil fuel are shipped to their storage tanks throughout the country *Erkut et al (2007)* and *Verter (2011)*. Release of Hazmats due to accidents during their transportation from their origin to their destination may bring about adverse effects to humans, environment and properties.

TDG unlike shipment of other type of commodities is regulated and monitored by governments at federal, provincial and municipal levels throughout the globe in order to mitigate the risk of transportation of dangerous goods while the industry does not impose such regulations on shipment of other type of commodities; this makes the TDG logistics even more complicated since governments at different levels often have different jurisdiction, thereby abiding by their respective

jurisdictional regulation. Furthermore, there are various nongovernmental companies monitoring the conformance of transpiration of Hazmats throughout the nation and internationally.

Size of a country and its level of industrialization defines the magnitude of the role of transportation for Hazmats in that country. According to the statistics of Trucking Commodity Origin and Destination Survey (TTCOD), *Provencher (2008)* reported that 106 million tons of Hazmats were hauled via trucks in 2004, amounting to 17.4% of all Canadian road freight shipments; in the same year, 36 millions of dangerous commodities have been shipped through Canadian National (CN) and Canadian Pacific (CP), representing 12.5% of all rail freight *Provencher (2008)* and *Verter (2011)*.

In 2009, Transport Canada reported that there were 30 million shipments of dangerous goods each year, half of which pertains to road transportation, and there were 396 accidents involving dangerous goods; accidents occurred during loading / unloading were twice as those occurred during transport TC (2009). Transport Canada estimates that nearly 80,000 shipments of dangerous goods are moved by road, rail, water, and air in Canada.

As depicted in Table 1-1, in 2015, Hazmat Shipments through railway accounted for 11% of the total shipment via rail (TC, TDG Newsletter, 2017). Table 1-2 elaborates on the Hazmat constituents accounting for 11% of the total railway freight volume in 2015 within Canada.

Commodity Type Shipped via Rail	Volume Percentage		
Non-Regulated	89%		
Hazmats 11%			
Source: TDG Newsletter 2017, Government of Canada			

Table 1-1: Rail Shipment in Canada (Non-regulated & Hazmats) - 2015

Table 1-2: Hazmat Types and Volumes Transported via Railroad in Canada - 2015

Hazmat Type Shipped via Rail	Hazmat Breakdown of 11%
Petroleum Crude Oil	25 %
FAK1 -Hazardous Materials	20 %
Liquidized Petroleum Gas	7 %
Ammonia, Anhydrous	7 %
Elevated Temperature Liquid, Liquid, N.O.S.2	6 %
Hydrocarbons, Liquid, N.O.S.	4 %
Environmentally Hazardous Substances, N.O.S.	3 %
Diesel Fuel	3 %
Sulfur, Molten	2 %
Octanes	2 %
Others	21 %

Source: TDG Newsletter 2017, Government of Canada

In the same fashion, Table 1-3 indicates the volume of Hazmats shipped via railway in Canada in 2016 amounted to 9.71% of the total railway freights in the same year; this figure shows a slight decrease of 1.29% from its previous year. Table 1-4 elaborates on the Hazmat constituents accounting for 9.71% of the total railway freight volume in 2015 within Canada.

Table 1-3: Rail Shipment in Canada (Non-regulated & Hazmats) - 2016

Commodity Type Shipped via Rail	Volume Percentage
Non-Regulated	90.29 %
Hazmats	9.71 %

Source: Protective Direction 36 for disclosure of dangerous goods shipments on CP – QC

¹ FAK, stands for Freight All Kinds; this is a common term in freight transportation industry which is used in carrier's

² Not Otherwise Specified

Hazmat Type Shipped via Rail	Hazmat Breakdown of 9.71%
Balance (miscellaneous)	30.7 %
Petroleum Crude Oil	13.4 %
FAK-Contains Dangerous Goods	12.3 %
Ammonia, Anhydrous	7.5 %
Alcohol, N.O.S.	7.5 %
Propane	7.2 %
Diesel Fuel	6.4 %
Elevated Temp Liquid, N.O.S.	4.8 %
Environmentally Hazardous Substances, Liquid	2.9 %
Sulfuric Acid	3.2 %
Sulfur, Molten	4.0 %

Table 1-4: Hazmat Types and Volumes Transported via Railroad in in Canada - 2016

Source: Protective Direction 36 for disclosure of dangerous goods shipments on CP - QC

Also, operating companies, Canadian Class I Railways, Canadian National (CN) and Canadian Pacific (CP), have to provide yearly and interim (6-month) reports to the designated emergency planner for the jurisdiction *TC TDG Newsletter (2017)*.

Hazmat Type Shipped via Rail	Hazmat Breakdown of 9.71%
Alcohol, N.O.S.	26.1 %
FAK-Hazardous Materials	17.9 %
Petroleum Crude Oil	14.7 %
Propane	3.5 %
Methanol	3 %
Elevated Temperature Liquid, N.O.S.	2.3 %
Environmentally Hazardous Substances	1.9 %
Sodium Chlorine	1.8 %
Engine, Internal Combustion	1.8 %
Petroleum Gases, Liquid	1.7 %
Others	25.4 %

Table 1-5: Dangerous Goods Shipment in Quebec – 2016

Source: Protective Direction 36 for disclosure of dangerous goods shipments on CP – QC

Table 1-5 and Table 1-6 demonstrate the percentage of dangerous goods of all types shipped through railways in 2016 in Quebec and Ontario, respectively. Table 1-5 illustrated that 74.6% of the total amount of Hazmats shipped through railroad is comprised of the top 10 products shipped within Quebec jurisdiction while the remaining 25.4% are many different products, each constituting 1.7% or less of the total TC, PD-36-QC-en (2017).

As shown in Table 1-6, 79.7% of the total amount of Hazmats shipped through railroad is comprised of the top 10 products shipped within Ontario jurisdiction while the remaining 20.3% are many different products, each forming 1.5% or less of the total source: *TC*, *PD-36-ON-en* (2017).

Hazmat Type Shipped via Rail Hazmat Breakdown of 9.71% **FAK-Hazardous Materials** 31.0 % 20.7 % Alcohol, N.O.S. Petroleum Crude Oil 8.4 % Sulfuric Acid 6.2 % Diesel Fuel 2.9 % Sodium Hydroxide Solution 2.5 % Gasoline 2.4 % 2.4 % Propane Elevated Temperature Liquid, N.O.S. 1.6 % Methanol 1.5 % Others 20.3 %

Table 1-6: Dangerous Goods Shipment in Ontario - 2016

Source: Protective Direction 36 for disclosure of dangerous goods shipments on CP - ON

Office of Hazardous Materials Safety (OHMS) of the US Department of Transportation (DOT), in their 2005–2006 biennial report, estimated 800,000 shipments per day, amounting to approximately 9 million tons of shipments per day in 1998, *DOT/PHMSA: 2013-2014 biennial report (2015)*. Also, *Research and Innovative Technology Administration (2012)* reported that annually, more than 2.5 billion tons regulated Hazmats of all types including: poisonous, explosive, flammables, corrosive, and radioactive materials with a value around \$2.3 trillion is transported 307 billion miles within the interconnected network in the US *DOT/PHMSA: 2013-2014 biennial report (2015)*.

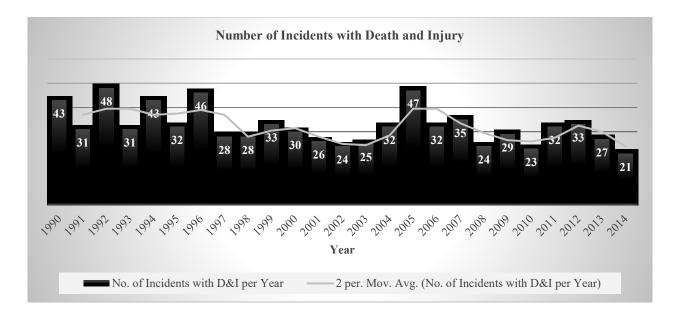


Figure 1-2: Deaths and Injuries (D&I) Statistics (US PHMSA) 1990 - 2014

Source: PHMSA - Transportation of Hazardous Materials: Biennial Report to Congress 2013 - 2014 PHMSA's aim is to mitigate the consequences of risks of hazmat transportation pursuing the goal of reducing the number of death and injuries (D&I) to zero *DOT/PHMSA: 2013-2014 biennial report (2015)*; however, incidents leading to death and injury are intrinsic to dangerous goods transportations. Figure 1-2 is a statistical compilation of casualties associated with TDGs, demonstrating (D&I) incidents have declined by 10% every 7 years.

Backing to the nationwide statistics on accidents involving TDG, there were 358 incidents reported that involved Hazmats, where more than 70% of them occurred during handling operations in terminals, yards, ports, while less than 30% of them happened on the course of transit. 96 road-mode accidents, accounted for 92% of in-transit accidents whereas the remainder 6% and 2% were associated with rail and air modes, respectively. Table 1-7 shows the number of accidents involved TDG from 2002 to 2007 by categorizing them into "in-transit" and "not-in-transit" main classes. Moreover, Table 1-8 provides some statistics about the number of death and injuries (D&I) involving TDG in Canada from 2002 to 2007, *TC Statistical Addendum 2007 (2008)*.

Year		In-Transit			Not-in-	Total	
i cai	Road	Rail	Air	Marine	Subtotal	Transit	Total
2002	170	16	8	1	195	344	439
2003	101	5	5	1	112	244	356
2004	106	9	6	0	121	248	369
2005	129	8	5	0	142	244	386
2006	102	4	7	0	113	272	385
2002 – 2006 Average	122	8	6	1	137	250	387
2007	124	9	7	1	141	280	421

Table 1-7: Statistics on the Number of Accidents Involving TDG 2002 -2007

Source: Transportation in Canada: Statistical Addendum 2007

Table 1-8: Deaths and Injuries (D&I) Statistics 2002 - 2007

Year	Deaths		Total		
i eai	Deatins	Major	Moderate	Minor	Total
2002	12	25	42	5	72
2003	5	21	17	1	39
2004	11	12	20	4	36
2005	7	18	22	4	44
2006	5	6	30	6	42
2002 - 2006	0	16	26	4	47
Average	0	10	20	4	47
2007	7	12	29	11	52

Source: Transportation in Canada: Statistical Addendum 2007

Table 1-9 shows the number of accidents involved TDG in Canada from 2006 to 2011 by categorizing them into "in-transit" and "not-in-transit" main classes. Moreover, Table 1-10 provides some statistics on the number of death and injuries (D&I) involving TDG in Canada from 2006 to 2011 *TC, Statistical Addendum 2011 (2012)*.

Comparing statistics associating with the number of accidents between 2006 and 2011 with that of 2002 to 2007, we can see the improvement in TDG safety in terms of reduction in the number of accidents. On the other hand, as we compare statistics associating with the number of D&Is between 2006 and 2011 with that of 2002 to 2007, we can see an improving trend in the protection of people exposed to the risk of transportation of Hazmats.

Year	In-Transit				Not-in-	Total	
rear	Road	Rail	Air	Marine ³	Subtotal	Transit	Total
2006	102	4	7	0	113	272	358
2007	125	9	8	0	142	282	424
2008	115	6	4	0	125	310	435
2009	78	5	0	0	83	242	325
2010	95	5	1	0	101	203	304
2006 - 2010	103.0	5.8	4.0	0.0	112.8	261.8	374.6
Average	105.0	5.8	4.0	0.0	112.0	201.8	574.0
2011	96	6	2	0	104	254	358

Table 1-9: Statistics on the Number of Accidents Involving TDG 2006 - 2011

Source: Transportation in Canada - Statistical Addendum 2011

Table 1-10: Deaths and Injuries (D&I) Statistics 2006 - 2011

Year Deaths			Tetal		
rear	Year Deaths		Moderate	Minor	Total
2006	1	0	17	0	17
2007	0	2	8	3	13
2008	0	1	8	2	11
2009	0	1	4	2	7
2010	0	2	7	0	9
2006 - 2010	0.2	1.2	8.8	1.4	11.4
Average	0.2	1.2	0.0	1.4	11.4
2011	0	2	3	2	7

Source: Transportation in Canada - Statistical Addendum 2011

1.1.3. Hazmat Transportation Optimization Models

Hazmats of any type are essential element of our contemporary life, and like any other type of goods, they need to be hauled from their origins like production facilities and factories, mines and refineries, to their temporal or final destinations like to hubs, retailers and eventually to their consumers. Hence, they need to be circulated into the supply chain and transportation networks. However, what makes transportation system of Hazmat different from that of regular commodities is the risk of incident, which, in case of Hazmats, is an accident leading to spill or leakage, thereby exacerbating the consequences of casualties and accidents as their spill and leakage may affect

³ The TDG Regulations do not cover in-transit marine accidents involving bulk shipments of dangerous goods.

people, environment and properties, adversely. Since risk is inherent in transportation of dangerous goods (TDG), these commodities are construed as "regulated" goods in terms of regulatory restrictions that have been imposed onto their transportation unlike the globally deregulation of the industry *Verter (2011)*.

Reviewing some harmful results of accidents involving Hazmats in Canada, we can refer to Toronto's 1979 incident that 200,000 people were forced to evacuate the area because of the release of Chlorine, leaking from damaged tank cars. Another tragic incident happened when 2.7 million liters of petroleum products released due to the derailment of 35 tank cars as of a CN Ultratrain just outside of Montréal in 1999 *Railway Investigation Report (2002)*. A more recent one was four years ago, in 2013, TDG was highlighted in catastrophic fashion when 47 people were killed as a result of derailment of an oil-laden runaway train which crashed in the center of Lac-Mégantic, Québec, Canada.

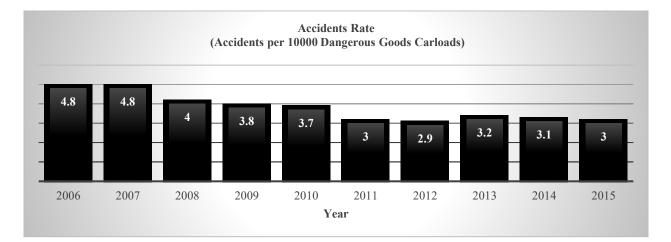




Figure 1-3 and Table 1-11 give statistics of the accidents involving TDG through Railroad transportation from 2006 to 2015, *RAC, Rail Trends (2016)*.

Year	Total Accidents Involving Dangerous Goods	Dangerous goods Carloads	Accidents Rate (Accidents per 1000 Dangerous Goods Carloads)			
2006	196	406425	0.48			
2007	206	426789	0.48			
2008	170	422467	0.40			
2009	145	379650	0.38			
2010	149	400318	0.37			
2011	129	425124	0.30			
2012	124	428660	0.29			
2013	157	493360	0.32			
2014	179	576226	0.31			
2015	147	491802	0.30			
Source: Rail Trends 2016						

Table 1-11: Accidents Involving Dangerous Goods - Rail Trends 2016 - 2006 to 2015

Source: Rail Trends 2016

Catastrophic consequences of incidents urge researchers to thoroughly investigate the causes of accidents in a root-cause manner considering every environmental, technological and managerial aspect of TDG in order to reduce the probability of accidents through suggesting preventive transportation modeling approaches, as well as suggesting ways to minimize the harmful consequences threatening people exposed to the health issues caused by dangerous accidental releases of Hazmats.

With this background about the risk of TDG, we move to the next section to review some articles and literature pertinent to mathematical modeling approaches for TDG.

1.2. Scope

This thesis aims to study railway transportation of dangerous goods using multicommodity-based Mixed Integer Nonlinear Linear Programming (MINLP) optimization models. The specific mathematical formulations of the problem addressed in this dissertation is a multi-order, multicommodity capacitated network flow problem with commodity-specific upper bounds on the number of railcars traversing arcs and nodes. Meteorological concepts concerning weather stability classes, pollutant dispersion models have been effectively used to develop the mathematical MINLP formulations. Once defined, the mathematical formulations will be applied to solve various hypothetical instances beginning from smaller instances, then evolving to some greater instances which are as large as those presented in the state-of-the-art and referee-reviewed papers. Finally, we will perform experiments with industry-scale data using IBM ILOG CPLEX software package. We will perform an in-depth analysis of the results and draw conclusions in the end.

1.3. Research Objectives

The following sections briefly explain the milestones to be realized throughout the dissertation. However, each and every topic throughout this section, will be elaborated on throughout the remaining chapters of the thesis.

1.3.1. Mathematical Model

A multicommodity, mixed integer nonlinear mathematical model have been proposed, variants of which are also included w.r.t the bifurcation of flows. For each variant, we consider singleobjective model in order to minimize the costs of transportation, yard operations and fixed train costs; we also consider multiobjective function for each model variants, which examine a set of nondominated Pareto-optimal paths for each traffic class. By incorporating risk evaluation function in terms of population exposure into our objective function, we address interests of the main stakeholders, i.e., the transport companies and regulatory agencies, which are the minimization of costs and risk, respectively. We have also considered the equity in spatial distribution of risk within the underlying network to prevent potential link segments and yards of the network from being overloaded w.r.t. risk exposed to the population residing near the links, thereby considering the interest of local and provincial authorities.

1.3.2. Hazmat Constraints

In order for our model to effectively take geographical and meteorological aspects into account, we had made use of a commonly used mathematical air dispersion model called Gaussian Plume Model. We have also considered the proportion of urbanity and rurality of areas along each serviceleg of all train services, as well as defining a yard is located in an either urban or rural area. More importantly, considering the maximum tolerable threshold for the risk in terms of population exposure, two sets of constraints have been introduced to set that upper limit on the value of risk on each and every service-leg of train services and yards; those upper limits, as enforced in the models, should not exceed a predefined proportion of the total risk on all service-legs and yards cross the underlying network, respectively. In addition, in the single-objective model variants, the total risk is also restricted not to be more than a predefined value which can be set by primary stakeholders and decision makers. However, due to the complexity and the controversial characteristic of setting such an upper limit on the total risk, we have incorporated this term into the objective function of the multiobjective model variants. As well, looking at the problem from a slightly different dimension by integrating the concept of a fixed bandwidth as the radius of evacuation area, estimated using GPM, we set Hazmat-specific upper limits on the maximum level of concentration of Hazmats, which should not exceed the Immediately Dangerous to Life and Health (IDLH) limit, suggested by NIOSH; for this, we made use of crosswind and vertical dispersion formulations of Brigg's Scheme to compute the Hazmat buoyant contaminants at a predefined distance from service-legs and yards.

We believe, from a practical point of view, this modeling approach can help us in prompt decision making about routing problem under both Hazmat and other technological constraints.

1.3.3. Numerical Experiments

We conduct experiments on small and large instances of the problem for each type of the abovementioned mathematical formulations to validate the functionality of the proposed model. Inspired by the state-of-the-art, *Verma et al (2011)*, the larger instance of the problem comprises of 25 yards and service-legs of 31 train services. We show the smaller instances of the problem can be solved within seconds, and the larger instances can be solved within a reasonable time if we consider the complexity of the problem.

1.4. Organization of the Thesis

The thesis is consisting of five chapters. We begin with presenting a review of recent literature relevant to the topic of interest in chapter 2. We categorize the articles associating with railway freight transportation into four main subsections: Hazmat Freights Risk Assessment, Routing, Facility Location, and Network Design. Hazmat Freights Risk Assessment has been divided into six subsections, through which we are going to cover various risk measuring approaches that have been taken in assessing the risk of transportation of dangerous goods. In chapter 3, single objective and multiobjective mathematical models have been developed. Moreover, for each of the model variants, two approaches have been taken to either allow the split of the flows or to restrict the bifurcation of the flow such that just a single path can be determined for each of the traffic classes to be shipped from their origin yards to their destination yards. Subsequently, in chapter 4, we will first perform experiments on a simple hypothetical network and then, on large-scale and real-life-size data sets. Further, we will run the models with various data sets by changing the number of train services, size and sparsity of the network, and number of the traffic classes. Then, results will be reported, providing insights into the performance of the models. Finally, in chapter 5, the

dissertation ends with an overall summary of the whole discussion, mathematical modelling approaches as well as potential future research directions.

Chapter 2

2. Literature Review

Throughout this chapter, we are going to review the most pertinent scholarly papers investigating Hazmat and regular freight transportation. Since there is a rigorous stream of papers in the realm of transportation, we have categorized them into VRP, TDG risk assessment, facility location problem, global and local route planning problems. However, in some cases, a given paper may be dealing with various aspects that allows it to be investigated under other categories; in those cases, however, we have focused on the most relevant content of the paper which may enrich our discussion.

2.1. Railway Freight Transportation, VRP, and Risk Assessment

Transportation of dangerous goods involves both transportation problems and risk due to transportation. Thus, TDG problems can include a variety of significant problems, mainly in combinatorial optimization, including vehicle routing problems (VRP) which is sometimes denoted as Hazmat vehicle routing problems (HVRP). VRP has a very rich literature, HVRP, on the contrary, has not been extensively investigated. Most of the papers dealing with Hazmat transportation focus on the route planning, solely, without focusing on vehicle routing. Nonetheless, we will be reviewing some of the most relevant papers in both VRP and HVRP in sections (2.1.1) and (2.1.2), respectively.

2.1.1. Vehicle Routing Problem (VRP)

In general terms, VRP deals with *route planning* and *vehicle routing*. Route planning aims to find paths comprising of a set of links and a set of intermediate depots (yards) and one origin and one

destination depot (yard), under a set of constraint. The underlying network, may be capacitated, i.e. some limits have been imposed on the number of vehicles or the amount of the volume of goods they contain, traversing through and arc or a node within the network. Those type of constraints may involve infrastructural restrictions, regulatory restrictions, or commodity-specific limitations, and etc. On the other hand, the vehicle routing includes assigning O/D demands, customers, to vehicles as well as finding the optimal sequence of visiting those customers by the vehicles that they have been assigned to.

Dantzig G.B. and Ramser J.H. (1959) applied VRP, for the first time, to find the optimum routing of a fleet of gasoline delivery trucks between an origin terminal (bulk terminal) and a large number of destination points (various service stations that were supplied by that terminal). Their mathematical model, a generalization of Traveling Sales Person (TSP), was the first formulation for VPR. They also proposed an algorithm to solve their model which was later effectively enhanced through a greedy heuristic suggested by *Clarke and Wright (1964)*.

Since 1959 that the first VRP model suggested till now, researchers have worked in developing mathematical models and solution approaches to deal with VRPs. Thus, there exists a wide variety of VRPs like capacitated vehicle routing problem (CVRP), or vehicle routing problem with time windows (VRPTW). Due to the broad literature in VRPs *Laporte (1992)*, we may not cover them all within the current document. However, we are going to mention some of the articles involving CVRP and VRPTW, using either exact methods or heuristic approaches to solve their VRPs, and we will provide the interested reader with the pertinent references to obtain more knowledge about various solution approaches in this area. Furthermore, we encourage the interested reader to refer to *Samuel R. (1983)*; *Bodin and Golden (1981)*; *Christofides (1985)*; *Cordeau, Laporte et al (2007)*; *Laporte and Nobert (1987)*; *Gendreau et al (2008)*; *Toth and Vigo (2002)* and other

references to obtain information about VRPs and their solution approaches. Nonetheless, we are going over some recent papers dealing with exact methods or heuristics to solve VPRs through the following subsections.

2.1.1.1. CVRP

CVRPs are NP-hard problems and they are actually harder than TSP; i.e. in practice, the best algorithms suggested to solve CVRP can barely solve handle instances more than 100 vertices while large TSP instances, with more than hundreds and thousands vertices, can be solved *Cordeau et al* (2007). Exact methods used to solve VPRs include: Branch and Bound (BB), Set Partitioning (SP), and Branch and Cut algorithms (BC).

Miller (1995) suggested a BB algorithm for a CVRP problem of a size of 61 vertices. They relaxed the subtour elimination and vehicle capacity constraints, thereby yielding a b-matching problem (b-MP); their algorithm solved all problems in TSPLIB having 51 or fewer vertices except the 48 vertex instance (att48.vrp).

In a weighted undirected graph G(V, E), with arbitrary edge capacities, *Miller and Pekny (1995)* suggested an algorithm to find a minimum cost perfect (b-MP), which was based on staged approach that sequentially applies increasingly more expensive steps until a solution is found. Computational results show the algorithm to be effective on problems derived from TSPLIB ranging in size from 532 to 3795 vertices for various b values.

Other than (b-MP) relaxation of the problem used for the (BB) algorithms, other relaxations suggested by researchers based on Assignment Problem (AP). *Dell'Amico and Toth (2000)* suggested an AP relaxation of the problem that could be solved within polynomial time; they developed codes to solve a classic linear AP with a min-sum objective function. Then, they

selected eight codes and performed experiments with a broad set of dense instances containing both randomly generated and benchmark problems.

Relaxations for BB based on degree-constrained spanning trees were applied to solve CVRP later several years after b-MP and AP based relaxations for BB. *Christofides et al (1981a)* proposed a VRP with a central facility where vehicles are stationed and are prepared to supply customers with known demands. For the exact solution of their VRP, they presented tree search algorithms incorporating lowerbounds (LBs) through: shortest spanning k-degree center tree (K-DCT), and q-routes. Reduction and dominance tests were included in their final algorithms. They drew conclusions about the LBs computed through each of the methods and reported that the LBs found through q-routes were superior to those found from k-DCT. They also reported that problems with up to 25 customers could be solved exactly.

Fisher (1994) considered a scheduling a fleet of k vehicles to make deliveries to n customers under capacity constraints. K-tree is defined to be a set of n+k edges that span a graph of n+1 nodes. Under vehicle capacity constraints and the requirement that each customer be visited exactly once, they modeled their VRP problem such that to find the minimum cost K-tree with two edges incident on the depot. To obtain lowerbounds in the BB algorithm through solving Lagrangian problem, the side constraints were dualized. Then, their algorithm could solve a well-known problem with 100 customers, as well as problems with 25 to 75 customers, to optimality.

Martinhon et al (2000) introduce a Lagrangian-based exact solution algorithm for their VRP problem; in their algorithm, they could obtain LBs by allowing exponentially many inequalities as candidates to Lagrangian dualization. They considered comb and multistar inequalities, which eventually led to a moderately improved Lagrangian bounds.

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Based on a Set-partitioning-based formulation of the VRP, *Agarwal et al (1989)* proposed a computationally viable algorithm. They solved a modified version of the well-known Set-partitioning-based formulation of the VRP through column generation. Their algorithm could help them solve Euclidean CVRP instances with up to 25 customers. *Bramel and Simchi-Levi (2001)* elaborates on Set-partitioning-based algorithms for capacitated VRPs.

Fischetti et al (1994) considered a specific variation of a standard asymmetric CVRP where the only vehicle capacities are imposed. Based on additive-approach proposed by *Fischetti and Toth (1989)*, they suggested two bounding procedures for CVRP; combining into an additive bounding procedure two new lower bounds based on disjunctions on infeasible arc subsets and on minimum cost flows led to the improvement of their AP relaxation. Then, they proposed an exact BB algorithm enhanced through reduction procedures, dominance criteria, and feasibility checks. They also presented extensive computational results using both real-world and random problems, showing their proposed algorithm was competitive compared to the previous algorithms from the literature.

Further, the methods proposed in symmetric CVRP could be generalized to find other bounds for the asymmetric CVRP. For instance, *Fisher (1994)* suggested a way to extend the m-tree based Lagrangian bound to the asymmetric CVRP. However, if the asymmetry of the problem is taken into consideration, better bounds may be obtained potentially; capacitated shortest spanning arborescence problem in *Toth and Vigo (1995)* and VRP with backhauls in *Toth and Vigo (1997)*, could be referred to as two examples of using m-arborescences instead of m-trees, and strengthening the bound in Lagrangian method, respectively.

On the other hand, Branch and Cut (BC) could be mentioned to be the best available exact approach for CVRP *Cordeau et al (2007)*.

For solving CVRP to optimality, *Augerat et al (1995)* presented a BC algorithm based on the partial polyhedral description of the corresponding polytope. For this, they made use of the valid inequalities introduced and implemented by *Cornuejols and Harche (1993)*; *De Vitis at al (1999)*; *Naddef and Rinaldi (2002)* and *Naddef and Rinaldi (1999)*. They focused on the design of separation procedures for several classes of valid inequalities; generalized subtour elimination inequalities (capacity constraints) turned out to be playing a significant role in developing cutting plane algorithms for the CVRP. They found better LBs as a result of implementing their algorithm to a set of instances taken from literature. The main results are the solution of two versions of an instance proposed by Fisher comprising of 134 customers.

Fukasawa et al (2006) proposed and algorithm comprised of both BC and Lagrangian Relaxation / Column Generation. Their algorithm works at the intersection of the polytope of a traditional Lagrangian relaxation over q-routes, and the one defined by bound, degree and capacity constraints, thereby leading to Branch-and-Cut-and-Price algorithm which helps finding tighter bounds than those produced by previously proposed BC algorithms.

Baldacci et al (2006) addressed multiple inventory locations rollon–rolloff vehicle routing problem (M-RRVRP); they modeled the M-RRVRP as a time constrained vehicle routing problem on a multigraph (TVRP-MG). Then, they suggested an exact method for solving their TVRP-MG problem formulated as a set partitioning problem. Their exact model could produce three different lowerbounds computed from different relaxations of the formulation of the problem. They, further, obtain an upperbound, which, along with the three LBs, could transform the solution of the Lagrangian relaxation into a feasible solution. Their algorithm could yield bounds of a quality levels comparable to those produced by the algorithm described in *Fukasawa et al (2006)*, but much quicker.

Muter et al (2014) addressed the multidepot VRP with interdepot routes that was an extension of a the multidepot VRP where vehicles can stop at some interdepot stops to replenish. They modeled their problem as a set covering problem such that variables are rotations corresponding to feasible combinations of routes. Then, two pricing algorithms were considered to generate rotations. By solving the first subproblem, an elementary shortest path problem with resource constraints on a modified version of the original customer-depot network, rotations are generated directly. The second subproblem results in a model with many columns as a result of exploiting the relationship between the sets of routes and rotations. To alleviate the difficulties in solving the second subproblem by column generation, they introduced an alternative approach. Further, they show, through experiments, that the second pricing subproblem performs better than the first one to produce lowerbounds of the LP relaxation. They solved the problem to optimality by computing the optimal integer solution by embedding the above-mentioned mechanism of computing LBs within a BB algorithm.

Classical Heuristic Category	Some of the Contributions to CVRP	
Route construction heuristics.	Clarke and Wright (1964), Laporte and Semet (2002),	
	Golden et al (1997), Paessens (1988), Nelson et al	
	(1985), Desrochers and Verhoog (1989), Altinkemer	
	and Gavish (1991), Wark and Holt (1994), Mole and	
	Jameson (1976), Christofides et al (1979)	
Two-phase heuristics.	Wren (1971), Wren and Holliday (1972), Gillett and	
	Miller (1974), Fisher and Jaikumar (1981), Bramel and	
	Simchi-Levi (1997), Foster and Ryan (1976), Ryan et al	
	(1993), Renaud et al (1996a), Beasley (1983),	
	Haimovich and Rinnooy Kan (1985), Bertsimas and	
	Howell (1986)	
Route improvement heuristics.	Lin (1965), Or (1976), Renaud at al (1996a), Laporte	
	and Semet (2002), Thompson and Psaraftis (1993), Van	
	Breedam (1994), Kindervater and Savelsbergh (1997)	

Table 2-1: Classical Heuristics Proposed for Solving CVRP

Moreover, there has been a rich stream of articles involving heuristics and metaheuristics to solve variants of the CVRP. Classical heuristics applied to solve CVRP include Route Construction, Two-phase, and Route Improvement heuristics. On the other hand, metaheuristics that have been used to solve CVRP include Local Search (simulated annealing, deterministic annealing, and tabu search), Population Search (including genetic search and adaptive memory procedures), and Learning Mechanisms (including neural networks and ant colony optimization).

Due to the impressive number of papers dealing with heuristics and metaheuristics to solve CVRP, we refer the interested reader to *Gendreau et al (2002); Cordeau and Laporte (2005); Cordeau et al (2005); Gendreau et al (2008)* to obtain more knowledge in this area. However, some of the most pertinent articles have been listed in Table 2-2 and Table 2-3 to be consulted.

Metaheuristic Category	Some of the Contributions to CVRP	
Local Search	Willard (1989), Osman (1993), Taillard (1993),	
	Gendreau et al (1994), Gendreau et al (1992), Rego and	
	Roucairol (1966), Rego (1998), Xu and Kelly (1996),	
	Ergun Ö. Et al (2006), Toth Vigo (2003), Golden et al	
	(1998), Dueck (1993), Li at al (2005), Shaw (1998),	
	Solomon (1987)	
Population Search	Rochat and Taillard (1995), Bozkaya et al (2003),	
	Tarantilis and Kiranoudis (2002), Prins (2004), Moscato	
	and Cotta (2003), Berger and Barkaoui (2004), Mester,	
	Bräysy O. (2005), Voudouris (1997), Rechenberg	
	(1973), (Potvin and Rousseau (1995)	
Learning Mechanisms	Reimann et al (2004)	

Table 2-2: Metaheuristics Proposed for Solving CVRP

2.1.1.2. VRPTW

Vehicle Routing Problem with Time Window, as a generalization of CVRP, is NP-hard. That is, even finding a feasible solution for VRPTW, given a fixed fleet size, is and NP-Complete Problem *Savelsbergh (1985)*. Although in case of narrow time window, problems with a realistic size can

be solved to optimality through exact algorithms, the concentration of the solution approaches for VRPTW has been on heuristic algorithms. Through what follows in this section, we will go over some of the solution approaches to this type of problem. However, reviewing all pertinent articles to VRPTW is out of the scope of this document. Nonetheless, we will provide some of the significant papers, e.g. *Cordeau et al (2002b)* and *Gendreau et al (2008)*, as a clue for the interested reader to follow the stream of the associated scholarly papers in this area of study.

The first algorithm to solve VRPTW was introduce in *Kolen et al (1987)*. They addressed the VRPTW with a fixed fleet of vehicles at hand at a depot to serve customers. They described a B&B algorithm to minimize the total route length, by making use of dynamic programming coupled with state space relaxation *Christofides et al (1981b)* to compute lowerbounds. Their algorithm, however, could solve instances less than 15 customers.

Solomon (1987) addressed the design and analysis of VRPTW; they described a variety of heuristics as well as carrying out extensive computational study which helped them conclude that insertion-type heuristic consistently gave very good results with different problem environments.

Solomon et al (1988) proposed various heuristics for solving VRPTW, including both route construction and route improvement procedures. They extended the branch exchange solution improvement procedures, that has previously applied to the standard VRP, to solve vehicle routing and scheduling problems with time window constraints.

Kohl et al (1999) developed the 2-path cut, valid inequalities, to compute lowerbounds for VRPTW. An effective separation algorithm was also developed to find inequalities. They applied B&B algorithm to find integer solutions to their problem, after incorporating the inequalities into the master of Dantzig-Wolf decomposition where the coupling constraints enforce that all customers to be served. The subproblem was a shortest path problem with time window and

capacity constraints. Their proposed algorithm The algorithm has been implemented and tested on problems of up to 100 customers from the *Solomon (1987)* datasets; it has succeeded in solving to optimality several previously unsolved problems and a new 150-customer problem.

Kallehauge et al (2006) proposed a Lagrangian branch-and-cut-and-price (LBCP) algorithm for the VRPTW; a significant speed-up gained through making use of acceleration strategy at the master problem compared to algorithms based on the Column Generation (CG) in the literature. They solved problem instances with 400 and 1000 customers.

Desrochers et al (1992) solved the relaxation of the set partitioning formulation of the VRPTW by column generation such that they added columns as needed by solving a shortest path problem with time windows and capacity constraints through Dynamic Programming (DP); then, they used the computed lowerbounds to find integer solution of the set partitioning formulation by means of B&B algorithm. They solve a problem of size of 100 customers to optimality by their proposed algorithm.

Irnich and Villeneuve (2006) they made use of elementary shortest-path problem with resource constraints (ESPPRC) to formulate the VRPTW; through carrying out experiments, they showed the lower bounds found through k-cycle elimination, for $k \ge 3$, could strengthen the lower bounds. Embedding this with CG, resulted in solving 15 unsolved instances of the (Solomon, 1987), to optimality.

Usually, the elementary shortest path subproblem of the CG model for the VRP is relaxed due to the too complexity of the problem. The same optimal integer solutions are found with and without elementary-path constraint as each of the customers must be visited just once. *Chabrier (2006)* proposed a modified labeling algorithm to enhance the algorithm for elementary path, resulting in

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better lower bounds. Consequently, they could solve 17 instances of the *Solomon (1987)* benchmark to optimality which have not been solved to the date.

In order to find integer solutions earlier through branch-and-price algorithm, *Danna and Le Pape* (2005) proposed a general cooperation scheme between branch-and-price and local search, thereby yielding high-quality upper bounds (UB) at earlier stages which leads to a smaller tree. On the other hand, en effective form of diversification is gained as branch-and-price provides the local search with different initial solutions.

Bard et al (2002) considered the problem of minimization of the number of required vehicles to meet the demand of customers in the VRPTW. For this, they proposed a Branch-and-cut algorithm; solving a series of relaxed problems incorporating newly found inequalities, resulted in obtaining ever increasing lower bounds. They made use of greedy randomized adaptive search procedure (GRASP) to obtain feasible solutions (UBs). Solving a separation problem helped finding violated cuts. Their suggested algorithm could solve benchmark problems of size 50 and 100 to optimality.

Heuristic Category	Some of the Contributions to VRPTW	
Route Construction Heuristics	Solomon (1987), Potvin and Rousseau (1993), Ioannou et al (2001)	
Route Improvement Heuristics	Russell (1977), Russell (1995), Baker and Schaffer (1986), Croes (1958), Lin (1965), Or (1976), Savelsbergh (1985), Solomon et al (1988), Savelsbergh, (1990), Savelsbergh (1992), Potvin and Rousseau (1995), Thompson and Psaraftis (1993), Cordone and Calvo (2001), Bräysy (2002), Glover (1996)	

Table 2-3: Heuristics Proposed for Solving VRPTW

Although we tried to mention some of the most significant papers dealing with VRPTW, due to the complexity of this problem, many of the researchers have focused on heuristic and metaheuristic approaches to solve the problem. We refer the interested researcher to discuss the following surveys to obtain profound knowledge about the evolution of heuristics and metaheuristics for solving VRPTW: *Bräysy and Gendreau (2005a, 2005b)* and *Gendreau et al (2008)*.

Metaheuristic Category	Some of the Contributions to VRPTW	
	Semet and Taillard (1993), Potvin and Bengio (2006), Taillard et al (1997), Rochat and Taillard (1995),	
Tabu Search	Taillard (1993), Badeau (1997), Battiti and Tecchiolli	
	(1994), Russell (1995), Chiang and Russell (1997),	
	Osman (1993)	
Genetic Algorithm	Homberger and Gehring (1999), Gehring and	
	Homberger (2002), Berger and Barkaoui (2004),	
	(Mester and Bräysy (2005), Potvin and Bengio (2006),	
	Thangiah and Petrovic (1998), Tan et al (2001)	
Other Metaheuristics	Kontoravdis and Bard (1995), Kilby at al (1998), De	
	Backer et al (2000), Gambardella et al (1999), Bent and	
	Van Hentenryck (2004), Shaw (1998), Bräysy (2003),	
	Mladenović and Hansen (1997), Taillard et al (1997), Li	
	and Lim (2003)	

Table 2-4: Metaheuristics	Proposed for	r Solving VRPTW
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Nonetheless, we provide you with some of the significant articles dealing with VRPTW directly, or whose results have been used to develop new heuristics for solving VRPTW, involving heuristics in Table 2-3 and metaheuristics in Table 2-4.

Although we tried to mention some of the most significant papers dealing with VRPTW, due to the complexity of this problem, many of the researchers have focused on heuristic and metaheuristic approaches to solve the problem. We refer the interested researcher to discuss the following surveys to obtain profound knowledge about the evolution of heuristics and metaheuristics for solving VRPTW: *Bräysy and Gendreau (2005a, 2005b)* and *Gendreau et al (2008)*.

2.1.2. Hazmat Vehicle Route Planning (HVRP)

We can observe the rarity of the implied Hazard assessment problems within the VRP literature since most of the Hazmat routing literature focuses on shortest path selection rather than forming complete tours *Eksioglu et al (2009)*.

One differentiating aspect of HVRP is the associated risk which leads to adding some additional commodity-specific constraints into a typical VRP which may, in effect, exert some crucially significant changes to the way we approach a typical VRP. That is, in a typical VRP, in general, we are trying to find the optimum paths for each and every O/D pair of orders under some networkspecific and operational constraints; in such problems, we aim to meet all demands at the minimum transportation cost. Such optimum solutions, could benefit not just the carrier, but the shipper and the customer, as well as the governments. These problems target to augment the volume of commodities to be shipped throughout the underlying network. Transportation of dangerous goods, on the contrary, cannot enjoy such conditions due to the risks it imposes on the environment and the society, hence, TDG has been regulated by the authorities. Such regulatory restrictions, in conjunction with some other Hazmat-related restrictions, should be incorporated into a Hazmat-VRP variant. Consequently, the inherent risk of transport of Hazmats, in effect, exert influence on both route planning and vehicle routing decisions while a typical VRP with non-regulated commodities concentrates on the latter part of the problem since the route planning decisions could be reached *a priori* by finding the shortest path or the cheapest one for each O/D pair of a demand. Considering that most of the articles developed for transportation of dangerous goods use single or multiple objective shortest path algorithms to minimize the risks due to shipment of Hazmats for each O/D pair. Tarantilis and Kiranoudis (2001) focused on a variant of VRP that determines a set of routes used by a fleet of trucks to serve a set of customers, reflecting many real-life

applications such as transportation of gas cylinders. They focused on mitigation of risk of population exposure through truck-route production, by solving a variant of VRP. They proposed a population exposure risk measure for each point in the risk space as product of population of a geographic population object such as a city, and distance-length between the point and the population point. They, further, suggested a single parameter metaheuristic algorithm called List Based Threshold Accepting (LBTA) that minimize risk by minimizing the total distance travelled by trucks in the so-called risk space. Moreover, they experimented with real-life data to show the performance of their proposed model and solution method.

Considering the overwhelming research on the O/D Hazmat routing problems, and the lesser focus that had been placed on Hazmat vehicle routing and scheduling problem, *Zografos and Androutsopoulos (2004)* addressed Hazardous materials distribution problem within a Hazmat vehicle routing and scheduling problem context. They proposed a biobjective VRPTW in order to minimize both risk and cost. Further, they proposed a new heuristic algorithm to solve their problem. Then, carrying out experiments with benchmark problem sets, they found the result of their algorithm encouraging. Moreover, incorporating their suggested algorithm with a GIS-based decision support system (DSS) for Hazmat logistics operations logistics which led to valid preliminary results on a set of case studies.

Du et al (2017) addressed a multi-depot vehicle routing problem. They developed a fuzzy bi-level model which seeks for minimization of total expected risk due transportation of dangerous goods when delivering Hazmat products to customers from multiple depots. Within their bilevel optimization formulation, the leader allots customers to depots subject to depot capacities and customer demands, while the follower determines the optimal path for each group of depot and customers. They, further, proposed and applied four fuzzy simulation-based heuristics to solve the

model and showed the effectiveness of their proposed model and heuristics through computational and illustrative experiments.

Hamdi-Dhaoui et al (2011) considered incompatible nature of some of the Hazardous materials in terms on storage and transportation; that is, some of the Hazmats neither can be stored in the same storage or building, nor can be transported in a same vehicle. They explained the first methods used vehicle routing problem with conflicts (VRPC); them, they presented a model that incorporates incompatibility of some of the materials such as Hazmats, into their mathematical model (VRPC). Further, they presented heuristic and metaheuristic methods, Iterated Local Search (ILS), and Greedy Randomized Adaptive Search Procedure-Evolutionary Local Search GRASP-ELS, to solve their model.

Bula et al (2017) addressed the Heterogeneous Fleet Vehicle Routing Problem (HFVRP) for transportation of Hazmats. Their proposed model's objective was to minimize total expected routing risk, which was a nonlinear function of vehicle load and the population exposure. They estimated the value of the objective function through piecewise linear approximation. They used a variable neighbor search (VNS) to solve their problem; they also enhance the performance of their algorithm through set-partitioning (SP) problem, as post-optimization procedure. They carried out computational experiments to verify their model and algorithm, which led to competitive results.

2.2. Hazmat Transportation Risk Assessment and Decision Making

One remarkable feature of transportation of Hazmats is its risk component which contrasts it from transportation of all other types of regular commodities. In the railway context, if we assume the same incident probability for both Hazmats and regular commodities, the differentiating aspect in transportation of Hazmats would be the adverse consequences like population exposure. Hence,

risk component of TDG plays a crucial role in decision making at all levels (strategic, tactical and operational). In the following sections, we will elaborate on the risk assessment measures and their effects on route planning, facility location and network design problems.

2.2.1. TDG Risk Constituents

The constituent parts of risk associating with TDG could be considered as *probability* of an accident which leads to the release and / or spill of Hazmat containers, referred to as "incident" in the context of transportation of dangerous goods, and harmful *consequences* imposed to the receptor that is located within the impact zone. Therefore, we will go over some articles dealing with probability of an incident and its catastrophic consequences.

2.2.1.1. Probability of Incident

To the best of our knowledge, *Ang and Briscoe (1979)* is the first research with an aim to develop a quantitative procedure for the predictive risk assessment for various transportation systems. For any given modes of transport, they suggested ways to evaluate certain factors on the safety of the system. Their effort led to many lots of theoretical and practical outcomes, one of which was that their offered methodology could estimate the accident rate / frequency in an existing or proposed system. As part of the quantitative risk analysis (QRA), they focused of the *frequency* of accidents and their expected *consequences*. Further, they elaborated on the computation of the probability of accidents given the frequency of faults affecting the system; they showed that identification of faults and their occurrence rate / frequency can be done systematically using a *fault tree*, referred to as fault tree analysis (FTA). As well, determination of accident probability can be done systematically through an *event tree*, referred to as event tree analysis (ETA).

Boykin et al (1984) addressed the equipment improvement of a chemical storage facility. They used various risk evaluation methods such as FTA and ETA, which is referred to as FETA in the

literature, and risk perspective techniques. Their work could be referred to as a successful application of FETA in risk assessment process.

Alp (1995) investigated quantitative risk assessment techniques mainly to quantify risks near transportation corridors. He showed the results of a real life example of application of the risk assessment methods to estimate probability and consequences of risks due to transportation of Hazmats in Toronto, Canada. They also made use of FETA on the process of assessment of the risk.

Jonkmana et al (2003) was an attempt to summarize 25 quantitative risk measures from the literature. They focused, mainly, on risk measures for loss of life, both individual and societal loss, as well as economic risk. They defined the Individual Risk (IR) as $IR = P_f \times P_{d|f}$, where P_f is the probability of failure and $P_{d|f}$ is the probability of death of an individual due to the failure. This measurement is used by Dutch Ministry of Housing, Spatial Planning and Environment (VROM). They also stated that $IR < 10^{-6}$, the standard set by Housing, Spatial Planning and Environment (VROM) Bottelberghs (2000), should always be reduced to a level which is as low as reasonably achievable (ALARA). Using the definition of Societal Risk given by Institution of Chemical Engineers (Great Britain, Engineering Practice Committee, Working Party (1985), "the relationship between frequency and the number of people suffering from a specified level of harm in a given population from the realization of a specified hazards", they computed the Aggregated Weight Risk (AWR), described by Piers (1998), by multiplying the number of houses inside a certain area with their IR level. They also showed that the probability distribution function of the number of fatalities per year can be used to derive societal risk. Further, they elaborated on the usage of FN-curve as a graphical representation of societal risk, where the probability of exceedance is represented as a function of the number of fatalities per year, on a double algorithmic

scale. Moreover, they showed that FN-curves are used as a tool for decision making about Hazmat installations in Denmark, Netherlands and the UK. One can find examples of FN-curve for PCB transport through Edmonton, Canada, in *Erkut and Verter (1995)*.

Probability of catastrophic event involving fatality or injury, due to an incident involving Hazmats container could be computed using *Bayes' theorem Erkut et al (2007)*.

Chow et al (1990) designed prediction models to estimate the likelihood of the most severe nuclear accidents such as complete core melts. They introduced Random Escalation Model (REM) which uses *Bayes*' methods, including multiple levels of event severity, to predict severe nuclear accidents and to assess the associating risk.

Glickman (1991) considered the transportation of flammable liquid chemicals in bulk through New York city. Under the both average and worst-case assumptions, he estimated the risks of transporting the Hazmats on two different routes, through a Bayesian model.

Mumpower (1986) and *Leonelli et al (2000)* showed that individual risk can be computed as frequency of death per year considering an average person at a given distance from the impact area. *Mumpower (1986)* also showed that this figure could be compared to de minimis of 10^{-6} or 10^{-5} deaths per year. However, Hazmat incidents usually involve a number of people exposed to the risk of death, injury or evacuation of area, thus we need to compute the risk imposed to those individuals, societal risk.

List and Mirchandani (1991) presented a model with a multiobjective function comprising of both risk cost and risk equity terms. Their model could be used by both carriers and authorities in the process of decision making about optimization of logistics plan, and setting regulations for routing of Hazmat materials and siting of Hazmat facilities, respectively. In their model, they did not use the conditional probability based on Bayesian theory; instead, for the sake of simplification, they

used the expected risk as the product of the probability of a release accident and the consequence of the incident, mostly referred to as *technical risk Erkut and Verter (1998)*.

2.2.1.2. Impact Area and Harmful Consequences

Consequences in case of an incident involving spill or release of Hazmats depends on several factors, one of which is the size and shape of the impact area or exposure zone, which is dependent on some other variables such as speed and direction of wind, topology, weather stability, and so on. Estimating, *a priori*, the dimensions and shape the exposure zone is sophisticated. However, researchers have proposed various approaches to model the exposure zone; we will review the most significant articles that have either proposed or applied one of the impact area modeling methods in the following subsections.

2.2.1.2.1. Fixed bandwidth

Batta and Chiu (1988) considered routing an undesirable vehicle like a truck carrying a Hazmat, on a network embedded on an Euclidean plane where the distribution of population centers or demand points at nodes and on links (straight-line) are distributed discretely and continuously, respectively. They sought for finding optimal path for the vehicle, regardless of the probability of Hazmat accidental leakage, which minimizes the weighted sum of lengths over which the vehicle keeps at least a lambda threshold distance from population centers along its journey from origin to destination nodes. They showed that shortest path algorithm can be used to solve their model if link lengths are appropriately redefined.

ReVelle et al (1991) showed that for the transportation of the hazardous wastes, spent nuclear duel rods, two measures of arc impedance can be postulated: transportation cost and actual or perceived risk of accident or exposure. Then, an arc impedance for each arc between any two given nodes is attributed which is a function of both arc length and the number of people living within a fixed

bandwidth of the arc. They made use of shortest path algorithm, 0-1 mathematical program for siting and the weighted sum method for solving multiobjective programming, for finding optimal solutions to the problem.

2.2.2. Danger Circle and Rectangular Impact Area

Erkut and Verter (1998) addressed the problem of lack of a unanimous agreement between all researchers in determining the risk due to transporting dangerous goods along its path from it s origin yard to its destination yard. They reviewed various methods that had been suggested to date, to show that different computation methods could lead to different "optimal" paths for routing Hazmat shipments. They also suggested a method to estimate the number of people affected in case of accident along a link segment by introducing danger circle method to determine the impact area. They suggested a danger circle with a radius between 0 to 7 miles around a link segment, which will carve out a band along a given arc where Hazmat is traversed through. Further, they justified the use of such a danger circle due to difficulties in computing the concentration level of a given type of Hazmats like Ammonia around a given link; they, further, explained that the concentration level is defined as a function of wind speed, release rate, distance from the container, and the topography. Thus, due to lack of data on the mentioned variables, on the one hand and lack of the knowledge about some other factors such as unknown dose-response of many chemicals, on the other, they found it practically impossible to estimate the incident consequences, thereby motivating them to make use of danger circles assuming the worst-case scenario where the chance of all people in the danger circle to be the same regardless of their distance from the incident spot, meteorological conditions and topography.

Kara et al (2003) investigated the differences between two methods suggested for determining the impact area: *semicircular exposure zone*, resulting from carving out the danger circle along a given link, and *rectangular* impact are.

They showed that by cutting off the circular areas at two nodes, we get the rectangular impact area which is also used by a special software, PC*HazRoute, developed for hazmat transportation, to compute population exposure. The radius or bandwidth is assumed to be substance-dependent; i.e. the effect of impact on any point within the impact area is not altered by the distance from the incident spot. Then, they further showed that the former method may result in significant errors stemming from double-counting at the nodes. The latter, rectangular impact area, as they illustrated, results in negligible errors in many cases. Nonetheless, nontrivial value of errors may be expected depending on the density of the population around the link intersections and the angle between link segment pairs. Furthermore, they proposed a link-labeling shortest-path algorithm, as adaptation of the algorithm developed by *Namkoong et al (1998)*, to find the path with the least population exposure.

Such predefined thresholds are suggested as a guideline for radius of isolation and evacuation areas for each type of Hazmats in ERG 2016 by CANUTEC, *Cloutier and Cushmac (2016)*. For instance, a circle of a radius of 800 *m* around a tank, tank-truck or railcar containing Chlorine, must be isolated and evacuated. For tanks, tank-truck and railcars containing explosives of (divisions 1.1, 1.2, 1.3 and 1.5) that may explode and throw fragments 1600 meters, as well as producing irritating, corrosive and / or toxic gases, at least 1600 meters must be isolated in all direction if the trailer or railcar is involved in fire.

2.2.2.1. GPM-based Eclipse

Of all hazardous materials, Toxic Inhalation Hazard (TIH), sometimes called Poisonous Inhalation Hazard (PIH), such as: Ammonia, Chlorine and Propane, may be among the most dangerous. Release of toxic inhalation hazards, whether the result of *attack (e.g. terrorist attacks)*, or *accident*, could result in devastating consequences. TIH / PIH material are *airborne* and their dispersion by wind is a very complex phenomenon. The level of concentration of TIH can help estimating the population exposure using mathematical air pollution dispersion models for airborne materials. Those models are mathematical simulation of the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere; in other words, we use them as means of estimating downwind air pollution concentrations given information about the pollutant emissions and nature of the atmosphere. The most popular air pollution model among researchers is *Gaussian Plume Model Arya (1999)*. The first formally published articles about GPM, however, to the best of our knowledge, backs to *Turner (1969)* and *Draxler (1980)* and *Draxler (1981)*. GPM, shows that airborne materials dispersion makes a shape of a *plume* like an *eclipse*, such as a pdf of a Gaussian probability distribution.

Hanna et al (1993) evaluated fifteen models for dispersion of gas-type Hazmats including; 7 of the models were publicly available, AFTOX, DEGADIS, HEGADAS, HGSYSTEM, INPUFF, OB/DG and SLAB, and six of them were proprietary models, AIRTOX, CHARM, FOCUS, GASTAR, PHAST and TRACE, and the remaining two models were two benchmark analytical models, GPM, and analytical approximations to the Britter and McQuaid Workbook nomograms. *Patel and Horowitz (1994)* considered determining the least risky path within a network for transporting Hazmats considering the diffusion of gases over wide areas from possible spills due to collision or improper operation of vehicle or container. They were the first to use GPM to model

the dispersion of the hazardous gases, thus estimating the expected number of affected people in case of an incident involving Hazmat. They showed that GIS could be coupled with optimization principles to solve difficult routing problems.

Chang et al (1997) considered developing of a decision support system (DSS) for the betterment of the decisions about chemical emergency and response. In urban environment, they used GIS for the management of chemical emergency response. They suggested that a computer-assisted DSS can be used to explore a real-time problem and find a set of acceptable solutions rapidly for emergency events. They incorporated four dispersion simulation model types: puff model, ISCST model which uses GPM, the three-dimensional numerical simulation model, and explosion model. *Zhang et al (2000)* used GPM to model the dispersion of airborne contaminants such as ammonia and chlorine, to determine the risk imposed on human populations. They modeled the likelihood of undesirable consequences such as injury, illness and death, as a function of concentration of contaminants. Using GIS, they could estimate the risk for each and every link of the network.

Puliafito et al (2003) addressed the problem of gaseous emissions of pollutant from auto-exhausts and industries causing airway diseases, decreasing productivity, and affecting artistic and cultural patrimony adversely in urban areas. They presented a model to determine air qualities in urban areas using GIS. Their model could be used to simulate and analyze both temporal and spatial pollutant concentration. Further, they model could also be used to test whether new industries in a given urban area would conform to the air quality standards, from air quality perspective.

Accidents involving Hazmats in railroad often involves multiple release sources (e.g. railcars) *Bagheri et al (2012)*. Thus, researchers tried to extend the application of GPM, from a single release source to multi-release sources. *Arya (1999)* and *Pasquill (1983)* showed that we can compute the total contamination level of Hazmats releasing from various sources with an arbitrary

position distribution and strength, by superposing the patterns of those sources and aggregating the contamination of each and every single source at any impact point. Considering this, Verma and Verter (2007) proposed a way to find the total concentration level at a given distance downwind from median, the first and the last railcar of a K-railcar block of Hazmats. They also proved that for a train containing n railcars, K of which are Hazmats, the greatest level of concentration of TIH at equidistant points from Hazmat block median, is when the wind direction is along with the rail segment through which train traverses. This result can be explained by GPM; that is, the highest level of hazmat particles will be reached at downwind distance from the release point where crosswind distance equals zero. In other words, when we are dealing with population exposure risk assessment method, we always consider the worst-case scenarios where the concentration of Hazmats are the most. Assuming equidistant points from a release point, the most concentration of releasing Hazmats, under GPM assumptions, will be at the point in downwind direction. So, for computing the worst-case scenario concentration levels, we assume that the elevation of the impact point is zero, the crosswind distance of the impact point from the release point is zero, and since in case of railroad transportation, the elevation of the source of release is almost zero as the railcar is derailed.

Verma et al (2011) addressed railway transportation of Hazmats at tactical level. They proposed a biobjective function comprising of terms of risk and cost of transportation, where risk was defined as the total number of people exposed to the risk of transporting Hazmat shipments along a given service-leg of train service carrying Hazmats. Impact area was determined through GPM by finding the longest downwind distance from rail segment computed from assuming the worst-case scenario for the contamination of Hazmats, IDLH level.

There is a profound discussion about air pollution modeling, and Gaussian Plume Models (GPM) and its parameters estimation in *Zannetti (1990)*; *Jørgensen and Johnsen (1981)*; *Moreira (2009)*; *Tirabassi (2009)*; *Pasquill (1983)* and *Arya (1999)*.

2.2.3. TDG Risk Evaluation Models

The main feature contrasting transportation of Hazmats with non-regulated commodities is its ingredient. Risk is inherent in commercial dangerous goods transportation. In terms of TDG optimization and mathematical modeling, we may take various types of risks, intrinsic to TDG, into consideration.

Table 2-5 depicts the categorization of TDG risk assessment measures from the literature. However, three main approaches, in general, have been taken to model TDG; one of then focuses on the probability of an incident, the other, concentrates on expected harmful consequences of an incident in TDG, the last one, takes the population exposure into account.

Expected consequence or Traditional Risk, might be the most popular risk assessment method, however due to the dearth of data, some researchers developed other ways to asses the risk. For instance, *Saccomanno and Chan (1985)* and *Abkowitz et al (1992)* took incident probability approach. Others, also, further developed other measures for risk analysis; *Batta and Chiu (1988)* and *ReVelle et al (1991)* focused on Population Exposure, the number of people exposed to the adverse effects and risk of evacuation of the area in case of incidents of cargos containing dangerous goods.

For each of the risk evaluation models shown in Table 2-5, we will go over some of the pertinent articles in the literature, in section (2.2.5).

Table 2-5: TDG Risk Evaluation Measures

Risk Evaluation Measures Recent	Classic	Expected / Traditional Risk (TR) Incident Probability (IP) Population Exposure (PE)
		Perceived Risk (PR)
		Maximum Risk (MM)
		Mean-Variance (MV)
		Expected Disutility (DU)
		Conditional Probability (CP)
		Demand Satisfaction (DS)
		Value at Risk (VaR)
	Recent	Conditional Value at Risk (CVaR)

2.2.4. Path Risk Axioms

Three axioms have been proposed by researchers for evaluating functions used in optimization models: Monotonicity Axiom for Path Evaluation Models, Optimality Principle for Path Selection Models, and Attribute Monotonicity Axiom.

The first axiom, monotonicity, was first proposed by *Erkut (1995)* which implies that as edges are added to a path, the evaluation value of the path will not decrease.

The second axiom, optimality principle for path selection, proposed by *Erkut and Verter (1998)* is could be construed as a restatement of Bellman's optimality principle which is a concatenating of the shortest path, i.e. an optimal path should be comprised of subpaths that are optimal themselves. Evaluation function satisfying this axiom should be order-preserving functions.

The third axiom, attribute monotonicity, proposed by *Erkut and Verter (1998)*, states that the path evaluation function is a nondecreasing function of edge attributes; i.e. edge attributes, incident probabilities and consequences, should be nondecreasing. Thus, path risk cannot decrease as probabilities and consequences of incident increase on an edge of the path.

Moreover, exact route evaluation models consider that edge impedances are path-dependent. That is, the likelihood of an incident on a given link segment on a path depends on the probability of the occurrence of the incident on the previous link segments of the path. This leads us to the assumption that vehicle carrying Hazmat on a route to its destination may experience several incidents with a small probability. Approximate method, on the contrary, assumes that any incident probability on a link on a path is not path-dependent, i.e. it does not depend on the probabilities of an incident on the previous links of the path. *Erkut and Verter (1998)* showed this approximation leads to a negligible error in computing incident probability along Hazmat route, less than 0.25% in most cases. The conditional probability of reaching an edge without experiencing an accident in the previous edges is very close to one owing to the very low incident rates, at most on the order of 10⁻⁶ per trip per kilometer *Harwood et al (1993)*.

Jin and Batta (1997) derived six exact risk models, by considering shipments as a sequence of Bernoulli trials. Their exact risk models, relate the number of shipments / trips to be made and the threshold number of accidents. Further, they assumed that if either an accident happens or trip is reached to its destination, the trip will be ended.

2.2.5. Risk Evaluation Measures

Throughout the following subsections, we will go over some contributions to the risk evaluation functions, which were listed in Table 2-5.

2.2.5.1. Traditional / Expected / Technical Risk (TR)

Batta and Chiu (1988) made use of traditional risk in their model such that the risk on each edge is the product of incident probability of the edge, accident per-unit length of movement, and its consequences, population exposure. They showed that the previous risk models in the literature used to assume that in case of an accident on a given link, risk (population exposure) would not consider the spot of the accident on the link. They, on the contrary, presented a model which attributes various risk parameters to an edge depending on the incident spot. Moreover, they showed that their model, contrary to the earlier models proposed by other researchers, could take this fact into account that the risk due to Hazmat shipments are higher on the intersections rather than along a link segment. Thus, they assigned penalties to the nodes of the transportation network to incorporate this concept. Moreover, the suggested model was the only approach by that time that went beyond point presentation of population center. They suggested risk model could incorporate the population density function associated with each edge.

Alp (1995) utilized quantitative risk assessment techniques to estimate the frequency of the release of Hazmats in case of accidents, then using this data, he defined the event risk as product of those frequencies to the estimated consequences, which conforms to the definition of traditional risk. He, also presented contrasting features of event risk and facility risk.

Zhang et al (2000) used traditional risk evaluation function as a product of probability of undesirable consequence due to the release of Hazmat and it its harmful consequences. Their aim was to develop a method of assessing risk of transportation of Hazmats whose results is more accurate using a dispersion model, GPM, and GIS. They used GIS and GPM to define the probability of adverse consequences of the spread of airborne Hazmats at any point around the link segment as the concentration level of the contaminant at that point divided by the maximum concentration of that pollutant computed through GPM.

Traditional risk has been used by the Department of Transportation in the US for many years in order to evaluate risk of paths and compare them for routing decision making *(DOT, 1994)*. Probability that a vehicle will be in a highway accident resulting in release of Hazmats along the highway route was multiplied to the potential number of people exposed to the risk of evacuation,

death or injury, to obtain risk value of the route. So that, for certain shipment, they could evaluate route risk values of two or more paths, thereby choosing the route with the minimum risk.

Erkut and Verter (1995) used TR in their risk modeling approach; they used the expected harmful consequences due to TDG as a measure of the associated societal risk; societal risk was obtained by multiplying the probability of a release event to the consequence of that event. Further, they presented a model which can be assumed to be a generalization of *Batta and Chiu (1988)*; they extended the basic model to compute risk of transporting Hazmats through large population center that cannot be modeled as a single point on a plane. Treating large population centers as two-dimensional objects on the plane, lead to more accuracy in treatment of consequences compared to the basic model.

Fang and Reed (1979) gathered and purified records of the location of derailed train railcars of 1975, 1976, and 1977, and found that 38.7 percent of the cars derailed were in the first third of the train, 36.2 percent were in the middle third, and 25.1 percent were in the last third. Hence, they proposed that hazmat railcars should be placed near the rear of the train because the front of the train is more prone to derailment under loaded conditions.

Verma (2011) suggested a way to incorporate the probability of incident in railway transportation, which could be used to compute the expected risk for route evaluation decisions. Analyzing Federal Railroad Administration (FRA) accident records, he concluded that front of the train is riskier, and safest position to place Hazmat railcars, freight-trains of any length, are the seventh to ninth train-deciles. Moreover, He developed a methodology using Bayes Theorem and Logical Diagrams. for risk assessment which accounts for the differentiating features of trains and train accidents. That is, the model incorporates the train-length, position of train-decile position of Hazmat railcars, the sequence of events leading to hazmat release, and the associated consequence

from ruptured railcars. the model, however, could estimate the risk of derailment associated with each decile of a train, but it failed to differentiate the probabilities of derailment of the cars within any given decile of the train. For instance, for a medium-size train containing 50 railcars, the probability of derailment of railcars 41 and 49 would be the same because they are both on the fifth decile.

Bagheri et al (2012) suggested a new risk assessment method to measure the risk of each and every railcar in short, medium and long trains. They showed that the causes behind derailment can be categorized based on the point of the derailment (POD), considering a train consist is divided into three parts: front, middle, and rear. Further, they put the train types into three different categories: short, medium and long, based on the number of railcars they carry in a similar fashion to Verma (2011). Then, having performed a nonparametric Kruskal-Wallis test to evaluate the significance of the effect of train types, short, medium and large, and derailment cause types, causes of derailment at the front, in the middle and at the rear part of train; it turned out that there was a significant explanation for the median point of derailment (POD). Through analysis of empirical dataset for 1997 to 2006, associating with the number of accidents (approx.5800), derailment of 885 Hazmat railcars, and 167 Hazmat railcar rupture and release (approx. 18.8%), they concluded that accidents involving Hazmats, often (e.g. 8 out of 11 accidents in 2006), result in multi railcar release episode. Moreover, they suggested that the probability of the release of a derailed Hazmat railcar, in a series of derailed cars, is independent from the probability of the release of any other derailed Hazmat railcar.

Bagheri et al (2014) compared road and rail modes of transportation of Hazmats w.r.t. the risk level and adverse consequences, they can bring about. They a novel and comprehensive assessment methodology to measure rail transport risk. Further, they made use of the proposed assessment

methodology to analyze hazmat transport risk resulting from meeting the demand for chlorine and ammonia in six distinct corridors in North America. Finally, they demonstrated that rail transport will reduce risk, irrespective of the risk measure and the transport corridor, and that every attempt must be made to use railroads to transport these shipments.

Cheng et al (2017) proposed a novel methodology which takes into account not just the characteristics of railroad accidents (i.e., quality of tracks, position-specific derailment and release probabilities, and consequence from multiple release sources viz., more than one hazmat railcar could be involved in an accident and release their contents) but also does not require any information on the train makeup as in *Bagheri et al (2014)*.

2.2.5.2. Incident Probability (IP)

Saccomanno and Chan (1985) addressed routing of trucks containing Hazmats through designated safe route to reduce the potential risk due to Hazmat spills. They used three different criteria for designating safe truck routes leading to various results in routing decisions: minimum risk, minimum accident likelihood, and minimum truck operating costs.

Minimum accident likelihood, implies the incident probability which is a simplification of traditional risk model which is reached by ignoring the variation in population density or considering all population densities, within a danger circle, are equal to some constant. However, this model for risk assessment may be appropriate if the transported Hazmat has a small danger circle; then, one can define the objective function such that the model could minimize the risks imposed on drivers, and costs due to incident.

Abkowitz et al (1992) used the definition of traditional risk, just as a measure to compare routing alternatives depending various path evaluation criteria. They assumed a fixed bandwidth of 5 miles around each link segment for estimating the population density. They proposed a bi-criteria

objective function to minimize risk and time of travel. They carried out various experiments with different criteria for designating routes for transportation of Hazmats; they defied the risk as a unitless-in-dimension expression obtained by multiplication of release-causing accident likelihood and population exposure (like traditional risk). They elaborated on their conclusions by comparing routing decision making under various criteria (incident probability, population exposure, traditional risk, and time of travel), like comparing the results obtained from perceived risk and traditional risk.

Bagheri et al (2011) addressed the placement of dangerous goods along a train consist and its relevance to the probability of derailment. They investigated the relationship between Hazmat railcar placement and derailment for different route attributes and Hazmat shipments. Their proposed model could estimate the probability of a railcar derailment by position given an estimated POD and the number of derailing railcars. Further, they presented a Hazmat railcar model that takes the derailment risk into account, to provide a reasonable scientific basis for effective dangerous goods (DG) marshalling in conventional rail hump yard operations.

2.2.5.3. Population Exposure (PE)

Batta and Chiu (1988) and *ReVelle et al (1991)* used population exposure in their risk assessment process. They assumed a fixed threshold, lambda, around the road segment, then computed the harmful consequences in terms of population exposure, using population density within the lambda-distance from the link. Since we have already reviewed those articles, in order to prevent duplication, we refer the reader to the section (2.2.1.2.1).

2.2.5.4. Perceived Risk (PR)

Slovic et al (1984) addressed perceived risk in terms of societal impact of fatal accidents. They showed that most of the models proposed for assessment of societal impact of accidents involving

fatalities are based on of disutility function of the number of fatalities in each accident, with a form like N^{α} ; where $\alpha = I$, $\alpha > I$, and $\alpha < I$ shows neutrality, aversion and proneness behaviors, respectively. Thus, perception of a society regarding risk is that a single large accident is more hazardous and serious than many small accidents producing the same consequences in terms of the aggregate number of fatalities. They argued that these models are inadequate partly due to the fact that accidents are alarming future troubles, meaning that societal impact is determined, to a great extent, by what it signifies. Therefore, an accident with little harm may bring about huge consequences should it amplify the judged probability and seriousness of future accidents. Further, they proposed that models, based solely on functions of the number of fatalities, be abandoned in favor of alternative models elaborating in the significant events and consequences due to accidents. Abkowitz et al (1992) showed that risk neutrality $\alpha = 1$ based on traditional / technical risk, assumes the same risk for an incident causing 100 fatalities and 100 incidents causing one fatality each. Risk aversion, $\alpha > 1$, on the contrary, associates more risk to the former case. They showed that risk aversion conforms to the public perception of risk when it comes to the safety of transportation. Carrying out various experiments, they concluded that the public perception of preferred routs is different from those determined using technical risk. Thus, in order to reconcile the differences, they offered to either the public perception of risk should be incorporated into the risk assessment methodologies or through the risk communication process.

Sherali et al (1997) addressed the development and analysis of a model seeking for minimization of risk of low-probability-high-consequence (LPHC) accidents associated with TDG. Their proposed model considers trade-offs between the conditional expectation of adverse consequences given an accident has occurred, and traditional risk which deals with the expected consequences and accident probabilities on a selected path. In other words, they wanted to find a path that minimizes conditional expectation value, under the constraints that expected value of the consequences being lesser than or equal to a specific value, and the aggregated path probability being less than another specific number. They solved their proposed model using a specialized branch-and-bound (BB) algorithm.

2.2.5.5. Maximum Risk (MM)

Addressing the deficiencies of the commonly used expected risk / traditional models for risk assessment, in considering the risk-averse attitudes of decision-makers in case of LPHC events,

Erkut and Ingolfsson (2000) proposed three models with three different criteria to address the catastrophic-avoidance models through: minimizing the maximum population exposure, in the first model. variance of route consequences is incorporated into the second model. The third model deals with an explicit disutility function. Moreover, they showed that all the suggested models can be reduced to a standard shortest path problem.

2.2.5.6. Mean-Variance (MV)

Sivakumar and Batta (1994) considered a variance-constraint shortest path problem, with all linear terms of objective function and both linear and nonlinear terms in constraints. Their proposed model could be used to model problems with probabilistic travel cost where travel costs on any two links are not correlated to with one another. The least expected length path is identified by their risk model subject to the constraint that the variance of the path length is within a prespecified upper bound. To ensure simple-path solution, subtour elimination constraints were added since the covariance terms could be negative. They could solve their models to optimality through exact solution methods and experimented with real-life routine scenario involving liquefied-gas Hazmats.

Erkut and Ingolfsson (2000) proposed three models (as explained in 2.2.5.5), one of which was variance of route consequences. In this model, the decisions about routing is based on the societal risk, he expected number of people affected in case of incident. Their model takes into account both the expected value and variance of the catastrophic potential of a Hazmat route. Since distribution of the consequences due to Hazmat release are bounded below by zero, with a mean close to zero, they considered the variance of the catastrophic events as measuring the extent of the right tail of the consequence distribution, where incidents are supposed to be following a spatial nonhomogeneous Poisson process over edges of the network, and they assumed a single trip may involve several incidents based on the approximate model, thus an incident would not terminate the trip. Since minimization of harmful consequences potential (variance) of paths, solely, do not make much sense without minimization of the expected value of those consequences, one ay consider these problems as a multiobjective problems to be solve by weighted sum, for instance. Thus, we may obtain a disutility model comprised of both mean and variance of path consequences for a given constant as a coefficient of variance, leading to various Pareto-optimal solutions, as a result.

2.2.5.7. Expected Disutility (DU)

Erkut and Ingolfsson (2000) proposed three models for path risk evaluation, one of which involved minimization of *expected disutility*. This model, unlike MV and MM, explicitly makes use of a utility function to account for risk-aversion attitude. Their proposed model has a catastrophe-aversion property such that considered the $(i + 1)^{st}$ life lost cost more than the i^{th} lost life. They assumed the incidents rate follow a spatial nonhomogeneous Poisson distribution. Population density is known and the number of the affected people as a result of an incident on each edge, *X*, is a function of population density function and incident probability. Thus, disutility function was

defined as follows: $u(X) := exp(\alpha X)$, where $\alpha > 0$ is a measure of catastrophe aversion. The greater the value of α , the less risk prone attitude towards selecting the associated link segment. Thus, expected disutility function for a given path *P* comprised of *n* consecutive links and incident likelihood of *P_i* on edge *i* of *P*, and *c_i* people exposed to risk, would be: $E[U(X)] = exp\left[\sum_{i=1}^{n} p_i(exp(\alpha c_i) - 1)\right]$. Thus, this model could be reduced to solving a shortest

path problem with $p_i(exp(\alpha c_i) - I)$ as edge impedance.

2.2.5.8. Conditional Probability (CP)

For modeling their problem, *Sivakumar et al (1993)* used conditional risk, and evaluate the expected consequences assuming the first accident surely happens. Their model minimizes the conditional risk; keeping the accident probability within a set threshold is also presented. They proposed two solution procedures.

Sivakumar et al (1995) considered routing of Hazmats for the case that that the occurrence of the first accident ends the routing. In their model, multiple route situation is permitted. The objective function is the minimization of the expected risk of the first accident under various constraints, such as constraints on probability of accidents, the expected *a priori* risk, cost of transportation, and risk equity. They used column generation to sole their model heuristically. Their model could be assumed as an extension to *Sivakumar et al (1993)*.

2.2.5.9. Demand Satisfaction (DS)

Erkut and Ingolfsson (2005) considered the fat that in reality the demands must be met even if the shipment happens to be involved in an accident. That is, assuming an accident can terminate a trip, as assumed in exact models; thus, incident will lead to subsequent shipments to satisfy the demand. They showed that assuming each trip without any accident as success in a Bernoulli trial, then the

number of trips on the same path before the first success follows a Geometric distribution. Thus, one could minimize the expected total consequence from all trips required to meet a given demand.

2.2.5.10. Value at Risk (VaR)

Kang et al (2014) introduced a VaR risk evaluation model which is used to routing decisions for a hazmat shipment given a predefined confidence interval for risk. On this basis, VaR could be assumed to be threshold value such that the probability of the consequences exceeding the VaR value is less than a probability level. Thus, their proposed model sought for routes with the minimum probability of the risk greater than a certain threshold. They solved their model to optimality for a single-trip problem, through exact solution approach. Through experiment they showed that VaR finds different routes for various confidence level.

Recently, *Siddiqui and Verma (2017)* addressed crude oid periodic fleet adjustment problem, and suggested a conditional value-at-risk based methodology to avoid extreme losses. They proposed a mixed integer nonlinear programming mode MINLP; theu made use of Monte-Carlo simulation to estimate their parameter. They tested the proposed model using a number of problem instances, and reported their results.

2.2.5.11. Conditional Value at Risk (CVaR)

Kwon (2011) investigated CVaR and its application in mitigating risk due to TDG. They proposed a new way to use CVaR as a measure for making decisions among possible choices of route for Hazmat shipments. They described their computational method to obtain the optimal path using CVaR; they illustrated how they model could determine the optimal CVaR route through a case study in the road network surrounding Albany, NY.

Before ending this section, we would like to discuss VaR and CVaR to some extent. These measures for risk assessment have been first suggested and applied in portfolio management and

financial investments. Both VaR and CVaR quantile-based risk measure (QBRMs). VaR is not a coherent measure whereas CVaR is tractable and assumed to be a coherent to VaR, and unlike VaR, a convex optimization framework could be provided by CVaR. However, although minimization of CVaR is convex in the context of financial optimization *Rockafellar and Uryasev* (2000), it is not the case for problems dealing with TDG.

Dowd and Blake (2006) discussed a number of QBRMs proposed for risk assessment such as VaR, CVaR, spectral risk measures, and distortion risk measures. Comparing the properties of various measures, they pointed out that VaR is seriously flawed.

Hosseini and Verma (2018) proposed a CVaR methodology for routing Hazmat frieghts, and considering the best train configurations, where train services are predefined, the showed that transport risk evaluated by CVaR is minimized. To estimate the conditional probabilities and to model the dynamics of the railroad accidents, they analyzed freight train derailment records. They tested their proposed methodology on several problem instances which indicated that their proposed methodology was superior to other measures for risk-averse routing of Hazmats.

Since most of the scholarly articles about VaR and CVaR involve risk assessment in the realm of financial investments, portfolio management and insurance plans, reviewing all of the literature dealing with these measures cannot be incorporated into the scope of this document. However, we encourage the interested researcher to review: *Kwon (2011)*; *Dowd and Blake (2006)*; *Sarykalin et al (2008)*; *Kang et al (2014)*; *Acerbi (2002)*; *Artzner (1999)*; *Acerbi (2004)*; *Mansini et al (2007)*; *Zhu and Fukushima (2009)* and *Pflug (2000)* to obtain more knowledge about the background, state-of-the-art methods and applications.

2.2.6. Contrasting Features of Railway TDG: Rail vs. Road

Most of models proposed for risk assessment have been developed to assess risks owing to transportation of Hazmats via road. *Erkut et al (2007)* indicated that most of the models proposed for targeting risks of road shipment may not be extended to the railroad transportation of dangerous goods due to the essential differences between those modes of transport. Table 2-6 lists some of the contrasting features of those modes of transportation.

Feature	Road	Rail
Infrastructure Ownership	Government	Private Rail Companies
Network Density	Dense	Sparse
Routing Decision	More Alternative	Less Alternative
Choice of circumventing major population centers	More Choice	Less Choice
Carriers per Shipment	Usually One	Usually More than One
Choice of circumventing major population centers	More Choice	Less Choice
Carriers per Shipment	Usually One	Usually More than One
Nonhazardous and Hazardous Cargo Together	Almost Never	Usually Yes
Approximate Tank Capacity	25 - 30 tons / truck tanker	80 tons / rail tank
Tanks Involved per Incident	1 per Truck	Several per Train
Variability of the number of Hazmat Tanks per Vehicle (Truck / Train)	Non (1 Hazmat per Truck)	High (Different No. of Hazmat Railcars / Train)

Table 2-6: Main Differences between Rail and Road Transport Modes

Some researchers, however, investigated the causes behind incident caused due to the derailment of train railcars, and the expected adverse consequences, to enhance risk evaluation models to capture the characteristics of the railway transportation. Causes may include speed and consist of train, or they could stem from infrastructure and maintenance. For instance, we can refer to *Bagheri et al (2012)* as an example of the studies that investigated cause due to consist of the train. Recently, *Liu (2017)* Analyzed the effect of rail defect inspection frequency on hazmat transportation risk. Also, evaluated segment-specific broken-rail-caused hazmat transportation

risk. Further proposed risk-based prioritization of rail defect inspection for hazmat transportation safety.

2.3. Facility Location Problem

Facility Location, as a crucially important topic in the realm of operations research, has been widely studied for decades. However, as sensitivity about environmental concerns increase over the last few decades, environmental aspects of facilities and their hazards to the environment and people, have been incorporated into these models. Since there are various surveys about Facility Location Problems in the literature, we will refer to some significant surveys and contributions to undesirable facility location problem in section (2.3.1), then we will cover more articles in Hazmat Location and Routing Problem (HLRP) in section (2.3.2). Moreover, Table 2-7 also provides some significant contributions to the subject by category.

2.3.1. Noxious and Obnoxious Facility Location Problems

Siting facilities, from the public perspective, could be classified into two main classes: desirable and undesirable. Problems addressing the latter class can also be categorized into two categories: problems dealing with siting of facilities that are hazardous, called noxious, or those dealing with nuisance facilities, called obnoxious.

Church and Garfinkel (1978) considered locating a point on a network so as to minimize the sum of its weighted distances (maxisum) to the nodes. They showed that there exists at least one optimal point in a finite set of points which can easily be generated. They proposed and algorithm, $O(mn \log n)$ time, for locating an optimal point (maxian) in this set. They showed that when network is a tree, this set consists of dangling nodes. In the field of location of undesirable facilities on networks, they are the precursors.

Minieka (1983) axiomatically characterized anticenter (maximax) and antemedian function on finite paths. the latter is a directed approach to that of *Church and Garfinkel (1978)*.

Erkut and Neuman (1989) considered undesirable facility location problem. They suggested that for this kind of problems, a model which maximizes some function of distance between facilities would be more appropriate than those most of them models minimizing some function of distance. They also provided a survey of maximization location models in the literature, whose objective functions involve distances. Further, they presented a synthesis of solution procedures emphasizing similarities and differences.

Cappanera (1999) presented a survey of mathematical methods for undesirable location problems in the plane and particularly on networks; solution procedures are briefly described. A review of extensive obnoxious facility location problems in networks is also given.

Current and Ratick (1995) considered the adverse effects due to facilities generating, processing, or disposing of such Hazmats. They also considered that most of the literature (to date) has considered siting and routing aspect of the problem separately. Hence, they proposed a multiobjective model to assist decision makers in location facilities handling Hazmats, and routing of Hazmats to those facilities. They also considered the equity in spatial dispersion of risk; on aggregate level, Risks and equity were addressed through minisum objectives, and at the individual level, they were addressed through minimax objectives.

Labbé (1990) considered an obnoxious facility location w.r.t. finite number of inhabitants with certain locations at vertices of a general network. She defined anti-Condorcet point, a voting solution, is a point in the network such that no other point is farther from a strict majority of inhabitants. Using an example, she showed that on a network with odd number of vertices (inhabitants), a finite set of points exists that contains all such solutions. However, an example was

used to show that this result cannot be extended to general networks with an even number of inhabitants. An algorithm is presented to find the solution of special case of a tree network, that the extreme vertices of a diameter is an anti-Condorcet point.

Tamir (1991) discussed new complexity results for several models dealing with the location of obnoxious or undesirable facilities on graphs, concerning the location of some p facilities, under Maximin and maxisum criteria, which are known as p-maximin and p-maxisum.

Colebrook and Sicilia (2006) addressed the problem of locating an undesirable facility location problem under the constraint. They could improve the *anti-cent-dian, as named by Moreno and Rodriguez (1999)*, facility location problem, on networks, providing an efficient O(mn) time algorithm. Their proposed algorithm is based on a new upper bound and on some specific properties of the anti-cent-dian problem.

Berman and Wang (2006) investigated 1-median and 1-antimedian problems with probabilistic demand; demand weights of users generated at nodes of the network are assumed to be independent and continuous random variables. The objective of 1-median problem with probabilistic demand, is to find a location of a desirable facility on a network that maximizes the probability that weighted sum distance does not exceed some predefined value *T*. On the contrary, the objective of 1-antimedian problem is to locate an undesirable facility, we maximize the probability that the total weighted distance is at least *T*. Moreover, they also discussed how to solve the problems under arbitrary distributions and for small and large networks.

Berman and Wang (2007) investigated the siting of semi-obnoxious facilities, where demand points within a certain distance from an open facility are expropriated at a given price. The objective of their proposed model was to minimize the total weighted transportation cost and expropriation cost. They considered developing the model for both single and multiple facilities. For a single facility, they developed an efficient algorithm for the problem on a network. a branch-

and-bound procedure using Lagrangian relaxation is proposed for the case involving locating problem of multiple facilities.

Berman et al (2007) proposed a novel methodology based on arc-covering in order to determine the optimal for the network so as to maximize the ability to respond to dangerous incidents; the emergency response capability to transport incidents in Quebec and Ontario (Canada) were assessed by their results.

Yamaguchi (2011) examined a model on a line network, where individuals collectively choose the location of an undesirable public facility through bargaining with the unanimity rule. They showed the existence of an stationary subgame perfect equilibrium (SSPE) and the characterization of SSPEs. They also showed that depending on the value of discount factor, as the discount factor tends to 1, the equilibrium location can converge to a location that is least desirable according to both the Benthamite and Rawlsian criteria.

Recently, *Ardjmand et al (2016)* presented a new stochastic model for transportation, location, and allocation of Hazmats. The objective function minimizes the total cost and risk of locating facilities and transportation of Hazmats, where cost of transportation is considered to be of a stochastic nature. They aim to make decision about (1) where to open the facilities and disposal sites; (2) to which facilities every customer should be assigned; (3) to which disposal site each facility should be assigned; and (4) which routes a facility should choose to reach the customers and disposal sites. Further, they a novel genetic algorithm (GA) for solving their model. The results revealed the efficiency of the proposed GA in terms of finding high quality solutions in a short time.

2.3.2. Hazmat Location-Routing Problem (HLRP)

Most of the time, both origin and destination of Hazmat shipments are noxious. For instance, supply chain of gas can be a good example of TDG where both origin and destination are hazardous, themselves; crude oil from oil fields is transported to refineries, where both sites are

hazardous. Subsequently, processed oil derivatives like petroleum or gas are transported to gas stations, and both origin and destinations may indeed impose threat to the society and environment. *List et (1991)* carried out a survey research on Hazmat materials transportation (rail and road), focusing on work done since 1980, dealing with risk assessment, routing / scheduling, and facility location. Tracing the evolution of models from single-criterion to multiobjective, the review highlights the emerging direction dealing with distributions of outcomes rather than the only optimizing the expected value. They discussed various aspects of TDG and offered significant challenges for further research.

Undesirable Facility Location on Network	Undesirable Facility Location on Simple Networks	1-Uncenter Problem	Melachrinoudis and Zhang (1999), Dyer (1984), Berman and Drezner (2000), Colebrook et al (2002), Church and Garfinkel (1978)
		Maxian Problem	Tamir (1991), Colebrook et al (2005), Colebrook and Sicilia (2006)
		Anti-cent-dian Problem	Moreno and Rodriguez (1999), Hansen et al (1991), Hershberger (1989)
	Undesirable Facility Location on Multicriteria Network	Uncenter	Zhang and Melachrinoudis (2001)
		Median	Hamacher et al (2002), Kalcsics et al (2014)
		λ-anti-cent-dian Problem	Moreno and Rodriguez (1999), Colebrook and Sicilia (2007)

Table 2-7: Some of the Contributions to Undesirable Facility Location Problem

Cappanera et al (2003) addressed the problem of simultaneously locating obnoxious facilities and routing obnoxious materials between a set of built-up areas and the facilities is addressed. They defined Obnoxious Facility Location and Routing model (OFLR) model, which is NP-hard discrete combined location-routing model. Further, they proposed a Lagrangian heuristic approach to solve the OFLR.

Erkut and Alp (2007) focused on designating Hazmat routes in and through major population centers. They restrict our attention to a minimally connected network (a tree) where we can predict accurately the flows on the network. We an aim to minimize the total transport risk, they formulated their integer programming problem. They could solve small-size problem instances to optimality by commercial solvers. However, they developed a constructive heuristic to expand the solution of the tree design problem by adding segments. Such additions usually increase the risk while reducing the transportation costs. The heuristic adds paths incrementally, which allows local authorities to trade off risk and cost. They also used the road network of the city of Ravenna, Italy, to demonstrate the solution of their integer programming model and their path-addition heuristic. Xie and (2012) considering the data derived from US Commodity Flow Survey, suggesting that transporting hazardous materials often involves multiple modes, especially for long-distance transportation, and due to the rarity of the articles on Hazmat location and routing on a multimodal transportation network, they proposed a multimodal Hazmat model that simultaneously optimizes the locations of transfer yards and transportation routes. They initially developed a nonlinear model which was converted into a mixed integer linear form. The new model could simultaneously optimize transfer yard locations and routing plans. They experiment their model with two case studies of different network sizes to test its applicability. They finally reported their results and suggestions for future work.

Bronfman et al (2016) addressed designing routes for Hazmat transportation in urban areas with muliple O/D pairs. Their proposed maxisum and maximin-maxisum models minimize the danger to which vulnerable centers are exposed by the routes. They proposed efficient IP formulations for both NP-Hard problems, as well as a polynomial heuristic that reaches gaps below 0.54% in a few seconds on the real case in the city of Santiago, Chile.

2.4. Hazmat Global Route Planning

Global route planning involves minimization of total risk and equity in the spatial distribution of risks within a jurisdiction, which are the two main concerns of governments within their jurisdiction. Risk mitigation measures taken by governments, local and provincial authorities could be put into two main categories: *proactive measures* and *reactive measures*. The former class involves establishment of inspection stations *Gendreau et al (2000)*, insurance requirements *Verter and Erkut (1997)*, container specifications *Barkan et al (2000)*. The latter class, however, involves establishment of hazmat emergency response networks *Berman et al (2007)*, and banning the use of certain rail segments *TC, Dangerous Goods Transportation and Handling Act (2002)*. Global route planning entails both proactive and reactive measures. However, those measures involving equity in spatial distribution of risk and minimization of total risk is of our interest. Hence, we will go over the literature on global route planning in the following order: risk equity and network design.

2.4.1. Spatial Risk Dispersion Equity

Risk equity can be achieved through various ways such as imposing risk equity constraints, generating dissimilar paths w.r.t. spatial risk distribution and risk load on links.

Keeney (1980) was the first article, to the best of our knowledge, that addressed equity of risk. He defined the public risk as possible fatalities to the member of the public. He, then, differentiated

between the risk risks of intrinsic into normal operations, like driving a car, and the risk due to hazards such as explosion. The paper explains that the risk due to private operations such as driving a car is accepted by the public since publics perception about them is their advantages outweigh their disadvantages. On the contrary, larger technological projects, for instance, concern the public because they are not sure if the risks would be worth the and / or if the risk is equitably distributed among the public. They proposed a measure of public risk which explicitly addresses the equity of risk. *Keeney (1980)* considered equity of risks in large-scale projects such as power plants where a group of people may incur the risks while some other group of the public may benefit from the project. On this basis, to address the equity of fairness of risk, equitable distribution of risk is developed to address the equity issue. They also proposed utility function that are consistent with different value attitudes involving risk equity.

Keeney and Winkler (1985) was one of the first efforts to address the equity of risk explicitly. They defined *ex ante* risk equity (equity of the processes resulting in harmful consequences like fatalities) and *ex post* risk equity. They incorporated both types of the risk equities as well as loss of life into von Neumann-Morgenstern utility model to evaluate public risks.

Zografos and Davis (1989) investigated system-wide routing of Hazmats and addressed the reduction of risk to the people living along links of a transportation network. For this, they proposed both capacitated and noncapacitated multiobjective optimization problem including terms for *Minimization of risk; minimization of risk of special population categories; minimization of travel time; and minimization of property damages*. Computational experiments revealed that adding capacity constraints leads to equitable distribution of risk throughout the network links while leading to an increase of 35% of the total risk.

Gopalan et al (1990a) considered a shortest path problem subject to equity constraints. Complicating constraints of the problem are relaxed through Lagrangian dual bounding approach. Duality gap is closed by finding t-shortest path regarding Lagrangian function. They considered both looping and loopless paths. They also proposed quick-and-dirty procedure and carried out experiments to show the performance of the model and algorithm.

Gopalan et al (1990b) proposed a model which minimizes the risk of travel and spreads the risk equitably throughout the geographical zones of the network. They develop a model to generate equitable set of routes Hazmats transportations. They also suggested a heuristic repeatedly solves single-trip problems, where a Lagrangian dual problem with gap closing procedure is used to solve single-trip problems to optimality. Computational experiments revealed high degree of equity can be achieved by modestly increasing total risk and through embarking on different routes to evenly spread risk among zones. Further, results indicate their proposed heuristic works efficiently computational requirements as well as solution quality.

Bell (2006,2007) proposed a minmax formulation considering both loss due to accident and cost of transportation, which minimizes the maximum risk. Thus, risk equity is achieved by balancing the risk through the links of the network. Useful insights into the nature of the solution could be obtained through connections to game theory. for risk equity by balancing the risk through the links of the network.

Akgün et al (2000) considered the problem of finding a number of spatially dissimilar paths between each O/D pair, which could be used in selecting routes for Hazmats considering risk equity, and in solving capacitated flow problems. Further, they explained that generating dissimilar path could be useful for transportation of dangerous goods for at least two reasons. Bad weather conditions can increase accident probabilities; therefore, a set of dissimilar paths can increase the

probability of being able to select a path which is not impacted by an adverse weather condition. It also required to ensure spatial risk equity for multiple shipments of Hazmats. They made use of p-dispersion location model of *Erkut (1990)* and *Erkut et al (1994)* as part of path generation procedure.

Carotenuto et al (2007a) addressed generation of paths between each pair of O/D shipments, with minimal risk for road transportation of Hazmats. They focused on minimization of total risk while considering equity of the risk induce on the population. They proposed two algorithms, as a modified version of Yen's algorithm *Yen (1971)*, for k-shortest path problem, considering risk propagation resulting from close paths and risk equity among geographical zones where transportation network is embedded. They, further, suggested a lower bound based on Lagrangian relaxation. They showed the results of their computational experiments.

Carotenuto et al (2007b) considered vehicle routing and scheduling problem involving Hazmats. A set of minimum and equitable risk alternative routes from O/D nodes and a preferred time are given. Their proposed job-shop scheduling problem, with no-wait constraints, assigns a route to a shipment and schedule the shipments on the assigned routes. They sought for minimization of total shipment delay, while equitably spreading the risk spatially and preventing the risk induced by vehicles traveling too close to each other. They also suggested a tabu search algorithm and reported the results of their computational experiments.

Dell'Olmo et al (2005) aimed to generate a set of alternative paths for one or a set of Hazmat shipments. Determining spatially dissimilar paths, could let equitable spatial distribution of total population exposure risk. They, initially find a set of Pareto-optimal paths for each O/D pair of shipments through solving a multicriteria shortest path problem. Then, for each of the found path, making use of GIS, they construct a Buffer Zone for approximating the impact area in case of

incident. Using the Buffer Zones, for every pair of paths, a dissimilarity index is derived which is used to find the most spatially different routes. Finally, they compare their proposed method with Iterative Penalty Method (IPM) *Johnson et al (1992)*, and discuss the computational results.

Dadkar et al (2008) developed a k-shortest path algorithm for which the performance of each highway facility, with respect to each objective, can be stochastic and can vary over time. Using a genetic algorithm, they solved a mixed integer program to identify a subset of paths which represents an acceptable trade-off between geographic diversity and performance. These models and algorithms are then applied to a realistic case study.

Martí et al (2009) considered the a bi-objective optimization problem, where a single solution consists of a set of p different paths; average path lengths must be kept low while another conflicting objective is that dissimilarity among the paths in the set should be kept high. They reviewed the previous methods and adapted to this bi-objective problem; thus they could compare the methods using the standard measures in multi-objective optimization. A new GRASP procedure is proposed and tested against the revised methods. Further, they show that it is able to create better approximations of efficient frontiers than existing methods.

Caramia and Giordani (2009) proposed a clustering-based approach for selecting k efficient paths maximizing their representativeness with respect to the cost vectors of all the efficient paths or with respect to the dissimilarity among the k selected paths; in the first stage, the set of efficient paths is determined e.g., with the use of the algorithm of *Martins (1984)*, In the second phase, a fuzzy k-means based routine is used to compute fuzzy path-class memberships representing a fuzzy k-class partition of the efficient paths. In the third phase, a Monte Carlo method, repeated for a certain number of times that exploits fuzzy memberships as path-class assignment

probabilities, generates a k-class partition of the efficient paths, and from each one of the k path classes it selects the path with the closest cost vector to the class centroid. The k-class

partition of the efficient paths (along with the related selection of k paths) is chosen by minimizing the sum over all the classes of the total square distance between the cost vector values of the paths of a class and the class centroid (i.e., maximizing path representativeness), or maximizing the dissimilarity among the k selected paths.

Caramia et al 2010 proposed a new approach for planning routes for hazmat shipments that selects k efficient paths with respect to the minimization of length, time (cost) and risk; in particular, the selection is made by choosing k representative paths among the set of efficient paths, with high spatial dissimilarity. This allows one to guarantee an equitable distribution of the risk over the network. Through the first stage, they made use of algorithm proposed in *Martins (1984)*, to find a set of paths. Over the second stage, they used a k-means algorithm to partition the latter set into k classes of paths, minimizing the total variance of the objective vector values of the paths in the same class. Finally, one path from each one of the k classes is chosen by heuristically solving the problem of selecting paths maximizing the total spatial dissimilarity.

Bonvicini and Spadoni (2008) considered a linear multicommodity, multi-origin destination problem with global arc capacities that reduce risk overloading on certain links, thereby looking for risk equity. Flow decision variables represented yearly Hazmat vehicle flow. They solved their model using commercial software.

2.4.2. Network Design Problem (NDP)

Network Design Problems (NDP) has been broadly studied, and has long been recognised as one of the most challenging problems in transportation. One can refer to *Balakrishnan at al (1997)*;

Ahuja (1993); Bertsekas (1998); Yang and Bell (1998); Magnanti and Wong (1984) and Pióro and Medhi (2004), to obtain more knowledge in NDPs.

Referring to the mathematical models associating with NDPs, we can put them into two categories: Bi-level Optimization Problems (*Bard, 2006*), and Mathematical Program with Equilibrium Constraints (MPEC) (*Luo et al (1996); Outrata et al (1998*). While most of the classical NDPs look for the optimum way of expanding infrastructure, Hazmat transportation network design problems (HTNDPs) aim to find most appropriate road segments to be wither partially or entirely banned to Hazmat shipments, in order to control link segments' of Hazmats to minimize the risk imposed to population, environment, and properties. Nonetheless, we are going over the most pertinent articles involving route planning problems that simultaneously incorporate interests of both the authorities and carriers. As well, we will discuss toll setting problems as a way to ensure the equity of risk distribution with the underlying network where Hazmats are transported.

2.4.2.1. Game Theory

Kara and Verter (2004) provided a bilevel optimization model for HNDP to incorporate the relationship between the regulator and carriers. In their proposed bilevel model, leader, the first level, designs the network through selecting the paths with minimum total risk, while the follower, the second level, associates with the carriers and looks for the routes, among the ones permitted by the leader, with minimum cost of travel. They further showed that due to the unimodularity of the inner problem, which is an integer linear problem, their model can be reduced to a single level problem, given the outer design variables as parameter; the bilevel problem is discrete-linear and in particular since the followers' problem is linear we can represent it with its primal-dual optimality (or KKT) conditions. Moreover, they showed the application of their suggested methodology in Western Ontario, Canada.

Marcotte et al (2009) proposed a bilevel network design problem which was reduced to a single level MIP which was more efficient that the single level proposed by *Kara and Verter (2004)*.

Both *Kara and Verter (2004)* and *Marcotte et al (2009)* may fail to find an optimal "stable" solution for the bilevel model. It is because in case of multiple minimum-cost routes for carriers (within the designated network by the leader), both models assume that carriers would also choose the route with minimum risk. However, it is not always the case; hence both of the single level reformulations could be assumed to be considering the optimistic case.

Erkut and Gzara (2008) considered a bilevel HTNDP where government designates a network and carriers chooses the routes of the network. They generalized *Kara and Verter (2004)* to incorporate a cost term in the objective function of the leader problem in order to overcome the abovementioned instability problem. They, further, proposed a heuristic to solve their bi-level biobjective model, which proved to be efficient through computational experiments as reported in the article.

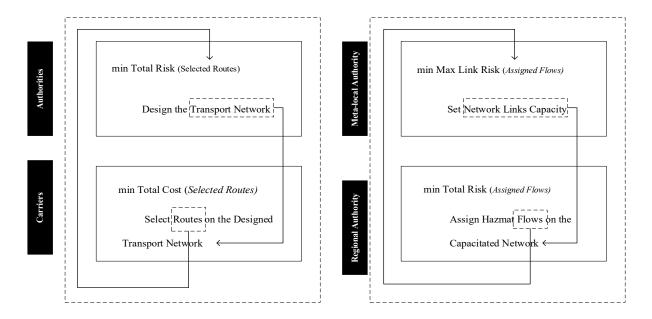


Figure 2-1: Various Approaches towards HTND

Source: Bianco et al (2009)

Bianco et al (2009) considered a bi-level HTNDP where the outer problem involves meta-local authority and the inner problem involves regional authorities. Obviously, this model differs form the previously-reviewed models since it does not involve carriers' interests. Moreover, this model considers just the minimization of total risk, but does it also look for equity if the spatial distribution of risk within the underlying network. The leader tries to minimize the maximum link total risk by imposing capacities on the flow over the links of the network in order to achieve risk equity as result of balancing the links load of Hazmat flows. The follower, on the other hand, specifies the optimal amount of Hazmats to be routed through already capacitated links of the network so as to minimize the total risk of the network.

Figure 2-1 illustrates the differences in HTNDP approaches taken by *Bianco et al (2009)* and others like *Kara and Verter (2004)*.

Minciardi and Robba (2012) considered a general decision architecture and provided an application to the case of the management of fleets of vehicles carrying Hazmats. They proposed a bilevel multiobjective model. They also reported the results of a specific case study relevant to the management of vehicles carrying hazmat through a critical infrastructure.

Taslimi et al (2017) considered a bilevel HTNDP with O/D pair for each shipment, with regulatory authorities as leader, and carriers as follower problems, respectively. Considering risk equity, the leader aims to minimize the maximum transport risk incurred by transportation zone; locations Hazmat response teams are the control variables for the regulatory authority. A tractable single level MILP is driven from reformulation of the original bilevel model, which can be solved to optimality through commercial solvers for medium-size problems. They, further, proposed a greedy heuristic for solving large-size problems. Moreover, they sought a robust solution to

capture the stochastic characteristics of the model. They reported their experimental results which were based on popular test networks from the Sioux Falls and Albany areas.

2.4.2.2. Toll Setting

Toll setting (TS) is another policy where the regulator set tolls on a set of links of the network to deter the carrier from using more populated road segments and motivates them to use the ones with less arc load.

Marcotte et al (2009) proposed a bilevel model as an extension of *(Labbé et al (1988)*, where they made use of toll setting (TS) to regulate road shipments of Hazmats. They also proposed a solution approach to solve their suggested model. Through computational experiments, they showed that their TS policies work better than HTSNP that consider closing road links to Hazmat shipments.

Bianco et al (2015) proposed a toll setting policy for regulation Hazmat shipments where government authorities aim not just to minimize the network total risk, but also do they look for equity in spread of risk over a given road network. In their proposed model, route selection of a carrier depends on the other carriers' choices. Hence, TS policy will deter the carriers from using road segments with higher value of total risk. Their proposed model, thus, is a mathematical programming with equilibrium constraints (MPEC) problem; inner problem is a Nash equilibrium problem with carriers as players, each one wishing to minimize his or her travel cost (including tolls); the outer problem considers government authority, whose aim is finding the link tolls that induce the carriers to choose route plans that minimize both the network total risk and the maximum link total risk among the network links (to address risk equity). Further, they proposed a local search heuristic for the MPEC problem and carried out experiments with examples from literature to test the performance of the model and the heuristic.

Wang et al (2012) proposed a dual toll pricing for Hazmat transportation risk mitigation. They aimed to control both regular and Hazmat vehicles, at the same time, to reduce risks. Considering duration-population-frequency of exposure, they suggested a new risk evaluation measure. Their proposed model is a Mathematical Program with Equilibrium Constraints (MPEC). They solved their model through decomposing the MPEC into first-stage and second stage problems; they developed separate methods to solve each stage, afterwards. They presented a report of their computational experiments.

Assadipour et al (2016) proposed a bi-level, bi-objective model for the purpose of regulating the usage of rail intermodal terminals for Hazmat shipments, where TS policy of government deters carriers from using certain terminals. They proposed a hybrid speed-constrained, multi-objective, particle swarm optimization algorithm, which is then integrated with CPLEX, to solve the model. Their model and algorithm were tested with a real problem instance based on the intermodal service chain of Norfolk Southern in US. Through comparative experiments, they showed that toll setting policies are more practical and efficient than a HTNDP approach, where certain terminals are closed to hazmat containers. two models can be combined as a two-stage strategy in long-term hazmat transportation regulations.

2.4.3. Multicommodity Network Flow Problem and Railway Freight Transportation

MCNFP deserves to be discussed separately because it cannot be considered just under either of NDP or Route Planning sections, as MCNFP-based formulations could be used to model problems associating with both NDP and Route Planning. On the other hand, since there is a rich literature in multicommodity-based models in freight transportation and since the mathematical model variants presented in chapter three of this document are Multicommodity Network Flow Problems

(MCNFP), some of the relevant significant articles will be reviewed after giving a brief introduction into MCNFPs.

Contrasting feature of the MCNFP from a single-commodity problem, in a sense, could be sharing of common arc and node capacities, sometimes referred to as set of bundle constraints, binding different commodities together.

We can find applications of MCNFP in telecommunications as in *Minoux (1989, 2001)*, transportations *Magnanti and Wong (1984)* and location problems *Crainic et al (1989)* and manufacturing and distribution problems *Folie and Tiffin (1976)* and *Geoffrion, and Graves (1974)*. Even though any MCNFP-based modeling within each application area may have some specific features and technological constraints due to some specific modes, but the underlying mathematical formulations have similarities with one another *Magnanti and Wong (1984)*; most of them are seeking for satisfying all of them O/D pair of orders at minimum cost.

Bertsekas (1998) thoroughly investigates specific properties of variants of linear and nonlinear MCNFP models with convex and nonconvex functions; it also categorizes MCNFP into Constraint-Separable MCNFP, Separable MCNFP, and Separable MCNFP with arc capacity constraints.

Ahuja et al (1993) introduces general MCNFP and sets out the optimality conditions, then elaborates on price-directive, resource-directive and partitioning solution methodologies for MILP MCPs.

Pióro and Medhi (2004) introduces many lots of applications of MCFP in communications and computer science by going over all variants of both link-based and path-based mathematical models.

One can investigate *Crainic and Laporte (1997)* to gain obtain more information about the various modeling approaches, various applications-specific modeling variants at strategical, tactical and operational levels.

2.4.3.1. MCNFP and Railway Freight Transportation

Assad (1981) provided an annotated bibliography aiming collect and classify the available literature on analytical models for rail systems. Various network, yard, and scheduling models are cited, together with some references providing the institutional background. Both simulation and optimization models are discussed with special emphasis on the latter.

Assad (1980) considering railway freight transportation, explained that freight flow management in rail systems involves multicommodity flows on a network complicated by node activities such as queueing and classification of cars at marshalling yards. Furthermore, he stated that routing in these systems should account for technology requirements of motive power and traction as well as resource allocation at each stage of rail operations (shown in Figure 2-2), such as assigning cars to blocks and assigning blocks to trains. In addition, he classified the rail freight transportation planning, based on their planning horizon, into three main categories: strategic, tactical and operational.

Bodin et al (1980) developed a nonlinear, MIP model for the railroad blocking problem, which can be viewed as a multicommodity flow problem with many additional side conditions including capacity constraints at each yard in terms of the maximum number of blocks and the maximum car volume that can be handled. Their proposed model sought for determining a classification strategy for all the classification yards in a railroad system at one time. To find feasible solutions to the problem, most of them have to be set heuristically due to the large number of binary variables. *Crainic et al (1984)* considered the problems of routing freight traffic, scheduling train services and allocating classification operations. They proposed a MIP multicommodity flow problem.

Crainic and Rousseau (1984) investigated the multimode, multicommodity freight transportation problem which occurs when the same authority supplies or regulates the supply of transportation services (including terminal operations) and also controls, at least partially, the routing of the goods through this service network. They solved their proposed model through column generation (CG) and decomposition heuristics, and reported the performance of their model through providing the results of their experimentations.

Barnhart et al (2000) considered the railroad blocking problem and proposed a capacitated multicommodity problem; they decomposed their complicated MIP problem into two simple problems so that the storage requirement and computational effort were greatly reduced. They added a set of inequalities to one subproblem to tighten the lower bounds and facilitate generating feasible solutions. They used subgradient optimization to solve the Lagrangian dual.

Newton et al (1998) proposed a model similar to *Bodin et al (1980)*; both models were MIPs that include constraints on the number and total volume of the blocks assembled at each terminal, but with many fewer binary variables. Their proposed MIP, accommodates different priority classes of traffic, like the model proposed by *Crainic et al (1984)*.

Ahuja et al (2007) indicated that the railroad blocking problem is a multicommodity flow, network design, and routing problem where one needs to design the underlying blocking network and to route different commodities (where each set of railcars with the same origin-destination pair of nodes defines a separate commodity) on the blocking network to minimize the system wide transportation costs.

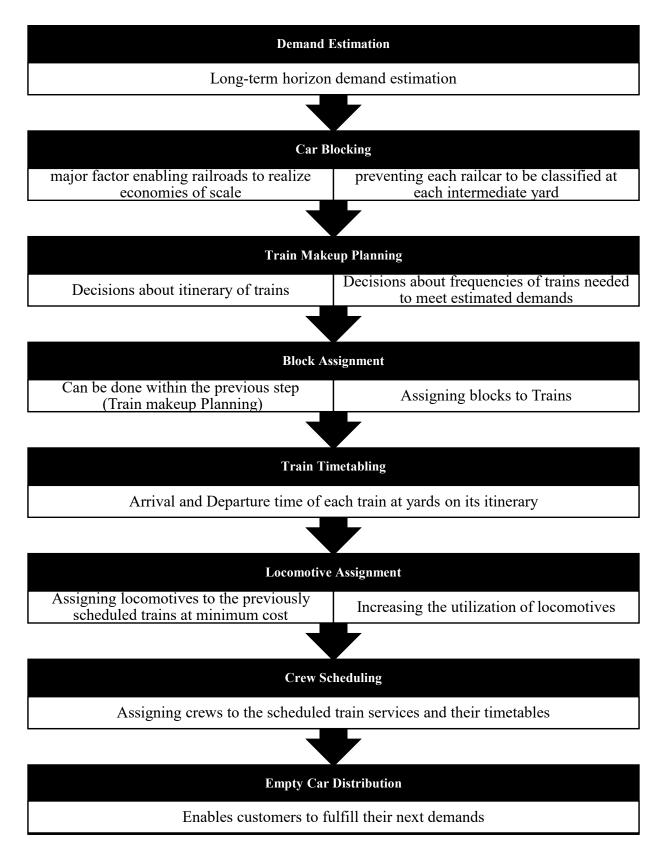


Figure 2-2: High-level Flowchart of Railway Freight Transportation Planning

They developed an algorithm using large-scale neighborhood search (VLSN) to solve their proposed model which could solve the problem to near optimality using one to two hours of computer time on a standard workstation computer

Hasany and Shafahi (2017) developed a model the uncertain railroad blocking problem as a twostage stochastic program. Further, they developed two exact algorithms based on the L-Shaped method. They evaluated the performance of their proposed algorithms for the test networks. They showed that the application of the stochastic model could reduce total cost by more than 12 million dollars per three-month horizon compared with the deterministic solution.

2.4.3.2. MCNFP and TDG

Iakovou et al (1999) considered routing Hazmats, at the strategic level, in marine waters over a multicommodity network flow with multiple O/D pairs. The reason behind multicommodity approach taken to develop the model is that selecting optimal routes by either O/D pair or by Hazmat type is myopic and may result in overloading certain links of the transportation network and, consequently, in poor overall system performance.

Bianco et al 2009 considered Hazmat network design problem (see also section 2.4.2.1). They explained that Although the transportation industry has been deregulated in many countries, hazmat transportation usually remains as part of the governments' mandate mainly due to the associated public and environmental risks, which leads to a harder class of problems that involve multi-commodity and multiple origin–destination routing decisions. On this basis, in their proposed bilevel model, the leader problem, authorities, determines the bundles capacity, maximum link total risk. once bundle capacities are fixed by the leader decision maker, the lower level (follower) problem that the follower decision maker wants to solve becomes a minimum cost multicommodity network flow problem, where the arc cost models the unit risk of traversing the

arc, with a specific hazmat shipment (commodity) $c \in C$ of d^c units being associated with a couple (s_c, t_c) of source-sink nodes.

Mohammadi et al (2017) considered designing a reliable Hazmat transportation network design (RHTND). They explained that classical approach taken in routing of hazardous materials which used to simplify the multicommodity, multimode shipments to single-commodity, and single-mode network, will lead to overload of certain links. This is because these models focus on route planning for a single-commodity and single O/D, at a time, ignoring the effect of interaction between different commodities, transportation modes, and selected routes. Thus, those model fail in taking into account the routing of the other shipments, certain links of the transportation network tend to be overloaded with Hazmat traffic, hence increasing the probabilities of accidents and risks associated with links.

Verma et al (2011) proposed, for the first time, a multiobjective multicommodity model, at the tactical service planning level, which considered Hazmat freight transportation by train. They developed a solution methodology based on a memetic algorithm suggested by *Moscato (1989)*, combining global and local searches. The reason behind this was that based on *Holland (1975)*, if there are a huge number of variables and relatively fewer constraints, a genetic algorithm based solution may be more effective and efficient (See also 2.5.2).

One can refer to the survey of *Yaghini and Akhavan (2012)* for a review of the works done in network design problems in the context of rail freight transportation planning; as well, *Cordeau et al (1998)* reviews optimization models associated with railway transportation.

2.5. Hazmat Local Route Planning and Scheduling

Most of the literature in Hazmat local route planning involve problems which seek for minimization of cost (money, time, risk). Risk measure is incorporated into the mathematical model either as arc impedance or as a term in objective function; the latter case, however, appear in multiobjective optimization problems which seek for a set of nondominated Pareto-optimal routes per O/D shipments w.r.t. risk, and travel cost minimization. Irrespective of the essence of the path evaluation function, such deterministic, static and single objective minimization problems can reduce to a classical shortest path problem; therefore, a label-setting algorithm (e.g. Djikstra's algorithm) can be applied to solve those problems. Other criteria have also considered in routing choices such as insurance cost, tardiness etc.

Due to the richness of the stream of literature on Hazmat local routing and scheduling, we will be reviewing the most significant and / or recent articles; we will review papers dealing with deterministic and stochastic problems with time-dependent variables.

2.5.1. Hazmat Road Route Planning and Scheduling

Nembhard and White III (1997) suggested a bi-criteria objective function to minimize risk to population and transportation cost. They sought for determining a path that maximizes a multi-attribute, non-order-preserving value function. They showed since a non-order-preserving value function, any sub-path of an optimal path may not be optimal, sub-optimal paths may be produced through a traditional application of dynamic programming; two approximation procedures were considered for two cases where in the first case, the number of intermediate stops between O/D pairs was zero, and the second case, considered this number to be more than zero. Through the first approximation, considering the sub-path of an optimal path is optimal, they applied DP, and for the second procedure, they applied DP after determining an order-preserving- criterion to

approximate a non-order-preserving value function. Subsequently, they used the best-first search algorithm to determine optimal routes for both cases.

Marianov and ReVelle (1998) proposed a bicriterion linear optimization model for routing vehicles through hazardous environments or routing vehicles carrying Hazmats. They also presented an example of the application of their model which sought for minimization of travel cost and risk.

Verter and Erkut (1997) Considering the increase in future cost of insurance that carriers would be incurred in case of accidents, although immediate costs are usually borne by insurers, they proposed a Hazmat routing problem subject insurance costs. They also proposed a solution approach to facilitate alternative routing policies evaluation. Results of computational experiments reveal that for each truck, the routing decision should be made based on expected increase in insurance costs due to possible accidents, and transportation costs.

Akgün et al (2000) focused on finding dissimilar path for routing Hazmats between each pair of O/D shipments (see also section 2.4.1).

Kara et al (2003) proposed two paths algorithms which are capable of dealing with path-dependent link impedances. One of their proposed algorithms as a modified version of Djikstra's algorithm, "impedance-adjusting node labeling shortest path algorithm", was used to find a route that minimizes the exact version of the path incident probability. They also suggested "impedance-adjusting link labeling shortest path algorithm" which prevents double counting of population exposed at risk. Their suggested approach is superior to standard shortest path algorithm, (see also 2.2.2).

Miller-Hooks and Mahmassani (1998) considered significance of optimal route selection for emergency response unites and vehicle carrying Hazmats in congested streets, where travel times are time-varying quantities that are best know *a priori* with uncertainty. They looked for

developing efficient algorithms to determine optimal paths in networks with time-varying random link costs, which also consider the trade-offs among various risk dimensions in route selection process. Hence, considering arc weights are discrete random variables whose probability distribution functions vary with time, they proposed two efficient algorithms to find paths with the least possible time between any two pair of O/Ds. The first algorithm could determine: the path with the least possible time from each node for each departure time interval, the least possible travel time and lower bound on the corresponding probability of occurrence of the travel time. The second algorithm determines up to k-least possible time paths, the associated travel times and the associated probabilities of occurrence of the travel times (or a lower bound on this probability). Their proposed algorithms for determining least time paths in stochastic, time-varying networks was novel. The algorithms provided a well-defined and efficiently-computed benchmark to evaluate paths obtained through heuristics which may consider other risk aspects. Moreover, they can be to solve problems including intelligent transportation systems (ITS), emergency response systems operations (medical, police, fire), and communications network.

Erkut and Alp (2006) addressed a routing and scheduling problem where link attributes (accident rates, population exposure, link durations) vary with time of day. Their model allowed for stopping at nodes. They, further, considered four versions of their problem with increasingly more realistic constraints on driving and waiting periods. Moreover, pseudo polynomial dynamic programming algorithms for each version of the problem were proposed. They also carried out experiments using a realistic example network to test the efficiency and effectiveness of their proposed algorithms. Results reveal that en-route stops resulted in generation of routes with much lower risk levels compared to those where no waiting is allowed.

Akgün et al (2007) considered the effects of weather systems on Hazmat routing. To characterize the time-dependent link attributes due to movement of weather systems, they analyzed the effect of a weather system on a vehicle passing thorough a link segment. Their analysis could be used as a building block for problems looking for the least-risk path for Hazmat shipments on network exposed to such weather systems. They also proposed different methods for solving the underlying problem, experimented with problem instances and reported their results. They concluded that determination of time-dependent link attributes is possible provided that some assumptions on the nature of the weather system. Also, they concluded that for practical-size problem instances, effective solutions can be obtained given while allowing for parking the vehicle to avoid weather system effects.

Androutsopoulos and Zografos (2010) considered a bicriterion routing and scheduling model with risk and cost, subject to time-dependent link attributes (both cost and risk). Given a fixed sequence of intermediate stops (customers), their model determines the non-dominated time-dependent paths for serving the customers within predefined time-windows. They proposed an algorithm determining the k-shortest time-dependent paths. Further, an algorithm is provided for solving the bicriterion problem. Using a set of problem instances developed the authors, they assessed the proximity of the solutions of the k-shortest time-dependent path problem with the non-dominated solutions.

Toumazis and Kwon (2013) proposed a new risk mitigating method for Hazmat routing problem, using Conditional Value at Risk method, CVaR, on time-dependent vehicular network. They extended the previous research by considering time-dependent nature of accident probabilities and accident consequences. They also provided a numerical method in order to determine the optimal departure time and the optimal route for a given O/ D pair of shipment. They presented the results of the experiments done to test their proposed algorithm in a road network in Buffalo, NY, US.

Recently, *Szeto et al (2017)* addressed Hazmat routing and scheduling problem involving multiple Hazmat classes with inaccurate and unknown incident probabilities. They proposed a link-based multi-demon formulation. They also suggested a solution approach to obtain route flow solutions without relying on heuristics for exhaustive route enumeration and generation.

Further they carried out a case study and reported their results and insights.

Recently, *Kumar et al (2018)* considered fleet mix and routing decision for hazmat transportation with a focus on a developing country. Although truck purchase cost is assumed to be the most important criteria for fleet acquisition-related decision in most of the developing countries, they also considered other type of costs such the cost being incurred due to the number of en-route stoppages based on the type of the truck, or recovery cost based on route choice decisions; they considered the above-mentioned costs for deciding the fleet mix and minimizing the overall costs for long-haul shipments. They proposed a nonlinear model and solved it through genetic algorithm. Their proposed model challenges the current truck purchasing strategy adopted in developing countries using the cheapest truck criteria.

2.5.2. Hazmat Rail Route Planning and Scheduling

Glickman (1983) addressed population-avoidance rerouting policies in the context of railroad transportation of Hazmats. Also, estimated the risk due to release of Hazmats from railcars in the US for a period of a year. Hazmat flow patterns were generated approximately for that year. Then, he considered alternative patterns, representing population-avoidance rerouting policies, for Hazmat flows. Further, some aggregate impacts both with and without track upgrade are estimated.

Moreover, it turned out that rerouting could reduce population exposure by 25 to 50 percent while traffic circuity increases by 15 to 30 percent.

Verma (2009) developed a biobjective MILP model, where characteristics of railroad industry have been incorporated into cost function, and dynamics of the railroad accidents are incorporated into the transport risk evaluation function. A solution framework is used to solve realistic-size problem instances based in South-east US. The results of the computational experiments are also reported; further, a risk-cost frontier illustrating non-dominated solutions is developed.

Verma et al (2011) presented a biobjective MILP model for railroad tactical planning problem. They aimed to determine the routes to be used for each shipment, the yard activities, and the number of trains of different types needed in the network. Differentiating characteristics of railroad transportation is incorporated into risk assessment component of their proposed model. They developed a memetic algorithm-based, combining genetic algorithm and local search *Holland (1975)*, solution methodology to solve their problem. Further, they experimented with real-size problem instances generated using railroad infrastructure in the Midwestern US. Results reveal that significant reduction in population exposure is achievable without having to incur unacceptable increases in operational costs.

Verma et al (2012) proposed a biobjective optimization framework for routing intermodal shipments with Hazmats, when both shippers and receivers have access to alternate intermodal terminals. Further, they proposed a solution methodology based on tabu search. They tested their proposed framework and heuristic with a realistic-size problem instance to obtain managerial insights. It turned out that drayage accounts for a significant portion of transport risk which could be reduced through scheduling direct and faster trains. Also, results indicate that the mix of

intermodal trains depends on the interest of decision-makers, where the resulting traffic can facilitate planning emergency response systems.

Recently, *Fang et al (2017)* considered routing and scheduling TDG through railway in the presence of due dates. Their focus was on the minimization of weighted sum of the earliness and tardiness for each demand as well as minimization of holding cost at yards, subject to risk threshold on service-legs at any time instant. Analyzing Federal Railroad Administration (FRA) accident records (1999 to 2013) revealed that the most important cause of derailment of railcars was train speed. They proposed a MIP model for preparing the shipment plan; further, a heuristic-based solution approach to solve their proposed model. They also presented results of computational experiments on a number of real-sized problem instances generated using infrastructure of a Class I railroad operator.

Recently, *Hosseini and Verma (2017)* proposed a Value at Risk (VaR) approach for TDG through railways, considering the risk-averse attitude towards Hazmats transportation as low-probabilityhigh-consequence (LPHC) event. They considered a limit on the number of train services available for routing Hazmats, considering the best train configuration, their model minimizes the risk of transportation measured by VaR method. They analyzed derailment reports of the Federal Railroad Administration (FRA) to develop expressions incorporating characteristics of railway accidents which helped them estimate various inputs. Several problem instances generated using the realistic network of a railroad operator were used to experiment with using their proposed methodology, which revealed the possibility of developing different routes for Hazmat shipments depending on the risk preference of the decision maker.

2.5.3. Hazmat Routing with Stochasticity of Link Attributes

Wijeratne et al (1993) described a method for determining a set of nondominated routes when there exist various uncertain measures for route evaluation. Their proposed Stochastic, Multiobjective Shortest Path (SMOSP) algorithm could be applied in TDG. They also showed an example of application to routing hazardous materials in the Albany-Schenectady-Troy area of New York State.

Recently, *Mohammadi et al (2017)* proposed a mathematical model for designing a reliable hazardous material transportation network (RHTND) based on hub location topology under uncertainties, where external event and Hazmat incidents may disrupt hub nodes. They developed a MILP model as well as providing a solution framework based on an integration of the well-known chance-constrained programing with a possibilistic programing approach to cope with uncertainties in the model. The model is solved to optimality for small-size problem instances while for larger-size instances, a metaheuristic algorithm was applied and the results are reported.

Static Stochastic Routing		
Transportation of Hazmats	Other Transportation Applications	
Wijeratne et al (1993), Sivakumar and Batta (1994), Erkut and Ingolfsson (2000)	Frank (1969), Mirchandani (1976), Kulkarni (1986), Corea and Kulkarni (1993)	

Table 2-8: Some Static Stochastic Route Planning Contributions

Stochastic Time-varying Network (STV)		
Category	Relevant Papers	
A priori Optimization	Hall (1986), Bellman (1958), Miller-Hooks and Mahmassani (2000), Fu and Rilett (1998), Chang et al (2005)	
Adaptive Route Selection	Hall (1986), Miller-Hooks (2001), Nguyen and Pallottino (1986)	
Adaptive Route Selection with real-time updates	Séguin et al (1997), Hoffman and Janko (1990), Koutsopoulos and Xu (1993), Yang (2001), Miller-Hooks and Mahmassani (2000), Miller-Hooks (2001)	

Table 2-8 and Table 2-9 provide the interested researcher with some relevant papers involving static stochastic routing, and routing in stochastic time-varying network (STV), respectively.

2.6. Hazmat Security Aspects

Nune (2007) addressed safe and secure transportation of Hazmats and the potential and risk imposed to society due to malicious entities who can carry Hazmat vehicles into weapons causing explosions in high profile locations. As part of his MSc thesis, he developed a neural network model to identify when a hazmat truck deviates from its pre-specified path based on its location in the road network. Further, he developed a methodology for predicting different paths that could be taken by malicious entities heading towards a target after successfully hijacking a hazmat vehicle. He also implemented his prediction methodology and neural network methodology on the network between Baltimore, Maryland and Washington, DC.

Murray-Tuite (2008) described the incorporation of two types of substitution (method and target) into a methodology to determine the risk profile for the transportation system because of attacks on the transportation system itself, collateral damage to the network because of targeting of adjacent assets, and pre-event and post-attack security measure implementation. They made use of Monte Carlo simulation to generate scenarios of target, attack methods, intelligence, security, substitution, target failure, and damage to the transportation network. Further, they characterized risk through a profile of scenario likelihood and consequences. It turned out that one instance of no targets was selected after applying the methodology to a hypothetical network with 5,000. Finally, she reported that although the scenario probabilities were very small, 18% of the cases resulted in the complete disconnection of the origin-destination pair. Thus, a city's decision makers should carefully consider the use of security measures in conjunction with the attacks if post-attack evacuation is a potential action.

Murray-Tuite and Fei (2010) considered a transportation network's capacity which is influenced by both the defender's protective measures and the attacker's actions, in an adversarial setting, which include substituting targets and attack methods in response to security measures. They addressed decision makers need of a methodology capturing the complicated attacker-defender interactions, which helps them understand the overall effects on the transportation system, as well as the consequences of asset failure. Thus, they proposed a methodology which probabilities of target–attack method combinations that are degree of belief based and updated using Bayes' Theorem after evidence of the attack is obtained. Probability of link capacity effects is generated by Monte Carlo simulation from by sampling from distributions of capacity reductions due to preevent security measures, substitutions, target failure, and post-event security measures. The average capacity reduction for a particular target–attack method combination was used as input to the traffic assignment–simulation package DYNASMART-P to determine travel time effects. They also applied the methodology to a sample network based on the northern Virginia area.

Dadkar et al (2010) developed a game-theoretic model of the interactions among government agencies, shippers/carriers and terrorists as a framework for the analysis. They also developed an effective solution procedure for this game. Finally, they illustrated the methodology on a realistic case study.

Nune and Murray-Tuite (2012) considered the potential malicious use of Hazmat which imposes threats to society; they explained that a way to combat this threat is detection of the vehicle deviations from their normal path. Hence, to identifying path deviations and classifying the threat level at each node in the network, they presented a probabilistic neural network approach. They also illustrated the methodology on the network between Baltimore, Maryland, and Washington,

D.C. Moreover, they elaborated on the accuracy of their proposed model, its positive and negative errors.

Khakzad et al (2017) addressed the linearity of the current security risk assessment, most of which, fail to incorporate the mutual interaction; hence, investigated the applicability of analytic network process (ANP) to security-based rank ordering of hazardous facilities such as chemical plants. While different techniques can be used to score individual risk parameters, ANP will enable considering mutual interactions, modifying the linearity of current security risk assessment methodologies.

One can obtain more knowledge about the variants of models proposed capturing security aspect of Hazmat transportations by referring to *Garrido (2013)*.

Chapter 3

3. Problem Statement and Mathematical Model

We address railway transportation of regular commodities, and toxic inhalation Hazmats (TIH) like Propane, Butane, Ammonia and Chlorine, where carriers aim to minimize the cost of travel and yards operational cost; on the other hand, authorities are looking for minimization of the number of people exposed to the risk of evacuation, injury, and fatality in case of incident. Thus, we will elaborate on the problem to be addressed in section (3.1), and we will discuss mathematical model variants throughout the following subsections. Looking at the problem from the carrier company's perspective, under functional and technological constraints along with Hazmat-specific constraints, we aim to find optimal paths for all traffic classes such that the total cost of transportation is minimized. As well, we need to find the minimum number of train services required to meet all demands. Hence, routing decisions for each and every traffic class, and makeup and the minimum number of train services, will be the constituents of our solution to the developed mixed freight tactical planning problem in section (3.2). In section (3.3), we considered the interest of both carriers and authorities, by incorporating transportation cost and risk into the objective function, thereby developing a comprehensive, MINLP model with multiobjective function.

In practice, at industry level, some other restrictions should be taken into account, which encouraged us to consider solving this problem with nonbifurcated flows. To elaborate more, we would refer to contractual considerations and customer requirements, railway system operating companies and carriers. For instance, customer of a given order would like to receive the whole volume of the order all together since this may decrease their overhead costs. On the other hand, some certain segments of underlying network are owned by different operators such as CN, PC, and some local carriers, (read also subsection 1.1.1). Therefore, the railway companies may indeed want to increase their profit through shipping their received orders using specific segments of the network, thereby, having to deal with fewer stakeholders, on the one hand, and incurring less transportations costs due to routing the order through the shortest path, on the other. Furthermore, splitting order can potentially result in increased yard operation costs, more train service costs, more holding costs, increased tardiness and potential penalties due to positive lateness in meeting the orders. Hence, for each of the models to be discussed in sections (3.2) and (3.3), we developed model variants w.r.t. bifurcation of flows; that is, we address each problem considering the situations where the bifurcation of flow is either allowed or not. While in the former case, commodities within any given traffic class can be routed using more than one path, the latter case considers the shortest path, w.r.t. arc and yard attributes, which may not necessarily be the cost of transportation, but also risk in terms of population exposure.

3.1. Problem Statements

We are considering a tactical planning problem of railway transportation of both regular commodities and dangerous goods. Hence, we limit the planning horizon to a one-week period, where freight demands / orders / shipments / traffic-classes of the week are identified based on their origin and destination nodes; each traffic-class, therefore, could be represented by its O/D pair associating with its origin and destination yards. However, since various traffic-classes may share the same origin and destination, each traffic-class is determined not just based on its O/D yards, but they are also assigned a unique index; thereby differentiating all traffic-classes that share the same origin and destination. We consider a railcar with a capacity of 80 tons, as unit of a traffic-class. Therefore, demands are expressed in terms of the number of railcars of certain commodities.

We focus on three main type of commodities: regular, Hazmat type I (e.g. Propane), Hazmat type II (e.g. Butane). Thus, each traffic-class may include both Hazmats (of either type or both) and regular commodities. Figure 3-1: Hazmat and Regular Commodities, Yards and a Service-leg shows a train carrying a block of regular commodities and a block of Hazmats.

Our physical network comprises of various nodes / stations / yards, as well as arcs / rail segments / tracks. Based on the physical underlying network, trains services are determined by their O/D yards, a set of intermediate yards and the track segments connecting the consecutive yards to one another, called service-legs. Each train service is unique while different train services may have some common yards and service-legs. O/D yards of a train service must be able to do classification, grouping and blocking operations while intermediate stops may do pick-up, drop-off and block-swap operations.

Each train service is determined by its origin yard, intermediate stop(s), destination yard, and a set of tracks vis á vis service-legs, as well as its capacity in terms of the maximum number of railcars it can carry through its itinerary. We suppose train services may share common service-legs and yards, however their itinerary cannot completely correspond; i.e. any of the itineraries of two train services are either comprised of two dissimilar and disjoint paths, or they may share one or more common service-legs, but their paths diverge at some common yard.

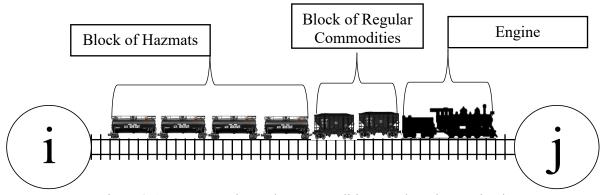


Figure 3-1: Hazmat and Regular Commodities, Yards and a Service-leg

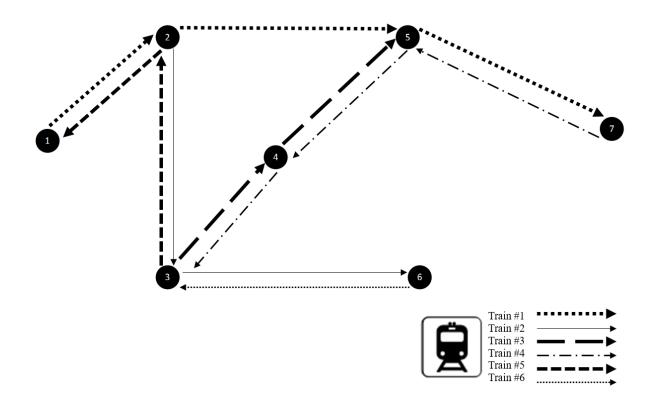


Figure 3-2: Hypothetical Network

Based on the available train services, itinerary of each traffic-class is defined as a feasible path from its origin yard to its destination yard; an itinerary of a certain traffic-class may include various service-legs of various train services. As well, any traffic class may be traversed through either transfer or classification yards, or both. For instance, if we consider the hypothetical network shown in Figure 3-2, then for a given traffic-class whose origin is yard 1, and its destination is yard 3, two possible itinerary could be considered; one itinerary is comprised of yards: 1,2, and 3. That is the traffic-class is using the first service-legs of train services 1 and 2. The other itinerary for this traffic-class, however, comprises of yards 1, 2, 5, 4 and 3. That is, to meet this traffic-class using the latter itinerary, the first two service-legs of train service 1, the second and the third service-legs of train service 4 are used. A given train on its predefined itinerary may do pick-up/drop-off operations on a certain number of transfer yards or it can simply stop at transfer yards

before continuing on its journey towards its destination yard. Transfer yards do not have the capability of grouping and blocking operations. Blocking is a significant factor in railway transportations to realize economies of scale. That is, in order to prevent the handling of railcars at every intermediate yards on its path from its origin to its destination, it is grouped to other railcars with common handling points. Thus, the blocked railcars are not disbanded before reaching the built-up block's destination; at the block destination, railcars of a given traffic class may need to be separated from their previously made blocks and join some railcars from other traffic classes to make a new block. Hence, for railway transportation of freight of all kinds, we should consider that the sequence of blocks which they can be assigned to, blocking path, is of high significance in generating feasible paths for each traffic-class. Referring to the example that we discussed earlier, for the second itinerary of the traffic-class, yard 1 and 5 and 3 can be considered a blocking path, yard 2 and 4 can be assumed to be transfer yards. Nonetheless, yard 2 for the same trafficclass, can be assumed to be either as a transfer yard or a classification yard. That is, railcars of this traffic-class can be blocked with those of other traffic-classes, for instance for a given traffic-class from yard 1 to yard 4, 1/4. In our models, we are differentiating between transfer and classification yards in terms of the costs incurred to the carrier company. Feasible itineraries for each of the traffic-classes are also determined in terms of defining their origin and destination yards, the service-legs of the train services that could be used to meet the demand, and the transfer and classification yards. Nonetheless, block-assignment decisions are not within the scope of this document.

3.1.1. Meteorology and Risk Evaluation Function

Throughout this section, we are going over Gaussian Plume Model for modeling air pollution concentration. This is because the Hazmats which we are concentrating on are Toxic Inhalation Hazards (TIH) which can become airborne and spread away into the air in case of incidents involving rupture and release of Hazmats. For instance, anhydrous Ammonia can create a billowing cloud which is propelling outward in downwind direction. Modeling the concentration of buoyant contaminants helps us with estimating the risk in terms of population exposure. Air pollution dispersion models can come in handy as we want to mathematically simulate the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere. Therefore, we can estimate the downwind concentration of buoyant Hazmats, given information about the pollutant emissions and nature of the atmosphere.

There are various dispersion model variants based on three main categories of dispersion models including: Eulerian models, Gaussian Models and Lagrangian Models. However, some of them are computationally more expensive and some others are more realistic.

During the last few years, great strides have been made to develop a framework for estimating population exposure due to release of Hazmats which become airborne on release like all types of TIH / PIH. For this, researchers have taken advantage of the capabilities of GPM to estimate the concentration levels at downwind distance from incident spot. Thus, concentration of toxic particles at a certain distance can be computed through GPM, then we could assume the total number of people exposed to levels of toxicity concentration equal or higher than Immediately Dangerous to Life and Health Level (IDLH), suggested as guideline by The National Institute for Occupational Safety and Health (NIOSH), as an estimate for assessing population exposure risk. Within this document, however, we focus on GPM to set limits on the level of contaminants concentration at certain downwind distances from release points located either on service-legs or yards. For this, we need to briefly elaborate on the mathematical formulations of GPM. Hence, we

refer to some assumptions which should be made, which might rarely be the case in reality, before we can use GMP, *Zhang et al (2000)*:

- the gas does not change its chemical properties during dispersion
- the terrain is unobstructed and flat
- the ground surface does not absorb the gas
- the wind speed and direction is stable during the dispersion period
- the emission rate is constant

Considering the above-mentioned assumptions, we may compute the concentration of airborne particles at a certain distance from the source of emission, using the following formulation:

$$C(x, y, z, h_e) = \frac{Q}{2 \pi \mu \sigma_y \sigma_z} exp\left(\frac{-l}{2}\left(\frac{y}{\sigma_y}\right)^2\right) \times \left[exp\left(\frac{-l}{2}\left(\frac{z-h_e}{\sigma_z}\right)^2\right) + exp\left(\frac{-l}{2}\left(\frac{z+h_e}{\sigma_z}\right)^2\right)\right]$$
(3.1.1)

In equation (3.1.1), concentration at impact point (x, y, z) in steady-state, $C (mg/m^3)$, is a function of release rate, Q (g/s), average wind speed, $\mu (m/s)$, crosswind and vertical dispersion, $\sigma_y (m)$ and $\sigma_z (m)$, respectively; $h_e(m)$ is the elevation of release-point. x, y, and z, are downwind distance, crosswind distance and elevation of the impact point. σ_y and σ_z , depend on weather stability classes, and the downwind distance from the release point. Figure A-2, demonstrates the Pasquill-Gifford proposed stability classes from the most unstable class, A, to the least unstable class, F. Based on the atmospheric stability classes and downwind distance from the source of release, one could estimate the crosswind and vertical dispersions by using empirically driven values (shown in Figure A-4); however, due to the complexity of reading from the curves, various estimation methods have been proposed such as the one known as the Brigg's Sigma Scheme, (shown in Figure A-6), to estimate the dispersions. Moreover, using sigma estimates derived from power-law enables us to compute the dispersions, $\sigma_y = ax^b$ and $\sigma_z = cx^d$, given the stability class and downwind distance. Dispersion coefficients: a, b, c and d, have been estimated by several researchers such as *Pasquill (1983)*, *Arya (1999)*, *McElroy and Pooler (1968)*, Figure A-7, *Singer and Smith (1966)*, Figure A-8, *Tadmor and Gur (1967)*, Figure A-9, and etc.

Accidents involving Hazmats in railroad often involves multiple railcars, and *Pasquill (1983)* and Arya (1999) showed that we can compute the total contamination level of Hazmats releasing from various sources with an arbitrary position distribution and strength, by superposing the patterns of those sources and aggregating the contamination of each and every single source at any impact point. Considering this, Verma and Verter (2007) proposed a way to find the total concentration level at X distance downwind from median, the first and the last railcar of a K-railcar block of Hazmats. They also proved that for a train containing n railcars, K of which are Hazmats, the greatest level of concentration of TIH at equidistant points from Hazmat block median, is when the wind direction is along with the rail segment through which train traverses. This result can be explained by GPM; that is, the highest level of hazmat particles will be reached at downwind distance from the release point where crosswind distance equals zero, y = 0. In other words, when we are dealing with population exposure risk assessment, we always consider the worst-case scenarios where the concentration of Hazmats are the most. Assuming equidistant points from a release point, the most concentration of releasing Hazmats, under GPM assumptions, will be at the point in downwind direction. So, for computing the worst-case scenario concentration levels, we assume that the elevation of the impact point is zero, z = 0, the crosswind distance of the impact point from the release point is zero, y = 0, and since in case of railroad transportation, the elevation of the source of release is almost zero as the railcar is derailed, then $h_e = 0$. So, we can use the

following equation (for a single release source) to compute the concentration of Hazmats at x distance in downwind direction from release point:

$$C(x) = \frac{Q}{2 \pi \mu \sigma_{y} \sigma_{z}}$$
(3.1.2)

As well, the following equation can be used to compute the maximum aggregate contaminant level of n-railcar hazmat block:

$$C_{n}(x) = \frac{Q}{2 \pi \mu c x^{b} x^{d}} + \frac{Q}{2 \pi \mu c (x-s)^{b} (x-s)^{d}} + \frac{Q}{2 \pi \mu c (x+s)^{b} (x+s)^{d}} + \dots$$

$$+ \frac{Q}{2 \pi \mu c (x-ns/2)^{b} (x-ns/2)^{d}} + \frac{Q}{2 \pi \mu c (x+ns/2)^{b} (x+ns/2)^{d}}$$
(3.1.3)

Where making use of power-law, crosswind and vertical dispersion can be estimated as follows: $\sigma_y = ax^b$ and $\sigma_z = cx^d$, respectively, where *a*, *b*, *c* and *d* are air pollutant dispersion parameters, and *s* denotes the length of each railcar. Moreover, the following estimation could be derived if we consider relative size difference between length of a railcar and length of Gaussian plume:

$$C_{n}(x) = n \times \frac{Q}{2 \pi \mu a c x^{b} x^{d}}$$
(3.1.4)

In equation (3.1.3), n represents the number of identical Hazmats railcars within a block of Hazmat railcars with a release rate of Q for each of the railcars. Alternatively, equation (3.1.4) can be presented as follows:

$$C_n(x) = n \times \frac{Q}{2 \pi \mu a c \sigma_y \sigma_z}$$
(3.1.5)

Furthermore, if we consider the concentration of a given buoyant Hazmat at IDLH level, then we may derive the maximum downwind distance from the release point, using equation (3.1.6), which

enables us to estimate the number of people exposed to the risk of injury or death in case of an incident, by dragging the derived radius along the service-leg where the incident has occurred; in case of incident occurrence at yards, we may just consider the density of people residing at a distance equal to the computed radius, far from the yard where the incident has occurred.

$$x = {}_{b+d} \sqrt{n \times \frac{Q}{ac\pi\mu C_{IDLH}}}$$
(3.1.6)

Please notice that, equation (3.1.6) considers all Hazmat railcars have the same rate of release and the Hazmat railcars contain the same type of Hazmat with the same IDLH level.

3.1.2. Notations

Considering Figure 3-1: Hazmat and Regular Commodities, Yards and a Service-leg which depicts the service-leg $\langle i, j \rangle \in SL$, where *i* and *j* are representing a pair of connected yards, and a train service $t \in T$, traversing through the service-leg and yards, we are going to define parameters and decision variables of both model variants with bifurcated flows and with nonbifurcated flows.

Sets	Y	Set of yards, indexed by: y, i and j
	SL	Set of service-legs, indexed by $\langle i,j \rangle$
	G	Set of goods / commodities, indexed by g
	K	Set of O/D traffic-classes, indexed by k
	R	Remoteness: Urban or Rural, indexed by r
	YT	<i>Classification or transfer yard, indexed by yt,</i> $yt \in \{cl, tr\}$
	BP	Breaking Points, indexed by bp
	DW	Downwind distance, indexed by d

Table 3-1: Notations of Model Variants with Bifurcated Flows

Parameters	$d^{k,g}$	Amount of commodity g in traffic-class k
	d_k	Total quantity of railcars in traffic-class k
		$\int d^{k,g} ; if \ y = or^k$
	$b^{y,k,g}$	$b^{y,k,g} = \begin{cases} 0 & \text{; if } y = \text{transshipment yard} \end{cases}$
		$b^{y,k,g} = \begin{cases} d^{k,g} & ; if \ y = or^k \\ 0 & ; if \ y = transshipment \ yard \\ -d^{k,g} & ; if \ y = ds^k \end{cases}$
	or^k	Origin yard of traffic-class k
	ds^k	Destination of yard of traffic-class k
	∂_y^k	$\partial_{y}^{k} = \begin{cases} 1 ; if: or^{k} = y \\ 0 ; Otherwise \end{cases}$
	yc ^{yt}	$yc^{yt} = \begin{cases} y^{cl}; \ yt = classification \ yard \\ y^{tr}; \ yt = transfer \ yard \end{cases}$
-	Y^{tr}	Yard Transfer cost per railcar (pick-up / drop-off)
_	Y^{cl}	Yard Classification cost (classification, etc.)
-	$u^g_{\langle i,j \rangle}$	<i>Limit on the number of railcars containing commodity g</i> <i>traversing service-leg s</i>
	$u^{\langle i,j \rangle}$	<i>Limit on the total number of railcars containing any commodity traversing service-leg s</i>
	$\boldsymbol{\upsilon}^{\scriptscriptstyle \mathcal{Y}}$	<i>Limit on yard operations on the total number of railcars on containing any commodity type</i>
	u_t	Capacity of train service t
	fc_t	Fixed cost of train service t
	$ heta$ g	IDLH level of commodity g
	l_s	Length of service-leg s
	Q^{g}	Rate of Release of commodity g
	\mathcal{E}^{r}	Used to determine the root of the radius function w.r.t. remoteness
	${\cal C}_g^{r,d}$	Concentration (ppm) of commodity g at d downwind distance from incident spot considering the remoteness (urban/rural)
	ψ_y^{yt}	$\psi_{y}^{k,yt} = \{0,1\}; \ \forall y \in Y; \forall k \in K$
	γ_y^{yt}	$\gamma_{y}^{yt} = \{0, 1\}; \ \forall y \in Y, \ yt \in YT$
	$ au^t_{< i, j>}$	$\tau_s^t = \{0, 1\}; \ \forall t \in T, \ \forall s \in Sl$
	$\delta^{r}_{\scriptscriptstyle\!\!\!\!<\!i,j\!\!\!\!>}$	$\delta_s^r = [0, 1]; \ \forall s \in legs, \ \forall r \in R$
F	ξ_y^r	$\xi_{y}^{r} = \{0, 1\}; \ \forall \in Y, \ \forall r \in R$
	$ ho^{r}{}_{{\scriptscriptstyle <}i,j{\scriptscriptstyle >}}$	Average population density around service-leg $s \in SL$ w.r.t. remoteness factor

Table 3-2: Notations of Model Variants with Bifurcated Flows (Cont'd)

Parameters	p_y	Average population density around yard $y \in Y$
	Υ^r_{bp}	Value of radius function around service-legs at breaking
		points w.r.t. remoteness
	λ	Value of adjusted radius function for yards at breaking points w.r.t. remoteness
	$\eta^{\scriptscriptstyle r}_{\scriptscriptstyle bp}$	Breaking points of radius curves w.r.t. Remoteness
	χ^{r}_{g}	Value of the coefficient of radius function for each commodity w.r.t. remoteness factor and weather stability class
	$u^{t,g}$	<i>Limit on the maximum number of commodity type g to be carried by train-service t</i>
	Р	Limit on the maximum tolerable risk
	ζ	$\zeta \in [0, I]$
	φ	$\phi \in [0, 1]$
	α	Weight factor for the travel and yard operations costs
	β	Weight factor for the risk term in the objective function, $\beta = 1 - \alpha$
Decision Variables	$X^{k,g,t}_{<\!i,j\!>} \!\in\! Z \!+\!$	integer variable presenting flow of commodity g of order k passing through s by train service t
	$N^t \in Z +$	Integer design variable for the total number of train service type t required to meet all weekly demands
	$Y^{r,t,g,bp}_{< i,j>} \ge 0$	Used for linearization of evacuation radius function at each service-leg
	$W^{r,t,g,bp}_{< i,j>} \in \{0,1\}$	Used for linearization of radius function for each yard service- leg
	$Q_i^{r,t,g,bp} \ge 0$	Used for linearization of evacuation radius function at each yard
	$V_i^{r,t,g,bp} \in \{0,1\}$	Used for linearization of radius function for each yard
Decision Expressions	$\varDelta^g_{\!$	Load of service-leg $s \in SL$ of commodity $g \in G$
Expressions	Π^{g}_{i}	Total Load of yard $i \in Y$ of all commodities $g \in G$
	$\wp^{g,r,d}_{< i,j>}$	Contamination level of Hazmat $g \in G$ at $d \in DW$ downwind distance from release spot on service-leg $s \in SL$ w.r.t.
	ard.	remoteness
	$arphi_i^{g,r,d}$	Contamination level of flows containing Hazmat $g \in G$ at $d \in DW$ downwind distance from release spot on yard $i \in Y$ w.r.t. remoteness
	$\mathcal{E} ho^{{}^{\langle i,j angle}}$	<i>Risk in terms of population exposure at service-leg</i> $\langle i, j \rangle \in SL$
	$\mathcal{E} \rho^i$	<i>Risk in terms of population exposure at yard</i> $i \in Y$

Table 3-3: Notations of Model Variants with Bifurcated Flows (Cont'd)

Sets	Y	Set of yards, indexed by: y, i and j
	SL	Set of service-legs, indexed by $\langle i, j \rangle$
	G	Set of goods / commodities, indexed by g
	K	Set of O/D traffic-classes, indexed by k
	R	Remoteness: Urban or Rural, indexed by r
	YT	Classification or transfer yard, indexed by $yt, yt \in \{cl, tr\}$
	BP	Breaking Points, indexed by bp
	DW	Downwind distance, indexed by d
Parameters	$d^{k,g}$	Amount of commodity g in Traffic-class k
	d_k	Total quantity of railcars in traffic-class k
		$\begin{bmatrix} 1 & ; if y = or^k \end{bmatrix}$
	$b^{^{y,k,g}}$	$b^{y,k,g} = \begin{cases} 1 & \text{; if } y = or^k \\ 0 & \text{; if } y = \text{transshipment yard} \end{cases}$
		-1 ; if $y = ds^k$
	or^k	Origin yard of traffic-class k
	ds^k	Destination of yard of traffic-class k
	∂_y^k	$\partial_{y}^{k} = \begin{cases} 1 \text{ ; } or^{k} = y \\ 0 \text{ ; otherwise} \end{cases}$
	<i>yc</i> ^{<i>yt</i>}	$yc^{yt} = \begin{cases} y^{cl}; yt = classification yard \\ y^{tr}; yt = transfer yard \end{cases}$
		y^{tr} ; $yt = transfer yard$
	Y^{tr}	Yard Transfer cost per railcar (pick-up / drop-off)
	Y^{cl}	Yard Classification cost (classification, etc.)
	$u^{\langle i,j \rangle}$	<i>Limit on the total number of railcars containing any commodity traversing service-leg s</i>
	$\mathcal{U}^{\mathcal{Y}}$	Limit on yard operations on the total number of railcars on containing any commodity type
	u_t	Capacity of train service t
	fc_t	Fixed cost of train service t
	$ heta^{ extsf{g}}$	IDLH level of commodity g
	$l_{\langle i,j \rangle}$	Length of service-legs
	$c_g^{r,d}$	Concentration (ppm) of commodity g at d downwind distance from incident spot considering the remoteness (urban/rural)
	ψ_y^{yt}	$\psi_{y}^{k,yt} = \{0,1\}; \ \forall y \in Y; \forall k \in K$
	γ_y^{yt}	$\gamma_{y}^{yt} = \{0, 1\}; \ \forall y \in Y, \ yt \in YT$
	$ au^t_{<\!i,j>}$	$\tau_s^t = \{0, 1\}; \ \forall t \in T, \ \forall s \in SL$

Table 3-4: Notations of Model Variants with Non-Bifurcated Flows

Parameters	S ^r	$S^r = [0, 1]$; $\forall a \in SL$, $\forall a \in P$
rarameters	$\delta^r_{}$	$\delta_s^r = [0, 1]; \ \forall s \in SL, \ \forall r \in R$
	ξ_y^r	$\xi_{y}^{r} = \{0, 1\}; \ \forall \in Y, \ \forall r \in R$
	${ ho^r}_{{\scriptscriptstyle <}i,j{\scriptscriptstyle >}}$	Average population density around service-leg $s \in SL$ w.r.t. remoteness factor
	p_y	Average population density around yard $y \in Y$
	Υ^r_{bp}	Value of radius function around service-legs at breaking points w.r.t. remoteness and weather stability class
	Â.	Value of adjusted radius function for yards at breaking points w.r.t. remoteness
	η^r_{bp}	Breaking points of radius curves w.r.t. Remoteness
	χ_{g}^{r}	Value of the coefficient of radius function for each commodity w.r.t. remoteness factor and weather stability class
	<i>u^{t,g}</i>	<i>Limit on the maximum number of commodity type g to be carried by train-service t</i>
	Р	Limit on the maximum tolerable risk
	5	$\zeta \in [0, 1]$
	ϕ	$\phi \in \left[0, 1\right]$
	α	Weight factor for the travel and yard operations costs
	β	Weight factor for the risk term in the objective function, $\beta = 1 - \alpha$
Decision Variables	$N^t \in Z +$	Integer design variable for the total number of train service type t required to meet all weekly demands
	$Z^{k,t}_{< i,j>}$	$\begin{bmatrix} 1 \\ j \end{bmatrix}$; if traffic-class k is passing through service-leg $\langle i, j \rangle$
		$Z_{}^{k,t} = \begin{cases} 1 \ ; \ if \ traffic-class \ k \ is \ passing \ through \ service-leg < i,j> \\ using \ train \ service \ t \\ 0 \ ; \ otherwise \end{cases}$
	$Y^{r,t,g,bp}_{< i,j>} \ge 0$	Used for linearization of evacuation radius function at each service-leg
	$W^{r,t,g,bp}_{< i,j>} \in \{0,1\}$	Used for linearization of radius function for each yard service- leg
	$Q_i^{r,t,g,bp} \ge 0$	Used for linearization of evacuation radius function at each yard
	$V_i^{r,t,g,bp} \in \{0,1\}$	Used for linearization of radius function for each yard

Table 3-5: Notations of Model Variants with Non-Bifurcated Flows (Cont'd)

Decision Expressions	$\varDelta^g_{\!$	Load of service-leg $s \in SL$ of commodity $g \in G$
	Π^{g}_{i}	Total Load of yard $i \in Y$ of all commodities $g \in G$
	$\wp^{g,r,d}_{\langle i,j \rangle}$	Contamination level of Hazmat $g \in G$ at $d \in DW$ downwind
	- 5	distance from release spot on service-leg $s \in SL$ w.r.t.
		remoteness
	$\varphi_i^{g,r,d}$	Contamination level of flows containing Hazmat $g \in G$ at
		$d \in DW$ downwind distance from release spot on yard $i \in Y$
		w.r.t. remoteness
	$arepsilon ho^{{<}i,j>}$	<i>Risk in terms of population exposure at service-leg</i> $\langle i, j \rangle \in SL$
	$\mathcal{E} \rho^i$	<i>Risk in terms of population exposure at yard</i> $i \in Y$

Table 3-6: Notations of Model Variants with Non-Bifurcated Flows (Cont'd)

3.2. Models with a Single Objective Function

Throughout this section, two model variants with single objective function will be discussed, whose objective functions comprise of transportation cost, yard operations cost and train fixed cost. Further, regarding predefined thresholds are suggested as a guideline for radius of isolation and evacuation areas for each type of Hazmats in ERG 2016 by CANUTEC, *Cloutier and Cushmac (2016)*, for each type of Hazmats, we have set two sets of constraints on the maximum contaminants concentration limits at those predefined thresholds, at downwind distances from yards and service-legs. Further the risk around each of the service-legs and yards have been constrained no to exceed a proportion of the total risk around all service-legs and total risk at all yards of the underlying network, respectively. Moreover, considering the interest of the regulatory agencies and insurance companies, a set of constraints which enforce limits, the maximum tolerable threshold, on the total number of people that are potentially exposed to the risk of evacuation, injury or fatality, have been added to the constraints. As explained earlier, setting such threshold can be controversial; as well, this constraint can become a complicating constraint given a tight upper limit which may result in infeasibility due to risk averseness of insurance companies.

Hence, we incorporated the term associating with the total risk into the objective function in the model variant that have been presented in section (3.3). Moreover, the risk function had a nonlinear, concave down, expression, which was piecewise linearized. Moreover, in order to avoid underestimation, we made use of linear regression to enhance the precision of the estimation between each breaking point.

Before presenting the models, we are going to briefly elaborate on the nonlinear radius function and its linearization. For each type of Hazmat under study and for each area type, urban and opencountry / rural, we have broken the radius function (3.1.6) into a coefficient and a function of a decision variable; for any train service traversing which traverses a given rail segment, we computed the radius function as follows:

$$rad_{\langle i,j\rangle}^{t,r,g} = (b+d)_r \sqrt{\mathfrak{I}_{\langle i,j\rangle}^{t,g} \times \frac{Q^g}{\left(ac\right)_r \pi \times \mu \times C_{IDLH}^g}} ; \forall r \in R, \forall g \in G, \langle i,j\rangle \in SL, \forall t \in T \quad (3.1.7)$$

In order to simplify the expression, we defined the following term to represent the root of the function w.r.t. remoteness.

$$\varepsilon^r = (b+d)_r \; ; \; \forall r \in R \tag{3.1.8}$$

So, if we separate the coefficients from the decision variable part, we get the following expressions:

$$\chi_g^r = \sqrt[\varepsilon^r]{\frac{Q^g}{(ac)_r \,\pi \times \mu \times C_{IDLH}^g}} ; \,\forall r \in R, \forall g \in G$$
(3.1.9)

Therefore, the radius function can be written as follows:

$$rad_{\langle i,j\rangle}^{t,r,g} = \chi_g^r \times \sqrt[c]{\mathfrak{T}_{\langle i,j\rangle}^{t,g}} ; \ \forall r \in \mathbb{R}, \forall g \in G, \langle i,j\rangle \in SL, \ t \in T$$
(3.1.10)

In the same fashion, for yards, the radius can be computed as follows:

$$rad_{j}^{t,r,g} = \varepsilon' \left(\sum_{k \in K} \sum_{\langle i,j \rangle \in Sl} X_{\langle i,j \rangle}^{k,g,t} + \sum_{k \in K} \sum_{\langle j,l \rangle \in Sl} \partial_{j}^{k} \times X_{\langle j,s \rangle}^{k,g,t} \right) \times \frac{Q^{g}}{(ac)_{r} \pi \times \mu \times C_{IDLH}^{g}} ; \forall r \in R, \forall g \in G,$$

$$\forall j \in Y, \forall t \in T$$

$$(3.1.11)$$

We define an expression for the number of railcars of train t which traverse through yard j as flows:

$$\Pi_{j}^{t,g} = \sum_{k \in K} \sum_{\langle i,j \rangle \in Sl} X_{\langle i,j \rangle}^{k,g,t} + \sum_{k \in K} \sum_{\langle j,l \rangle \in Sl} \partial_{j}^{k} \times X_{\langle j,s \rangle}^{k,g,t} ; \forall \langle i,j \rangle, \langle j,l \rangle \in SL, \forall j \in Y, \forall t \in T$$

$$(3.1.12)$$

Therefore, the dispersion radius function due Hazmat railcars on train t which traverses through yard j, can be computed as follows:

$$rad_{j}^{t,r,g} = \chi_{g}^{r} \times \sqrt[e^{r}]{\Pi_{j}^{t,g}} ; \forall r \in R, \forall g \in G, j \in Y, \forall t \in T$$

$$(3.1.13)$$

As depicted in Figure 3-3, radius function is a concave-down function. This figure demonstrates the curve of $rad_{<l,j>}^{l,r,g}$ and/or $rad_l^{l,r,g}$ for $0 \le \Im_{<l,j>}^{l,g} \le 300$ or $0 \le \Pi_j^{l,g} \le 300$, in urban and rural areas, we considered the worst case scenario, a very unstable weather condition in the urban areas will have PG: A, and in rural areas it barely gets worse than PG: D. Moreover, we applied the air dispersion parameters of *Tadmor and Gur (1967)*, to estimate the buoyant contaminants dispersion radius. Moreover, as shown in the Figure 3-3, there is a remarkable discrepancy between values of radius in urban and rural areas. In addition, the discrepancy between the radius due to incidents involving Propane and Butane, as demonstrated in Figure 3-4, increases as we move from urban to the rural areas. The reason behind the above-mentioned discrepancy between Hazmat dispersion radius in urban and rural areas stem from the fact that the crosswind and vertical dispersions of contaminants are much higher in urban areas than those of rural areas due to the turbulence and weather instability conditions. Furthermore, Figure 3-6 and Figure 3-5 demonstrate the radius of evacuation area for different number of Hazmat railcars, from the release spot in both rural and urban areas, respectively. Due to the concavity of the radius curves, linearization may indeed result in underestimation of the radius value within any given pair of breaking points. Moreover, as we discussed earlier, for $rad_i^{i,r,g}$ and $rad_{\langle i,j \rangle}^{\iota,r,g}$, where $i \in Y$ and $\langle i,j \rangle \in SL$, we linearize $\sqrt[q]{\Pi_j^{r,g}}$ and

 $\sqrt[s]{\mathfrak{T}_{\langle i,j \rangle}^{r,g}}$, respectively, then, we multiply it by χ_g^r , to compute the evacuation radius. In order to prevent too much underestimation of the value of radius, we make use of linear regression line between any two breaking points. Figure 3-7 and Figure 3-8 illustrate the application of linear regression in linearization of the radius function in both rural and urban areas, respectively.

In order to compute the risk in terms of the number of people exposed to the risk due to transportation of Hazmats around service-legs and yards, we consider a rectangular impact area and danger circle, respectively. Hence, population exposure risk is obtained as follows:

$$R_{\scriptscriptstyle (i,j)}^{t,r,g} = 2 \ rad_{\scriptscriptstyle (i,j)}^{t,r,g} \ l_{\scriptscriptstyle (i,j)} \ \rho_{\scriptscriptstyle (i,j)}^r \tag{3.1.14}$$

$$R_{j}^{t,r,g} = \pi \; (rad_{j}^{t,r,g})^{2} \rho^{j} \tag{3.1.15}$$

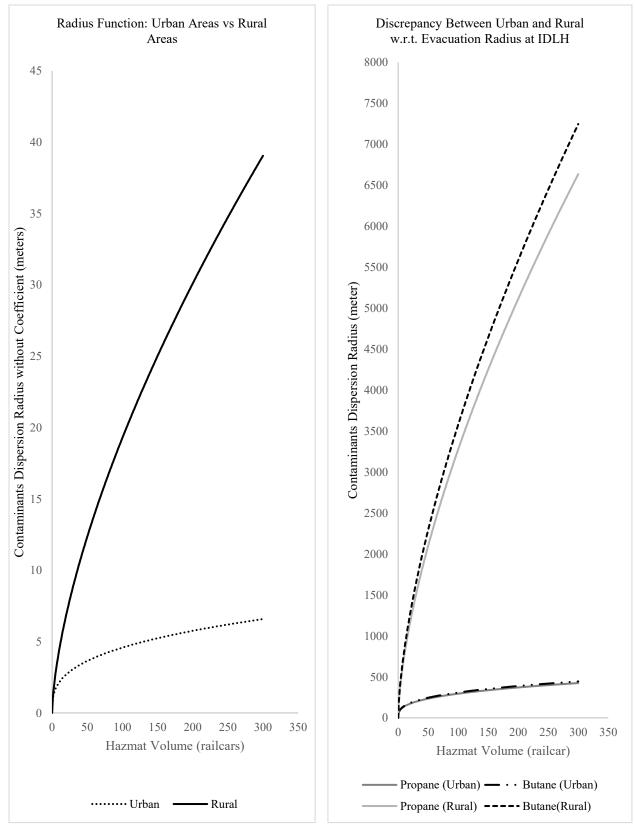


Figure 3-3: Evacuation Radius - Urban vs Rural Areas

Figure 3-4: Radius of Evacuation Area - A Concavedown Function

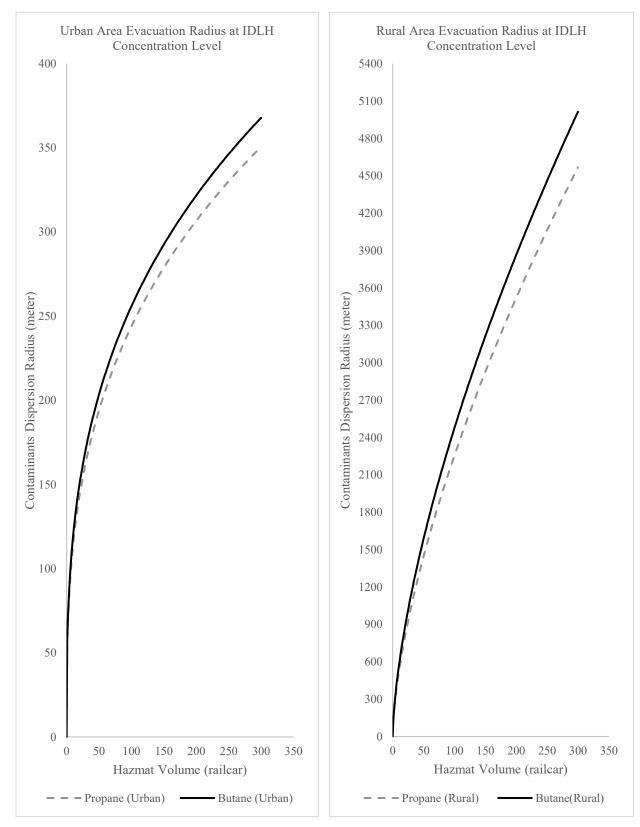


Figure 3-6: Evacuation Radius at IDLH Level in Urban Areas

Figure 3-5: Evacuation Radius at IDLH Level in Rural Areas

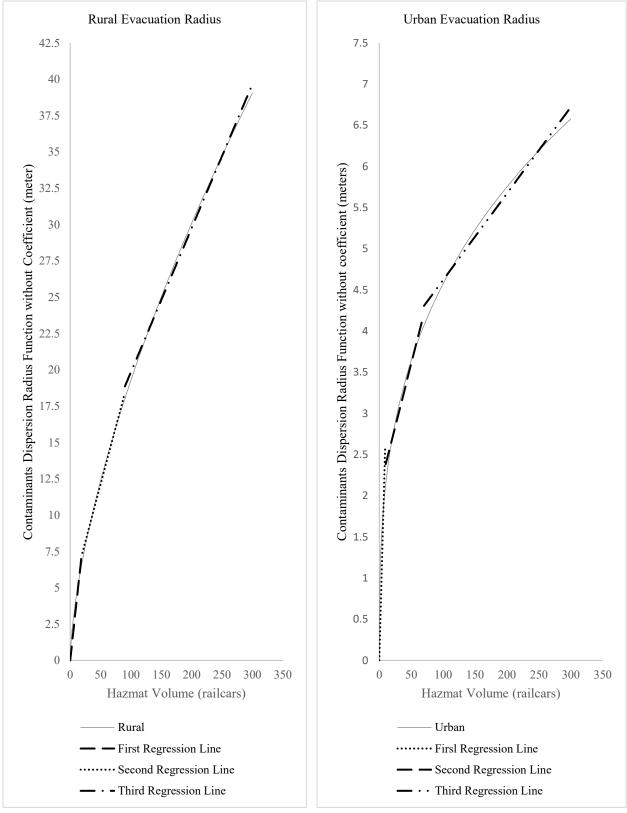
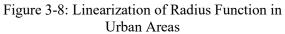


Figure 3-7: Linearization of Radius Function in Rural Areas



3.2.1. Single objective with Bifurcated Flows

$$Minimize \begin{pmatrix} \sum_{\langle i,j \rangle \in SI} \sum_{k \in K} \sum_{g \in G} \sum_{t \in T} X_{\langle i,j \rangle}^{kg,t} & l_{\langle i,j \rangle} & tc + \\ \sum_{\langle i,j \rangle SL} \sum_{k \in K} \sum_{g \in G} \sum_{t \in T} \sum_{y \in YT} \psi_i^{yt} & yc^{yt} & X_{\langle i,j \rangle}^{kg,t} + \sum_{k \in K} d_k & y^{tr} + \\ \sum_{t \in T} \sum_{\langle i,j \rangle \in SI} (fc_t / c) & N^t & \tau_{\langle i,j \rangle}^t & l^{\langle i,j \rangle} \end{pmatrix}$$
(3.1.16)

Subject to :

$$X_{\langle i,j \rangle}^{k,g,t} \le \tau_{\langle i,j \rangle}^{t} d^{k,g}; \ \forall k \in K, \ g \in G, \ t \in T, \ \forall < i,j > \in SL$$
(3.1.17)

$$\sum_{\langle i,j \rangle \in SL} \sum_{t \in T} X_{\langle i,j \rangle}^{k,g,t} - \sum_{\langle j,i \rangle \in SL} \sum_{t \in T} X_{\langle j,i \rangle}^{k,g,t} = b_i^{k,g} \ ; \ \forall i \in Y, \ \forall k \in K, \ \forall g \in G$$
(3.1.18)

$$\mathfrak{I}_{\langle i,j\rangle}^{t,g} \le N^t u^{t,g} ; \forall t \in T, \forall \langle i,j\rangle \in SL, \forall g \in G$$
(3.1.19)

$$\Delta_{\langle i,j\rangle}^g \le u_{\langle i,j\rangle}^g ; \forall \langle i,j\rangle \in SL; \forall g \in G$$

$$(3.1.20)$$

$$\Delta^{\langle i,j\rangle} \le u^{\langle i,j\rangle} ; \ \forall < i,j > \in SL$$
(3.1.21)

$$\Pi_i^g \le \upsilon_i^g \; ; \; \forall i \in Y, \; \forall g \in G \tag{3.1.22}$$

$$\Pi_i \le \upsilon^i \; ; \; \forall i \in Y \tag{3.1.23}$$

$$\wp_{}^{g,r,d} \le \theta^g \; ; \; \forall < i,j> \in SL, \; \forall g \in G, \; r \in R, \; \forall d \in DW$$

$$(3.1.24)$$

$$\varphi_i^{g,r,d} \le \theta^g \; ; \; \forall i \in Y, \; \forall g \in G, \; r \in R, \; \forall d \in DW \tag{3.1.25}$$

$$\varepsilon \rho^{\langle i,j \rangle} \leq \zeta \sum_{\langle m,n \rangle \in SL} \varepsilon \rho^{\langle m,n \rangle} ; \; \forall \langle i,j \rangle \in SL$$
(3.1.26)

$$\varepsilon \rho^{i} \le \phi \sum_{j \in Y} \varepsilon \rho^{j} \quad \forall i \in Y$$
(3.1.27)

$$\sum_{i\in Y} \varepsilon \rho^{j} + \sum_{\langle i,j\rangle \in Sl} \varepsilon \rho^{\langle i,j\rangle} \le P$$
(3.1.28)

$$\sum_{k \in K} X_{\langle i,j \rangle}^{k,g,i} - \sum_{bp \in BP} Y_{\langle i,j \rangle}^{t,r,g,bp} \ \eta_{bp}^{r} = 0 \ ; \ \forall < i,j \rangle \in SL, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.29)

$$Y_{}^{t,r,g,l} \le W_{}^{t,r,g,l}; \ \forall < i,j> \in SL, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.30)

$$Y_{}^{t,r,g,2} \le W_{}^{r,t,g,l} + W_{}^{t,r,g,2} ; \ \forall < i,j> \in SL, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.31)

$$Y_{\langle i,j \rangle}^{t,r,g,3} \le W_{\langle i,j \rangle}^{t,r,g,2} + W_{\langle i,j \rangle}^{t,r,g,3}; \ \forall < i,j > \in SL, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.32)

$$Y_{}^{t,r,g,4} \le W_{}^{t,r,g,3}; \ \forall < i,j> \in SL, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.33)

$$\sum_{bp \in BP} Y_{\langle i,j \rangle}^{t,r,g,bp} = 1 ; \forall \langle i,j \rangle \in SL, g \in G, r \in R, \forall t \in T$$

$$(3.1.34)$$

$$\sum_{i=l}^{bp-1} W_{}^{i,r,g,i} = 1; \, \forall < i,j> \in SL, \, g \in G, \, r \in R, \, \forall t \in T$$
(3.1.35)

$$\sum_{k \in K} \sum_{\langle i, j \rangle \in SI} X_{\langle i, j \rangle}^{k,g,t} + \sum_{k \in K} \sum_{\langle j, s \rangle \in SI} \partial_i^k X_{\langle j, s \rangle}^{k,g,t} - \sum_{bp \in BP} Q_i^{t,r,g,bp} \eta_{bp}^r = 0 ; \forall j \in Y, g \in G, r \in R, \forall t \in T$$
(3.1.36)

$$Q_i^{t,rg,l} \le V_i^{t,r,g,l}; \ \forall i \in Y, \ g \in G, \ r \in R, \ \forall t \in T$$

$$(3.1.37)$$

$$Q_i^{t,r,g,2} \le V_i^{t,r,g,1} + V_i^{t,r,g,2} ; \forall i \in Y, g \in G, r \in R, \forall t \in T$$
(3.1.38)

$$Q_i^{t,r,g,3} \le V_i^{t,r,g,2} + V_i^{t,r,g,3} ; \ \forall i \in Y, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.39)

$$Q_i^{t,r,g,4} \le V_i^{t,r,g,3}; \ \forall i \in Y, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.40)

$$\sum_{bp\in BP} \mathcal{Q}_i^{t,r,g,bp} = 1 ; \forall i \in Y, g \in G, r \in R, \forall t \in T$$

$$(3.1.41)$$

$$\sum_{i=l}^{bp-l} V_{}^{t,r,g,i} = l \; ; \; \forall i \in Y, \; g \in G, \; r \in R, \; \forall t \in T$$
(3.1.42)

Where:

$$\mathfrak{T}_{}^{t,g} = \sum_{k \in K} X_{}^{k,g,t} ; \ \forall < i,j> \in SL, \ t \in T, \ g \in G$$
(3.1.43)

$$\Delta_{}^{g} = \sum_{k \in K} \sum_{t \in T} X_{}^{k,g,t} ; \ \forall < i,j> \in SL, \ \forall g \in G$$
(3.1.44)

$$\Delta^{\langle i,j\rangle} = \sum_{k \in K} \sum_{g \in G} \sum_{t \in T} X^{k,g,t}_{\langle i,j\rangle} ; \forall \langle i,j\rangle \in SL$$
(3.1.45)

$$\varepsilon \rho^{} = \sum_{r \in R} \sum_{g \in G} \sum_{bp \in BP} \sum_{t \in T} \delta^{r}_{} \ \chi^{r}_{g} \ Y^{t,r,g,bp}_{} \ \Upsilon^{r}_{bp} \ l_{} \ \rho^{r}_{} \ ; \ \forall < i,j> \in SL$$
(3.1.46)

$$\varepsilon \rho^{i} = \sum_{r \in R} \sum_{g \in G} \sum_{bp \in BP} \sum_{t \in T} \xi_{y}^{r} \chi_{g}^{r} \mathcal{Q}_{i}^{t,r,g,bp} \hat{\mathcal{X}} \qquad i \in Y$$
(3.1.47)

$$\wp_{}^{g,r,d} = \sum_{r \in R} \sum_{k \in K} \sum_{t \in T} X_{}^{k,g,t} c_g^{r,d} ; \forall < i,j> \in SL, \forall g \in G, r \in R, d \in DW$$
(3.1.48)

$$\Pi_{i}^{g} = \sum_{k \in K} \sum_{t \in T} \sum_{\langle j, i \rangle \in Sl} X_{\langle j, i \rangle}^{k,g,t} + \sum_{k \in K} \partial_{i}^{k} b^{y,k,g} ; \forall i \in Y, g \in G, r \in R$$
(3.1.49)

$$\varphi_i^{g,r,d} = \Pi_i^g \ c_g^{r,d} \ ; \ i \in Y, \ g \in G, \ r \in R, \ d \in DW$$
(3.1.50)

The objective function of the model, (3.1.16), is comprised of four terms; the first term is computing the total travel cost, the second and the third terms are computing yard operations costs; the second term is considering the classification costs at the origin yards as well as the transfer costs at intermediate yards while the third term computes the unloading and sorting costs at the destination yards which is a fixed cost (and assumed to be incurring the same cost as transfer cost), thereby not affecting the optimal solution in terms of the routing decision making. However, we have incorporated this term into the objective function to obtain the total yard operation costs. The fourth term in the objective function computes the total train costs.

Constraints (3.1.17) enforce that flow can pass through a rail segment iff that service-leg has been defined as a service-leg of a train service. Set of constraints (3.1.18) are flow conservation / mass

balance constraints, which enforce all demands to be met. Constraints (3.1.19) enforce regulatory restriction on the maximum number of Hazmat of each type to be loaded on each train-service; as well, this set of constraints enforce the minimum number of train services required to meet all weekly demands. constraints (3.1.20) enforce upper limits on arc load of each type of commodities; constraints (3.1.21) enforce limits on the total number of railcars of any type of commodities traversing through each arc; constraints (3.1.22) enforce upper limits on yard load of each type of commodities; constraints (3.1.23) enforce limits on the total number of railcars of any type of commodities traversing through each yard; constraints (3.1.24) enforce the limit on the concentration of Hazmats of each type to be less than the IDLH limit at a predefined downwind distance from any given arc; constraints (3.1.25) enforce the limit on the concentration of Hazmats of each type to be less than the IDLH limit at a predefined downwind distance from any given yard. Set of constraints (3.1.26) and (3.1.27) enforce the maximum tolerable population exposure at service-legs and yards of the underlying network of the problem under study, respectively; these constraints ensure that the risk on a service-leg and at yards cannot exceed a predefined proportion of total risk of service-legs and yards, depending on the value of ζ and ϕ set by the authorities. Constraints (3.1.28) enforce a limit P on the maximum tolerable risk in terms of the number of people exposed to risk of transportation.

Constraints (3.1.29) to (3.1.35) are used to linearize the nonlinear dispersion radius function for any given rail segment. Constraints (3.1.36) to (3.1.42) are used to linearize the nonlinear dispersion radius function for any given yard.

Constraints (3.1.43) to (3.1.50) are used to define the decision expressions we made use of in previous constraints.

3.2.2. Single objective with Non-Bifurcated Flows

$$Minimize \begin{pmatrix} \sum_{\langle i,j \rangle \in Sl} \sum_{k \in K} \sum_{g \in G} \sum_{i \in T} Z_{\langle i,j \rangle}^{k,t} d^{k,g} l_{\langle i,j \rangle} tc + \\ \sum_{\langle i,j \rangle \in Sl} \sum_{k \in K} \sum_{g \in G} \sum_{i \in T} \sum_{yt \in YT} \psi_{i}^{yt} yc^{yt} X_{\langle i,j \rangle}^{k,g,t} + \sum_{k \in K} d_{k} y^{tr} + \\ \sum_{i \in T} \sum_{\langle i,j \rangle \in Sl} (fc_{i}/c) N^{t} \tau_{\langle i,j \rangle}^{t} l^{\langle i,j \rangle} \end{pmatrix}$$
(3.1.51)

Subject to:

$$Z_{\langle i,j\rangle}^{k,t} \le \tau_{\langle i,j\rangle}^{t} ; \forall k \in K, \ t \in T, \ \langle i,j\rangle \in SL$$

$$(3.1.52)$$

$$\sum_{\langle i,j\rangle\in SL}\sum_{t\in T} Z_{\langle i,j\rangle}^{k,t} - \sum_{\langle j,i\rangle\in SL}\sum_{t\in T} Z_{\langle i,j\rangle}^{k,t} = b_i^{k,g} ; \forall i \in Y, \forall k \in K, \forall g \in G$$

$$(3.1.53)$$

$$\mathfrak{I}_{\langle i,j\rangle}^{t,g} \leq N^{t} u^{t,g} ; \forall t \in T, \forall \langle i,j\rangle \in SL, \forall g \in G$$

$$(3.1.54)$$

$$\sum_{i \in T} Z_{\langle i,j \rangle}^{k,i} \leq 1 ; \forall k \in K, \forall \langle i,j \rangle \in SL$$

$$(3.1.55)$$

$$\Delta^g_{\langle i,j\rangle} \le u^g_{\langle i,j\rangle} ; \ \langle i,j\rangle \in SL; \ \forall g \in G$$

$$(3.1.56)$$

$$\Delta^{s} \le u^{} ; \ \in SL$$
(3.1.57)

$$\Pi_i^g \le \upsilon_i^g \; ; \; \forall i \in Y, \; \forall g \in G \tag{3.1.58}$$

$$\Pi_i \le \upsilon^i \; ; \; \forall i \in Y \tag{3.1.59}$$

$$\wp_{}^{g,r,d} \le \theta^g; \ \forall < i,j> \in Sl, \ \forall g \in G, \ r \in R, \ \forall d \in DW$$

$$(3.1.60)$$

$$\varphi_i^{g,r,d} \le \theta^g \; ; \; \forall i \in Y, \; \forall g \in G, \; r \in R, \; \forall d \in DW$$
(3.1.61)

$$\varepsilon \rho^{\langle i,j \rangle} \leq \zeta \sum_{\langle m,n \rangle \in SL} \varepsilon \rho^{\langle m,n \rangle} ; \ \forall \langle i,j \rangle \in SL$$
(3.1.62)

$$\varepsilon \rho^{i} \le \phi \sum_{j \in Y} \varepsilon \rho^{j} \quad \forall i \in Y$$
(3.1.63)

$$\sum_{i\in Y} \varepsilon \rho^{j} + \sum_{\langle i,j\rangle \in Sl} \varepsilon \rho^{\langle i,j\rangle} \le P$$
(3.1.64)

$$\sum_{k \in K} Z_{\langle i,j \rangle}^{k,t} d^{k,g} - \sum_{bp \in BP} Y_{\langle i,j \rangle}^{t,r,g,bp} \eta_{bp}^{r} = 0 ; \forall \langle i,j \rangle \in SL, g \in G, r \in R, t \in T$$
(3.1.65)

$$Y_{}^{t,r,g,l} \le W_{}^{t,r,g,l}; \ \forall < i,j>\in SL, \ g \in G, \ r \in R, \ t \in T$$
(3.1.66)

$$Y_{\langle i,j \rangle}^{t,r,2} \le W_{\langle i,j \rangle}^{t,r,g,l} + W_{\langle i,j \rangle}^{t,r,g,2} ; \forall < i,j \rangle \in SL, \ g \in G, \ r \in R, \ t \in T$$
(3.1.67)

$$Y_{}^{t,r,g,3} \le W_{}^{t,r,g,2} + W_{}^{t,r,g,3}; \ \forall < i,j> \in SL, \ g \in G, \ r \in R, \ t \in T$$
(3.1.68)

$$Y_{}^{t,r,g,4} \le W_{}^{t,r,g,3}; \ \forall < i,j>\in SL, \ g \in G, \ r \in R, \ t \in T$$
(3.1.69)

$$\sum_{bp \in BP} Y_{\langle i,j \rangle}^{t,r,g,bp} = 1 ; \ \forall < i,j \rangle \in SL, \ g \in G, \ r \in R, \ t \in T$$
(3.1.70)

$$\sum_{i=1}^{bp-1} W_{}^{t,r,g,i} = 1 ; \forall < i,j> \in SL, g \in G, r \in R, t \in T$$
(3.1.71)

$$\Pi_{i}^{g} - \sum_{bp \in BP} Q_{i}^{t,r,g,bp} \ \eta_{bp}^{r} = 0 \ ; \ \forall i \in Y, \ g \in G, \ r \in R, \ t \in T$$
(3.1.72)

$$Q_i^{t,r,g,l} \le V_i^{t,r,g,l}; \ \forall i \in Y, \ g \in G, \ r \in R, \ t \in T$$
(3.1.73)

$$Q_i^{t,r,g,2} \le V_i^{t,r,g,1} + V_i^{t,r,g,2} ; \forall i \in Y, g \in G, r \in R, t \in T$$
(3.1.74)

$$Q_i^{t,r,g,3} \le V_i^{t,r,g,2} + V_i^{t,r,g,3} ; \forall i \in Y, g \in G, r \in R, t \in T$$
(3.1.75)

$$Q_i^{t,r,g,4} \le V_i^{t,r,g,3}; \ \forall i \in Y, \ g \in G, \ r \in R, \ t \in T$$
(3.1.76)

$$\sum_{bp\in BP} Q_i^{t,r,g,bp} = 1 ; \forall i \in Y, g \in G, r \in R, t \in T$$

$$(3.1.77)$$

$$\sum_{i=1}^{bp-1} V_{\langle i,j \rangle}^{t,r,g,i} = 1 ; \ \forall i \in Y, \ g \in G, \ r \in R, \ t \in T$$
(3.1.78)

Where:

$$\mathfrak{T}_{}^{t,g} = \sum_{k \in K} Z_{}^{k,t} d^{k,g} ; \forall < i,j> \in SL, t \in T, g \in G$$
(3.1.79)

$$\Delta_{\langle i,j\rangle}^{g} = \sum_{k \in K} \sum_{t \in T} Z_{\langle i,j\rangle}^{k,t} d^{k,g} ; \forall \langle i,j\rangle \in SL, \forall g \in G$$

$$(3.1.80)$$

$$\Delta^{} = \sum_{k \in K} \sum_{g \in G} \sum_{i \in T} Z_{}^{k,i} d^{k,g} ; \forall < i,j> \in SL$$
(3.1.81)

$$\Pi_{i}^{g} = \sum_{k \in K} \sum_{t \in T} \sum_{\langle j, i \rangle \in Sl} Z_{\langle i, j \rangle}^{k, t} d^{k, g} + \sum_{k \in K} \partial_{i}^{k} b^{y, k, g} d^{k, g} ; \forall i \in Y, g \in G, r \in R$$
(3.1.82)

$$\varepsilon \rho^{} = \sum_{r \in R} \sum_{g \in G} \sum_{bp \in BP} \delta^{r}_{} \chi^{r}_{g} Y^{t,r,g,bp}_{} \Upsilon^{r}_{bp} l_{} \rho^{r}_{}; \forall < i,j> \in SL$$
(3.1.83)

$$\varepsilon \rho^{i} = \sum_{r \in \mathbb{R}} \sum_{g \in G} \sum_{bp \in BP} \partial_{i}^{r} \chi_{g}^{r} Q_{i}^{t,r,g,bp} \hat{\chi} \qquad i \in Y$$
(3.1.84)

$$\wp_{}^{g,r,d} = \sum_{r \in R} \sum_{k \in K} \sum_{t \in T} Z_{}^{k,t} d^{k,g} c_g^{r,d} ; \forall < i,j> \in SL, \forall g \in G, r \in R, d \in DW$$
(3.1.85)

$$\varphi_i^{g,r,d} = \Pi_i^g \ c_g^{r,d} \ ; \ i \in Y, \ g \in G, \ r \in R, \ d \in DW$$
(3.1.86)

What contrasts this model variant from the previously discussed model in section (3.2.1), is that this model considers no more than a single route for each pair of O/D traffic-class. In other words, the previously discussed model reduces to the current model if the carrier company would like to route all commodities $g \in G$ within the traffic-class $k \in K$, through the shortest path w.r.t. the transportation and yard operations costs, under the above-mentioned constraints.

The objective function is the same as the previously discussed model. Furthermore, all constraints are the same except the constraints (3.1.55) which enforce that each traffic-class cannot be carried by more than one train on each arc. This constraint can be neutral if two train-services passing

through any given arc have the same fixed costs and if we assume the length of their service-legs are the same.

3.3. Models with a Multiobjective Function

Throughout the following subsections, we look at the problem from a different angle, by incorporating the risk term into the objective function. Since setting upper limits on the maximum number of people to be exposed to the risk due to transportation of Hazmats, is controversial, on the one hand, and tightening the respective constraints which will result in infeasibility of the problem, on the other, we decided to find a set of nondominated Pareto-optimal paths depending on various weights assigned to the cost and risk terms into the objective function. Hence, the following multiobjective models have the same constraints expect that the constraint concerning population exposure is removed from the constraints and treated as risk evaluation measure into the objective function.

3.3.1. Biobjective with Bifurcated Flows

$$Minimize \begin{pmatrix} Cost: \alpha \begin{bmatrix} \sum_{\langle i,j \rangle \in SL} \sum_{k \in K} \sum_{g \in G} \sum_{t \in T} X_{\langle i,j \rangle}^{k,g,t} l_{\langle i,j \rangle} tc + \\ \begin{bmatrix} \sum_{\langle i,j \rangle \in SL} \sum_{k \in K} \sum_{g \in G} \sum_{t \in T} \sum_{y t \in YT} \psi_i^{yt} yc^{yt} X_{\langle i,j \rangle}^{k,g,t} + \sum_{k \in K} d_k y^{tr} \end{bmatrix} + \\ \sum_{t \in T} \sum_{\langle i,j \rangle \in SL} (fc_t/c) N^t \tau_{\langle i,j \rangle}^t l_{\langle i,j \rangle} l^{\langle i,j \rangle} \end{pmatrix} \\ Risk: \beta \begin{bmatrix} \sum_{\langle i,j \rangle \in SI} \sum_{t \in T} \sum_{r \in R} \sum_{g \in G} \sum_{bp \in BP} \delta_{\langle i,j \rangle}^r \chi_g^r Y_{\langle i,j \rangle}^{t,r,g,bp} \gamma_{bp}^r l_{\langle i,j \rangle} \rho_{\langle i,j \rangle}^r \end{bmatrix} + \\ \begin{bmatrix} \sum_{i \in Y} \sum_{t \in T} \sum_{r \in R} \sum_{g \in G} \sum_{bp \in BP} \partial_i^r (\chi_g^r)^2 Q_i^{t,r,g,bp} \tilde{\chi} \end{bmatrix} \end{bmatrix} \end{pmatrix}$$
(3.1.87)

Subject to:

$$X_{}^{k,g,t} \le \tau_{}^{t} d^{k,g}; \ \forall k \in K, \ g \in G, \ t \in T, \ \forall < i,j> \in SL$$
(3.1.88)

$$\sum_{\langle i,j \rangle \in SL} \sum_{t \in T} X_{\langle i,j \rangle}^{k,g,t} - \sum_{\langle j,i \rangle \in SL} \sum_{t \in T} X_{\langle j,i \rangle}^{k,g,t} = b_i^{k,g} ; \forall i \in Y, \forall k \in K, \forall g \in G$$
(3.1.89)

$$\mathfrak{I}^{i,g}_{\langle i,j\rangle} \le N^t u^{i,g} \; ; \; \forall t \in T, \; \forall \langle i,j\rangle \in SL, \; \forall g \in G$$

$$(3.1.90)$$

$$\Delta_{\langle i,j\rangle}^g \le u_{\langle i,j\rangle}^g ; \forall \langle i,j\rangle \in SL; \forall g \in G$$

$$(3.1.91)$$

$$\Delta^{\langle i,j \rangle} \le u^{\langle i,j \rangle} ; \ \forall \langle i,j \rangle \in SL$$
(3.1.92)

$$\Pi_i^g \le \upsilon_i^g \; ; \; \forall i \in Y, \; \forall g \in G \tag{3.1.93}$$

$$\Pi_i \le \upsilon^i \; ; \; \forall i \in Y \tag{3.1.94}$$

$$\wp_{}^{g,r,d} \le \theta^g \; ; \; \forall < i,j> \in Sl, \; \forall g \in G, \; r \in R, \; \forall d \in DW$$

$$(3.1.95)$$

$$\varphi_i^{g,r,d} \le \theta^g \; ; \; \forall i \in Y, \; \forall g \in G, \; r \in R, \; \forall d \in DW$$
(3.1.96)

$$\varepsilon \rho^{\langle i,j \rangle} \leq \zeta \sum_{\langle m,n \rangle \in Sl} \varepsilon \rho^{\langle m,n \rangle} ; \; \forall \langle i,j \rangle \in SL$$
(3.1.97)

$$\varepsilon \rho^{i} \le \phi \sum_{j \in Y} \varepsilon \rho^{j} \quad \forall i \in Y$$
(3.1.98)

$$\sum_{k \in K} X_{\langle i,j \rangle}^{k,g,t} - \sum_{bp \in BP} Y_{\langle i,j \rangle}^{t,r,g,bp} \ \eta_{bp}^{r} = 0 \ ; \ \forall < i,j \rangle \in SL, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.99)

$$Y_{}^{t,r,g,l} \le W_{}^{t,r,g,l}; \ \forall < i,j>\in SL, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.100)

$$Y_{}^{t,r,g,2} \le W_{}^{t,r,g,l} + W_{}^{t,r,g,2} \; ; \; \forall < i,j> \in SL, \; g \in G, \; r \in R, \; \forall t \in T$$
(3.1.101)

$$Y_{}^{t,rg,3} \le W_{}^{t,r,g,2} + W_{}^{t,r,g,3}; \ \forall < i,j> \in SL, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.102)

$$Y_{}^{t,r,g,4} \le W_{}^{t,r,g,3}; \ \forall < i,j>\in SL, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.103)

$$\sum_{bp \in BP} Y_{}^{t,r,g,bp} = 1 ; \forall < i,j > \in SL, g \in G, r \in R, \forall t \in T$$
(3.1.104)

$$\sum_{i=l}^{bp-l} W_{}^{i,r,g,i} = l \; ; \; \forall < i,j> \in SL, \; g \in G, \; r \in R, \; \forall t \in T$$
(3.1.105)

$$\sum_{k \in K} \sum_{\langle i,j \rangle \in Sl} X_{\langle i,j \rangle}^{k,g,t} + \sum_{k \in K} \sum_{\langle j,s \rangle \in Sl} \partial_i^k X_{\langle j,s \rangle}^{k,g,t} - \sum_{bp \in BP} Q_i^{t,r,g,bp} \eta_{bp}^r = 0 ; \forall j \in Y, g \in G, r \in R, \forall t \in T$$
(3.1.106)

$$Q_i^{t,r,g,l} \le V_i^{t,r,g,l}; \ \forall i \in Y, \ g \in G, \ r \in R, \ \forall t \in T$$

$$(3.1.107)$$

$$Q_i^{t,r,g,2} \le V_i^{t,r,g,1} + V_i^{r,g,2} \; ; \; \forall i \in Y, \; g \in G, \; r \in R, \; \forall t \in T$$
(3.1.108)

$$Q_i^{t,r,g,3} \le V_i^{t,r,g,2} + V_i^{t,r,g,3} ; \ \forall i \in Y, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.109)

$$Q_i^{t,r,g,4} \le V_i^{t,r,g,3}; \ \forall i \in Y, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.110)

$$\sum_{bp\in B^P} \mathcal{Q}_i^{t,r,g,bp} = 1 ; \forall i \in Y, g \in G, r \in R, \forall t \in T$$
(3.1.111)

$$\sum_{i=l}^{bp-1} V_{}^{t,r,g,i} = 1 ; \ \forall i \in Y, \ g \in G, \ r \in R, \ \forall t \in T$$
(3.1.112)

Where:

$$\mathfrak{T}_{}^{t,g} = \sum_{k \in K} X_{}^{k,g,t} ; \forall < i,j> \in SL, t \in T, g \in G$$
(3.1.113)

$$\Delta_{\langle i,j\rangle}^{g} = \sum_{k \in K} \sum_{t \in T} X_{\langle i,j\rangle}^{k,g,t} ; \forall \langle i,j\rangle \in SL, \; \forall g \in G$$

$$(3.1.114)$$

$$\Delta^{} = \sum_{k \in K} \sum_{g \in G} \sum_{t \in T} X_{}^{k,g,t} ; \forall < i,j> \in SL$$
(3.1.115)

$$\varepsilon \rho^{} = \sum_{r \in R} \sum_{g \in G} \sum_{bp \in BP} \sum_{i \in T} \delta^{r}_{} \ \chi^{r}_{g} \ Y^{r,t,g,bp}_{} \ \Upsilon^{r}_{bp} \ l_{} \ \rho^{r}_{} \ ; \ \forall < i,j> \in SL$$
(3.1.116)

$$\varepsilon \rho^{i} = \sum_{r \in R} \sum_{g \in G} \sum_{bp \in BP} \sum_{t \in T} \xi_{y}^{r} \chi_{g}^{r} Q_{i}^{r,t,g,bp} \hat{\mathcal{X}} \qquad i \in Y$$
(3.1.117)

$$\wp_{}^{g,r,d} = \sum_{r \in R} \sum_{k \in K} \sum_{t \in T} X_{}^{k,g,t} c_g^{r,d} ; \forall < i,j> \in SL, \forall g \in G, r \in R, d \in dw$$
(3.1.118)

$$\Pi_{i}^{g} = \sum_{k \in K} \sum_{i \in T} \sum_{\langle j, i \rangle \in Sl} X_{\langle j, i \rangle}^{k,g,i} + \sum_{k \in K} \hat{o}_{i}^{k} b^{y,k,g} ; \forall i \in Y, g \in G, r \in R$$
(3.1.119)

$$\varphi_i^{g,r,d} = \prod_i^g c_g^{r,d} \; ; \; i \in Y, \; g \in G, \; r \in R, \; d \in dw$$
(3.1.120)

The objective function of the model, (3.1.87), is comprised of six terms; the first four terms are computing the cost of transportation comprising of travel costs, yard operations costs, and train fixed costs. The fifth and sixth terms, on the other hand, account for the population exposure risk at service-legs and yards, respectively. Depending on the decision makers' policy and considerations, the weights on transportation costs, α , and risk weight, β , are determined. Thus, for different values of α and β , a set of nondominated Pareto-optimal paths will be obtained.

Constraints (3.1.88) enforce that flow can pass through a rail segment iff that service-leg has been defined as a service-leg of a train service. Set of constraints (3.1.89) are flow conservation / mass balance constraints, which enforce all demands to be met. constraints (3.1.90) enforce regulatory restriction on the maximum number of Hazmat of each type to be loaded on each train-service; as well, this set of constraints enforce the minimum number of train services required to meet all weekly demands. constraints (3.1.91) enforce upper limits on arc load of each type of commodities; constraints (3.1.92) enforce limits on the total number of railcars of any type of commodities traversing through each arc; constraints (3.1.93) enforce upper limits on yard load of each type of commodities traversing through each yard; constraints (3.1.95) enforce the limit on the concentration of Hazmats of each type to be less than the IDLH limit at a predefined downwind distance from any given arc; constraints (3.1.96) enforce the limit on the concentration of Hazmats

of each type to be less than the IDLH limit at a predefined downwind distance from any given yard. Set of constraints (3.1.97) and (3.1.98) enforce the maximum tolerable population exposure at service-legs and yards of the underlying network of the problem under study, respectively; these constraints ensure that the risk on a service-leg and yards cannot exceed a predefined proportion of total risk of service-legs and yards, depending on the value of ζ and ϕ set by the authorities.

Constraints (3.1.99) to (3.1.105) are used to linearize the nonlinear dispersion radius function for any given rail segment. Constraints (3.1.106) to (3.1.112) are used to linearize the nonlinear dispersion radius function for any given yard.

Constraints (3.1.113) to (3.1.120) are used to define the decision expressions we made use of in previous constraints.

3.3.2. Biobjective with Non-Bifurcated Flows

$$Minimize \begin{pmatrix} Cost: \alpha \begin{bmatrix} \sum_{\langle i,j \rangle \in SL} \sum_{k \in K} \sum_{g \in G} \sum_{t \in T} Z_{\langle i,j \rangle}^{k,t} d^{k,g} l_{\langle i,j \rangle} tc + \\ \begin{bmatrix} \sum_{\langle i,j \rangle \in SL} \sum_{k \in K} \sum_{g \in G} \sum_{t \in T} \sum_{y \in YT} \psi_{i}^{yt} YC^{yt} Z_{\langle i,j \rangle}^{k,t} d^{k,g} + \sum_{k \in K} d_{k} y^{tr} \end{bmatrix} + \\ \sum_{t \in T} \sum_{\langle i,j \rangle \in SL} (fc_{t}/c) N^{t} \tau_{\langle i,j \rangle}^{t} l^{\langle i,j \rangle} l^{\langle i,j \rangle} \\ Risk: \beta \begin{bmatrix} \sum_{\langle i,j \rangle \in SL} \sum_{t \in T} \sum_{r \in R} \sum_{g \in G} \sum_{bp \in BP} \delta_{\langle i,j \rangle}^{r} \chi_{g}^{r} Y_{\langle i,j \rangle}^{t,r,g,bp} Y_{bp}^{r} l_{\langle i,j \rangle} \rho_{\langle i,j \rangle}^{r} \end{bmatrix} + \\ \begin{bmatrix} \sum_{i \in Y} \sum_{t \in T} \sum_{r \in R} \sum_{g \in G} \sum_{bp \in BP} \delta_{i}^{r} (\chi_{g}^{r})^{2} Q_{i}^{t,r,g,bp} \chi_{g}^{r} \end{bmatrix} \end{pmatrix}$$
(3.1.121)

Subject to:

$$Z_{\langle i,j \rangle}^{k,t} \le \tau_{\langle i,j \rangle}^{t} ; \forall k \in K, \ t \in T, \ \langle i,j \rangle \in SL$$
(3.1.122)

$$\sum_{\langle i,j\rangle\in SL}\sum_{t\in T} \tau_{\langle i,j\rangle}^{t} Z_{\langle i,j\rangle}^{k,t} d^{k,g} - \sum_{\langle j,i\rangle\in SL}\sum_{t\in T} \tau_{\langle j,i\rangle}^{t} Z_{\langle j,i\rangle}^{k,t} d^{k,g} = b_{i}^{k,g} d^{k,g} ; \forall i \in Y, \ \forall k \in K, \ \forall g \in G$$
(3.1.123)

$$\mathfrak{I}_{\langle i,j\rangle}^{t,g} \leq N^{t} u^{t,g} \; ; \; \forall \; t \in T, \; \forall < i,j > \in SL \; , \; \forall \; g \in G \tag{3.1.124}$$

$$\sum_{t \in T} Z_{\langle i,j \rangle}^{k,t} \leq l \; ; \; \forall k \in K, \; \forall \langle i,j \rangle \in SL$$
(3.1.125)

$$\Delta^{g}_{} \le u^{g}_{} ; \ \in SL , \ \forall g \in G$$
(3.1.126)

$$\Delta^{} \le u^{} ; \in SL$$
(3.1.127)

$$\Pi_i^g \le \upsilon_i^g \; ; \; \forall i \in Y, \; \forall g \in G \tag{3.1.128}$$

$$\Pi_i \le \upsilon^i \; ; \; \forall i \in Y \tag{3.1.129}$$

$$\wp_{\langle i,j\rangle}^{g,r,d} \le \theta^g; \ \forall < i,j\rangle \in SL, \ \forall g \in G, \ r \in R, \ \forall d \in DW$$
(3.1.130)

$$\varphi_i^{g,r,d} \le \theta^g \; ; \; \forall i \in Y, \; \forall g \in G, \; r \in R, \; \forall d \in DW$$
(3.1.131)

$$\varepsilon \rho^{\langle i,j \rangle} \leq \zeta \sum_{\langle m,n \rangle \in SL} \varepsilon \rho^{\langle m,n \rangle} ; \; \forall \langle i,j \rangle \in SL$$
(3.1.132)

$$\varepsilon \rho^{i} \le \phi \sum_{j \in Y} \varepsilon \rho^{j} \quad \forall i \in Y$$
(3.1.133)

$$\sum_{k \in \mathcal{K}} Z_{\langle i, j \rangle}^{k, g} d^{k, g} - \sum_{bp \in BP} Y_{\langle i, j \rangle}^{i, r, g, bp} \eta_{bp}^{r} = 0 ; \forall \langle i, j \rangle \in SL, g \in G, r \in R, t \in T$$
(3.1.134)

$$Y_{}^{t,r,g,l} \le W_{}^{t,r,g,l}; \ \forall < i,j> \in SL, \ g \in G, \ r \in R, \ t \in T$$
(3.1.135)

$$Y_{\langle i,j \rangle}^{t,r,2} \le W_{\langle i,j \rangle}^{t,r,g,l} + W_{\langle i,j \rangle}^{t,r,g,2} ; \forall < i,j > \in SL, g \in G, r \in R, t \in T$$
(3.1.136)

$$Y_{}^{t,r,g,3} \le W_{}^{t,r,g,2} + W_{}^{t,r,g,3}; \ \forall < i,j> \in SL, \ g \in G, \ r \in R, \ t \in T$$
(3.1.137)

$$Y_{}^{t,r,g,4} \le W_{}^{t,r,g,3}; \ \forall < i,j> \in SL, \ g \in G, \ r \in R, \ t \in T$$
(3.1.138)

$$\sum_{bp \in BP} Y_{\langle i,j \rangle}^{t,r,g,bp} = 1 ; \forall \langle i,j \rangle \in SL, g \in G, r \in R, t \in T$$
(3.1.139)

$$\sum_{i=1}^{bp-1} W_{}^{t,r,g,i} = 1 ; \forall < i,j> \in SL, g \in G, r \in R, t \in T$$
(3.1.140)

$$\Pi_{i}^{g} - \sum_{bp \in B^{p}} Q_{i}^{t,r,g,bp} \ \eta_{bp}^{r} = 0 \ ; \ \forall i \in Y, \ g \in G, \ r \in R, \ t \in T$$
(3.1.141)

$$Q_i^{t,r,g,l} \le V_i^{t,r,g,l}; \ \forall i \in Y, \ g \in G, \ r \in R, \ t \in T$$
(3.1.142)

$$Q_i^{t,r,g,2} \le V_i^{t,r,g,1} + V_i^{t,r,g,2} ; \forall i \in Y, g \in G, r \in R, t \in T$$
(3.1.143)

$$Q_i^{t,r,g,3} \le V_i^{t,r,g,2} + V_i^{t,r,g,3} ; \forall i \in Y, g \in G, r \in R, t \in T$$
(3.1.144)

$$Q_i^{t,r,g,4} \le V_i^{t,r,g,3}; \ \forall i \in Y, \ g \in G, \ r \in R, \ t \in T$$
(3.1.145)

$$\sum_{bp\in BP} Q_i^{t,r,g,bp} = 1 ; \forall i \in Y, g \in G, r \in R, t \in T$$

$$(3.1.146)$$

$$\sum_{i=1}^{bp-l} V_{}^{t,r,g,i} = 1 ; \forall i \in Y, g \in G, r \in R, t \in T$$
(3.1.147)

Where:

$$\mathfrak{T}_{}^{i,g} = \sum_{k \in K} Z_{}^{k,t} d^{k,g} ; \forall < i,j> \in SL, t \in T, g \in G$$
(3.1.148)

$$\Delta_{}^{g} = \sum_{k \in K} \sum_{i \in T} Z_{}^{k,t} d^{k,g} ; \forall < i,j> \in SL, \forall g \in G$$
(3.1.149)

$$\Delta^{} = \sum_{k \in K} \sum_{g \in G} \sum_{t \in T} Z^{k,t}_{} d^{k,g} ; \forall < i,j> \in SL$$
(3.1.150)

$$\Pi_{i}^{g} = \sum_{k \in K} \sum_{t \in T} \sum_{\langle j, i \rangle \in SI} Z_{\langle i, j \rangle}^{k, t} d^{k, g} + \sum_{k \in K} \partial_{i}^{k} b^{y, k, g} d^{k, g} ; \forall i \in Y, g \in G, r \in R$$
(3.1.151)

$$\varepsilon \rho^{} = \sum_{r \in \mathbb{R}} \sum_{g \in G} \sum_{bp \in BP} \delta^{r}_{} \chi^{r}_{g} Y^{t,r,g,bp}_{} \Upsilon^{r}_{bp} l_{} \rho^{r}_{} ; \forall \in SL$$
(3.1.152)

$$\varepsilon \rho^{i} = \sum_{r \in R} \sum_{g \in G} \sum_{bp \in B^{P}} \hat{O}_{i}^{r} \chi_{g}^{r} Q_{i}^{t,r,g,bp} \hat{\mathcal{X}} \qquad i \in Y$$
(3.1.153)

$$\wp_{}^{g,r,d} = \sum_{r \in R} \sum_{k \in K} \sum_{t \in T} Z_{}^{k,t} d^{k,g} c_g^{r,d} ; \forall < i,j> \in SL, \forall g \in G, r \in R, d \in DW$$
(3.1.154)

$$\varphi_i^{g,r,d} = \Pi_i^g \ c_g^{r,d} \ ; \ i \in Y, \ g \in G, \ r \in R, \ d \in DW$$
(3.1.155)

The developed model in the current subsection, assumes shortest path for conveying each trafficclass from its origin to its destination, thereby restricting the slit of flows. Comparing this problem with the previous one, all constraints are the same except the constraints (3.1.125) which enforce that each traffic-class cannot be carried by more than one train on each track segment.

It is to mention that in terms of the complexity of the problem under study, based on Even et al (1975) and *Garey and Johnson (1979)*, the multicommodity routing problem with integral flows, is NP-complete even if the number of commodities is two.

In chapter 4, experiments will be carried out on the same network with all presented model variants, and results will be reported, which may shed light onto the pros and cons of each modeling approach.

Chapter 4

4. Computational Experiments and Problem Setting

Throughout this chapter of the dissertation experiments will be carried out to demonstrate the functionality of the mathematical models that have been developed in the previous chapter. As well, we will obtain managerial insights into the network design and route planning decisions, risk mitigation techniques and tactical planning of railways transportation of dangerous goods and regular commodities.

4.1. Parameters Estimation

In order to compute the population exposure, we made use of dispersion parameters of *Tadmor* and *Gur (1967)*, Figure A-9, considering weather stability condition PG: A and PG: E, for urban and rural areas, respectively. Rate of release of the Hazmat contents of the railcars can be computed by running various scenarios in ALOHA⁴ software which is offered by EPA, United States Environmental Protection Agency, and is widely used in risk response planning concerning chemical emergencies. *Verma and Verter (2007)* suggested that a 24-inch rupture on all Hazmat railcars since it can be assumed to be the worst case scenario; hence, considering the worst case scenario for the diameter of the rupture, we ran ALOHA for each type of Hazmats under study, Propane and Butane, which have several similarities regarding various aspects such as their chemical characteristics, transportation, demands and applications. Figure B-1 to Figure B-8 demonstrate the results of running ALOHA software for Propane and Butane in both urban and

⁴ https://www.epa.gov/cameo/aloha-software

rural vis open country environments, in weather stability classes PG: A and PG: E, respectively. It is significant to notice that considering the worst case scenario in evaluating risk of transportation of Hazmats in terms of population exposure, radius of dispersion of airborne contaminants affects the number of people exposed to the risk in case of incident, and the value of radius is greater in areas with more stable weather conditions. On the other hand, if we aim to compute Hazmat contaminant's concentration at a certain predefined radius from service-legs and yards, e.g. 800 meters from potential release spot, the worst-case scenario would be the most unstable weather condition, PG: A. Moreover, the least wind speed in any weather stability condition will result to the highest concentration of the contaminants at the vicinity of an incident spot.

Parameters of the problem such as transportation costs can be estimated from publicly available information or recent works such as *Ahuja et al (2007)*. For instance, based on *Ahuja et al (2007)*, we considered \$0.50 to move a railcar one mile, hence we assumed \$0.80 per kilometer per railcar. Fixed cost of all train services also have been considered to be \$500 per hour where the freight train speeds have been considered to be 22 miles per hour in average, which is almost 35.04 kilometers per hour for CN trains *Rail Performance Measures (2018)*.

According to *Statistics Canada, Census of Population (2011)*, if at least 1000 persons are living in a center or if a center has at least 400 persons per 1000 square meters, it falls into the category of population centers / urban area, otherwise, it is assumed to be rural. Hence, in our experiments, we assumed 400 and 150 persons per 1000 square meters as density of urban and rural areas respectively.

Like *Verma et al (2011)*, we also use randomly generated demand data roughly corresponding to the fuel oil consumption figures as reported by the Department of Energy (<u>http://tonto.eia.doe.gov</u>). Hence, to test the models with various data sets, for Case I, the order

sizes in our hypothetical order data may range between 10 to 30 railcars, wherein 5 to 15 railcars with Hazmat content of both types, Propane and Butane, may be included within each order. For Case II, however, we assumed the orders size can range between 3 to 15, wherein 2 to 10 railcars with Hazmat content of both types, Propane and Butane, may be included within each order. Moreover, it is to mention that all orders have been randomly generated using uniform probability distribution.

Moreover, while for various instances in our experiments to follow in this chapter we may consider different capacities for each of the train services, the volume of Hazmat contents to be loaded on each train, however, cannot exceed aggregate 150,000 imperial gallons amounting to 681,913.5 liters, to be complied with regulation of *Liquefied Petroleum Gases Bulk Storage Regulations C.R.C. c. 1152 (2018)*. Further, trains have been classified into three types of trains based on their capacity in terms of the number of railcars that they can carry; hence, we may have short, medium and long trains with (*capacity* < 40), (40 <*capacity* < 120) and (*capacity* > 120), respectively, *Bagheri et al (2011)*.

Furthermore, in each of the problem settings, other parameters and coefficients will be defined and elaborated on. As well, for the sake of simplicity and to avoid repetition, the models presented in subsections (3.2.1), (3.2.2), (3.3.1) and (3.3.2) will be referred to as P1, P2, P3 and P4, respectively.

4.2. Case I: Small Instances of the Problem

In this subsection, we will run small and medium instances of the problem on a network with seven yards and thirteen rail segments. For various number of train services and orders, we will be running the model and reporting the results, highlighting the major factors and insights. Further, we will compare the results of the multiobjective models, P3 and P4, and single-objective models, P1 and P2, separately.

Experiments have been done on a computer with an installed memory (RAM) of 16 GB, Intel [®] Core[™] i7 @ 3.4 GHz processor, and a 64-bit Windows 7 OS.

4.2.1. Description of Instances

Considering the sparse network depicted in Figure 4-1, models will be tested, and results will be reported throughout this subsection of the document.

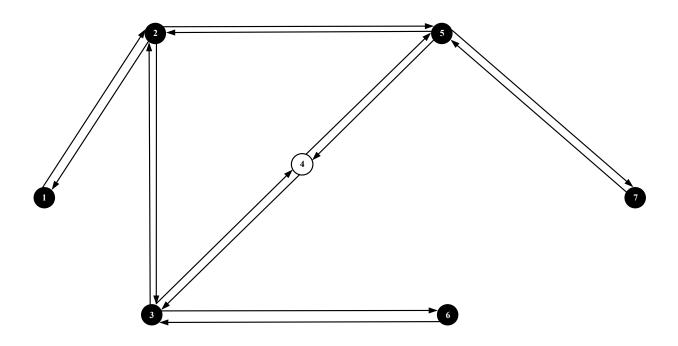


Figure 4-1: Hypothetical Network I, Case I

Yard	Remoteness: Urban / Rural
1	Urban
2	Urban
3	Rural
4	Urban
5	Urban
6	Rural
7	Urban

In the hypothetical network that has been depicted above, all yards except yard 4, have the

classification capability. Data of the five instances that have been considered for this network,

have been shown in the following tables:

D 11			
Rail	Proportion of Urban Areas	Proportion of Rural Areas	Length (km)
Segments	[0,1]	[0,1]	Length (Kill)
<1,2>	1.00	0.00	400
<2,5>	1.00	0.00	800
<5,7>	0.95	0.05	450
<2,5> <5,7> <2,3>	0.00	1.00	800
<3,6>	0.15	0.85	550
<3,4>	0.50	0.50	500
<3,4> <4,5>	0.05	0.95	500
<7,5>	0.05	0.95	450
<5,4>	1.00	0.00	500
<4,3>	0.50	0.50	400
<6,3>	0.00	1.00	550
<3,2>	0.95	0.05	700
<2,1> <5,2>	0.05	0.95	400
<5,2>	1.00	0.00	800

Table 4-2: Proportion of Urban and Rural Areas, and length of each Rail Segment

Table 4-3: Case I - Instance 1

Instance #1								
	Parameter		Value					
	ζ			0.50				
	¢			0.35				
	Р			400,000				
Number of Orders: 1								
Order No.	Origin	Destination	Order Size (railcars)					
Oldel No.		Destination	Regular	Propane	Butane			
1	1 4		11	5	5			
	Ν	Number of Train	Services: 4					
Train Service	Itina	40 M I	Capacity (railcars)					
No.	Itine	i ai y	Regular	Propane	Butane			
1	1-2-5-7		25	7	7			
2	2-3-6		25	7	7			
3	3-4	4-5	25	7	7			
4	7-5-	-4-3	40	7	7			

Instance #2							
	Parameter		Value				
	ζ			0.50			
	φ			0.35			
	Р			400,000			
Number of Orders:							
Order No.	Omicin	Destination -	Order Size (railcars)				
Order No.	Origin		Regular	Propane	Butane		
1	1 4		11	5	5		
	Ν	Number of Train	Services: 5				
Train Service	Itina	40 47 I	Capacity (railcars)				
No.	Itine	rary	Regular	Propane	Butane		
1	1-2-	-5-7	25	7	7		
2	2-3-6		20	7	7		
3	3-4-5		25	7	7		
4	7-5-	-4-3	40	7	7		
5	1-2-	-5-4	25	7	7		

Table 4-4: Case I - Instance 2

Table 4-5: Case I - Instance 3

Instance #3						
	Parameter		Value			
	ζ			0.40		
	φ			0.40		
	Р			400,000		
		Number of O	rders: 6			
Order No.				der Size (railcar	rs)	
Order No.	Origin	Destination	Regular	Propane	Butane	
1	1	3	16	3	7	
2	1	4	11	5	5	
3	5	4	10	10	7	
4	2	7	8	3	1	
5	2	3	10	7	4	
6	1	6	15	4	6	
	Ν	Number of Train	Services: 5			
Train Service	Itina	40 M I	Capacity (railcars)			
No.	Itine	rary	Regular	Propane	Butane	
1	1-2-	-5-7	25	7	7	
2	2-3-6		20	7	7	
3	3-4-5		25	7	7	
4	7-5-	-4-3	40	7	7	
5	6-	-3	25	7	7	

		Instance	#4			
	Parameter		Value			
	ζ			0.30		
	φ			0.30		
	P			500,000		
	1	Number of O	orders: 6	500,000		
				der Size (railcar	s)	
Order No.	Origin	Destination	Regular	Propane	Butane	
1	1	1 3		3	7	
2	1 4		11	5	5	
3	5	4	10	10	7	
4	2	7	8	3	1	
5	2	3	10	7	4	
6	1	6	15	4	6	
	Ν	Number of Train	Services: 6			
Train Service	Itina	140 HT I	Capacity (railcars)			
No.	Itine	stat y	Regular	Propane	Butane	
1	1-2-	-5-7	25	7	7	
2	2-3	3-6	20	7	7	
3	6-3-4-5		25	7	7	
4	7-5-4-3		40	7	7	
5	2-5	5-4	25	7	7	
6	7-5-	-2-1	25	7	7	

Table 4-6: Case I - Instance 4

Table 4-7: Case I - Instance 5

Instance #5							
	Parameter		Value				
	ζ			0.20			
	φ			0.20			
	Р			2,000,000			
		Number of Or	rders: 42				
Order No.	Origin	Destination	Order Size (railcars)				
Oldel No.	Origin		Regular	Propane	Butane		
1	1	2	10	2	1		
2	1	3	7	4	2		
3	1	4	5	4	3		
4	1	5	11	3	4		
5	1	6	8	3	4		
6	1	7	5	1	4		
7	2	1	6	3	3		
8	2	3	12	1	3		
9	2	4	9	2	1		

	0.1.1		Order Size (railcars)		
Order No.	Origin	Destination	Regular Propane 5 7 4 5 15 2 7 5 2 1 5 3 2 8 2 4 12 2 5 7 4 5 3 2 8 2 14 5 7 4 5 7 4 5 7 4 6 14 3 7 7 2 1 7 3 2 5 1 5 5 1 6 5 2 7 10 3 1 15 1 2 14 3 3 6 2 4 15 1 7 15 4 3 5 1 2 11 4 <td>Butane</td>	Butane	
10	2	5	7		4
11	2	6	15	2	3
12	2	7		2	1
13	3	1			3
14	3	2	8		3
15	3	4	12	2	2
16	3	5	7		3
17	3	6			3
18	3	7			2
19	4	1	7	3	4
20	4	2	5	1	4
21	4	3	11	4	3
22	4	5		1	1
23	4	6	5	2	1
24	4	7	10	3	3
25	5	1	15	1	4
26	5	2	14	3	3
27	5	3	6	2	4
28	5	4	15	1	2
29	5	6	15	1	2
30	5	7	15	4	3
31	6	1	5	1	4
32	6	2	11	4	3
33	6	3	5	1	1
34	6	4	9	2	1
35	6	5	7	4	4
36	6	7	15	2	3
37	7	1	5	4	3
38	7	2	11	3	4
39	7	3	8	3	4
40	7	4	11	4	3
41	7	5	5	1	1
42	7	6	9	2	1
	<u> </u>	Number of Train			
Train Service	Itine		C	apacity (railcars)
No.			Regular	Propane	Butane
1		-5-7	25	7	7
2		3-6	25	7	7
3		4-5	25	7	7
4		-4-3	25	7	7
5	6-3-	-2-1	25	7	7

Table 4-8: Case I - Instance 5 (Cont'd)

Instance #6									
	Number of Train Services: 6								
Train Service	Itinerary		Capacity (railcars	5)					
No.	Itilierary	Regular	Propane	Butane					
1	1-2-5-7	25	7	7					
2	2-3-6	20	7	7					
3	3-4-5	25	7	7					
4	7-5-4-3	40	7	7					
5	1-2-3-4	25	7	7					
6	2-5-4	25	7	7					
7	7-5-2-1	25	7	7					
8	6-3-2-1	25	7	7					
9	6-3-4-5	25	7	7					
10	5-2-3	25	7	7					

Table 4-9: Train Service for Instance 6

Data set of instances 5 and 6 are similar except that we have increased the number of train services from 5 to 10, as well as modifying the itineraries of train services to investigate the correlation between the number of train services and risk and cost values.

4.2.2. Computational Results (Case I)

For the models with multiobjective function, P3 and P4, we have defined the following weights for the terms of cost and risk in the objective function as shown in Table 4-10.

Weight Legend	α	β
Min Cost	1.00	0.00
А	0.90	0.10
В	0.80	0.20
С	0.70	0.30
D	0.60	0.40
Base Case	0.50	0.50
E	0.40	0.60
F	0.30	0.70
G	0.20	0.80
Н	0.10	0.90
Min Risk	0.00	1.00

Table 4-10: Cost and Risk Weights

Reports on the average run time, total cost of transportation (travel cost, yard operations cost and train fixed costs), under various weighting scenarios as depicted above, have been reported in the following tables. It is to mention that the number of people exposed to the risk of transportation of Propane and Butane Hazmat railcars have been reported in order, for each cost and risk weighting policy, in the column of risk. Since, to the best of our knowledge, the interaction of the chemicals under study and the consequences of such interactions on increasing the risk of population exposure have not been studied thoroughly, population exposure due to transportation of each type of Hazmats has been reported separately.

4.2.2.1. Computational Results of Single-objective Models

The results of running the model variants P1 and P2, for all of the instances have been reported in Table 4-11; in the risk column, table cells in gray represent risk due to transportation of propane, and those in white, represent the risk due to shipping Butane railcars.

		P1				P2				
Instance	Avg. Time	Cost \$ 1E6		ersons E6	No. of Trains	Avg. Time	Cost \$ 1E6		ersons E6	No. of Trains
	(S)	ILO	Propane	Butane	TTams	(S)	TEO	Propane	Butane	Trains
1	0.01	0.08	0.14	0.15	2	0.01	0.09	0.18	0.20	2
2	0.02	0.08	0.15	0.16	2	< 0.01	0.09	0.20	0.21	2
3	0.14	0.31	0.55	0.65	8	0.19	0.33	0.55	0.65	8
4	0.14	0.31	0.57	0.68	8	0.38	0.32	0.59	0.70	8
5	0.75	1.10	1.78	2.52	22	1.20	1.15	1.85	2.30	22
6	24.76	0.96	1.82	2.21	19	1630	0.97	1.80	2.17	19

Table 4-11: Computational Results of P1 & P2: Case I

The results of the experiments that have been summarized in Table 4-11, can give a better understanding of the advantages and disadvantages of each modeling approach if one compares the values of instances 1, 3 and 5 with those of instances 2, 4 and 6, for each of the model variants as well as comparing the figures associating with P1 with those of P2.

4.2.2.2. Computational Results of Multiobjective Models

This subsection of the document, provides the reader with the computational results associating with the multiobjective model variants. Based on the weights of cost and risk terms, as defined and labeled in Table 4-10, results of the experiments for both model variants, P3 and P4, and for various instances, have been reported in the following tables. Results associating with experiments carried out using data of instances 1, 3 and 5, should be compared with those pertaining to instances 2, 4 and 6, respectively.

	Р3					P4					
Weights	Avg. Time	Cost \$ 1E6		ersons E6	No. of Trains	Avg. Time			Risk Persons 1E6		
	(S)	ILU	Propane	Butane	Tams	(S)	ILU	Propane	Butane	Trains	
Min Cost	0.02	0.75	0.12	0.13	2	0.02	0.75	0.12	0.13	2	
А	0.02	0.75	0.12	0.13	2	< 0.01	0.75	0.12	0.13	2	
В	0.02	0.75	0.12	0.13	2	< 0.01	0.75	0.12	0.13	2	
С	0.02	0.75	0.12	0.13	2	0.01	0.75	0.12	0.13	2	
D	0.02	0.75	0.12	0.13	2	0.01	0.75	0.12	0.13	2	
Base Case	0.02	0.75	0.12	0.13	2	0.02	0.75	0.12	0.13	2	
Е	0.02	0.75	0.12	0.13	2	< 0.01	0.75	0.12	0.13	2	
F	0.02	0.75	0.12	0.13	2	< 0.01	0.75	0.12	0.13	2	
G	0.02	0.75	0.12	0.13	2	0.02	0.75	0.12	0.13	2	
Н	0.02	0.75	0.12	0.13	2	0.01	0.75	0.12	0.13	2	
Min Risk	0.02	0.75	0.12	0.13	2	0.01	0.75	0.12	0.13	2	

Table 4-12: Computational Results - P3 & P4 - Instances 1

			P3			P4					
Weights	Avg. Time	Cost \$ 1E6		ersons E6	No. of Trains	Avg. Time	Cost \$ 1E6		ersons E6	No. of Trains	
	(S)	ILO	Propane	Butane	Trains	(S)	ILO	Propane	Butane	Trains	
Min Cost	0.94	0.06	0.12	0.13	1	< 0.01	0.06	0.12	0.13	1	
А	2.53	0.06	0.12	0.13	1	0.58	0.06	0.12	0.13	1	
В	3.24	0.06	0.12	0.13	1	0.53	0.06	0.12	0.13	1	
С	0.80	0.06	0.12	0.13	1	0.56	0.06	0.12	0.13	1	
D	0.48	0.06	0.12	0.13	1	0.42	0.06	0.12	0.13	1	
Base Case	0.56	0.06	0.12	0.13	1	0.45	0.06	0.12	0.13	1	
Е	0.47	0.06	0.12	0.13	1	0.41	0.06	0.12	0.13	1	
F	0.42	0.06	0.12	0.13	1	0.48	0.06	0.12	0.13	1	
G	0.37	0.06	0.12	0.13	1	0.44	0.06	0.12	0.13	1	
Н	0.36	0.06	0.12	0.13	1	0.28	0.06	0.12	0.13	1	
Min Risk	0.14	0.13	0.12	0.13	5	0.33	0.08	0.12	0.13	2	

Table 4-13: Computational Results - P3 & P4 - Instances 2

Table 4-14: Computational Results - P3 & P4 - Instance 3

	Р3					P4				
Weights	Avg. Time	Cost \$ 1E6	Risk P 1I	ersons E6	No. of Trains	Avg. Time				No. of Trains
	(S)	ILO	Propane	Butane	Trains	(S)	ILO	Propane	Butane	Trains
Min Cost	0.2	0.31	0.54	0.65	8	0.11	0.33	0.54	0.63	8
А	0.26	0.31	0.54	0.65	8	0.13	0.33	0.54	0.63	8
В	0.25	0.31	0.54	0.65	8	0.16	0.33	0.54	0.63	8
С	0.23	0.31	0.54	0.65	8	0.17	0.34	0.54	0.63	8
D	0.23	0.35	0.54	0.65	8	0.09	0.34	0.54	0.63	8
Base Case	0.2	0.35	0.54	0.65	8	0.11	0.34	0.54	0.63	8
Е	0.13	0.35	0.54	0.65	8	0.09	0.41	0.51	0.60	10
F	0.16	0.35	0.52	0.61	8	0.13	0.41	0.51	0.60	10
G	0.14	0.39	0.51	0.60	10	0.09	0.41	0.51	0.60	10
Н	0.11	0.39	0.51	0.60	10	0.13	0.41	0.51	0.60	10
Min Risk	0.16	0.41	0.51	0.60	10	0.09	0.41	0.51	0.60	10

			P3			P4				
Weights	Avg. Time	Cost \$ 1E6	Risk P 1H	ersons E6	No. of Trains	Avg. Time	Cost \$ 1E6		ersons E6	No. of Trains
	(S)	TEO	Propane	Butane	TTams	(S)	ILO	Propane	Butane	TTallis
Min Cost	1.22	0.31	0.57	0.68	8	0.34	0.32	0.58	0.68	8
А	3.34	0.31	0.58	0.68	8	0.5	0.33	0.58	0.68	8
В	2.21	0.31	0.56	0.65	8	0.5	0.33	0.55	0.65	8
С	0.67	0.31	0.55	0.65	8	0.56	0.34	0.55	0.65	8
D	0.56	0.35	0.55	0.65	8	0.39	0.34	0.55	0.65	8
Base Case	0.45	0.35	0.55	0.65	8	0.41	0.34	0.52	0.65	8
Е	0.47	0.35	0.54	0.65	8	0.42	0.41	0.52	0.63	10
F	0.36	0.35	0.51	0.61	8	0.4	0.41	0.52	0.63	10
G	0.39	0.39	0.51	0.61	10	0.44	0.41	0.52	0.63	10
Н	0.33	0.39	0.51	0.51	10	0.42	0.41	0.52	063	10
Min Risk	0.3	0.51	0.51	0.61	10	0.39	0.44	0.52	0.63	12

Table 4-15: Computational Results - P3 & P4 - Instance 4

Table 4-16: Computational Results - P3 & P4 - Instance 5

	Р3				P4					
Weights	Avg. Time	Cost \$ 1E6		ersons E6	No. of Trains	Avg. Time	Cost \$ 1E6		ersons E6	No. of Trains
	(S)	ILO	Propane	Butane	Trains	(S)	ILO	Propane	Butane	Trains
Min Cost	0.9	1.11	1.78	2.25	22	0.22	1.15	1.85	2.30	22
А	0.65	1.11	1.67	2.25	22	0.34	1.16	1.78	2.30	22
В	0.55	1.16	1.67	2.16	22	0.64	1.21	1.78	2.21	24
С	0.62	1.22	1.67	2.25	24	0.25	1.21	1.68	2.21	24
D	0.62	1.22	1.67	2.16	25	0.36	1.28	1.68	2.07	25
Base Case	0.51	1.22	1.58	1.93	25	0.4	1.31	1.68	2.07	27
Е	0.42	1.25	1.58	1.93	25	0.36	1.31	1.68	2.07	27
F	0.47	1.25	1.58	1.93	26	0.39	1.34	1.63	2.07	28
G	0.31	1.29	1.58	1.93	26	0.33	1.34	1.63	2.00	28
Н	0.53	1.33	1.58	1.93	28	0.36	1.38	1.60	2.00	29
Min Risk	0.9	1.33	1.57	1.91	30	0.33	1.38	1.60	1.99	29

			P3			P4					
Weights	Avg. Time	Cost \$ 1E6	Risk P 1I	ersons E6	No. of Trains	Avg. Time	Cost \$ 1E6		ersons E6	No. of Trains	
	(S)	ILO	Propane	Butane	TTams	(S)	ILO	Propane	Butane	Trains	
Min Cost	2.06	0.96	1.80	2.16	19	2.73	0.97	1.83	2.18	19	
А	39.8	0.97	1.75	2.13	19	29.28	0.97	1.79	2.16	19	
В	53.06	0.97	1.75	2.13	19	44.54	0.99	1.76	2.14	19	
С	44.72	1.01	1.75	2.06	20	33.32	1.08	1.66	1.99	21	
D	40.92	1.12	1.75	1.93	23	33.71	1.09	1.64	1.98	21	
Base Case	39.8	1.12	1.67	1.93	23	28.45	1.16	1.61	1.93	23	
Е	36.22	1.12	1.67	1.93	23	27.6	1.16	1.61	1.93	23	
F	41.21	1.12	1.60	1.93	23	26.96	1.17	1.60	1.93	23	
G	34.43	1.20	1.60	1.91	26	30.8	1.20	1.60	1.92	24	
Н	32.87	1.25	1.60	1.91	28	18.97	1.27	1.59	1.91	25	
Min Risk	17.96	1.62	1.60	1.91	41	38.28	1.40	1.59	1.91	31	

Table 4-17: Computational Results - P3 & P4 - Instance 6

4.2.3. Analysis of the Experiments and Insights – Case I

While the results of experiments for all model variants with all instances have been reported in the previous subsections, our concentration will be more focused on the results of the last instance.

Results of experiments indicate that for the smaller instances of the problem with fewer number of orders and available train services, there is negligible discrepancy between the values of cost and risk in P3 and P4. For the larger instance of the problem with 42 orders and 10 available train service, however, there is a distinguishable discrepancy in those values associated with P3 and P4. To elaborate more and considering the results of instance 6, we see that the *min cost* solution to P4, entails cost of \$0.97E6 and exposes 1.83E6 people (due to Propane) and 2.18E6 people (due to Butane) whereas the *min cost* solution to P3, will cost \$0.96E6 and exposes 1.80E6 (due to Propane) and 2.16E6 (due to Butane) people. The *min risk* solution to P3 and P4, on the other hand, entail a cost of \$1.62 and \$1.40 million, respectively. The *min risk* solutions to P4 also exposes 1.59 and 1.91 million people due to transportation of Propane and Butane, respectively, while those value for P3 are 1.60 and 1.91 million people due to shipping Propane and Butane, respectively. Moreover, considering solution to the *Base Case*, we observe that not only the transportation cost of P3 is lower than that of P4, but also, the risk number for Butane is lower than that of P4, which effectively demonstrates the advantages of P3 over P4 which stems from the more choices that it offers in routing decisions for each railcar. This is also the case, as we compare the figures associating with P1 and P2 in Table 4-11.

In addition, considering P3 and risk due to Propane, as we increase the coefficient of risk term in the objective function from 0% to 10%, or in other words, by spending an extra \$5K, we can put approximately 45K fewer people into the risk due to transportation of Propane railcars, which can be translated to spending every extra \$1 can save almost 9 people. Similarly, considering P4 and risk due to Propane, as we increase the coefficient of risk term in the objective function from 0% to 20%, or in other words, by spending an extra \$12K, we can put approximately 67K fewer people into the risk due to transportation of Propane railcars, which can be translated to spending every extra \$1 can save almost 6 people. As well, considering P3 and risk due to Butane, as we increase the coefficient of risk term in the objective function from 0% to 10%, or in other words, by spending an extra \$5K, we can put approximately 33K fewer people into the risk due to transportation of Butane railcars, which can be translated to spending every extra \$1 can save almost 7 people. Similarly, considering P4 and risk due to Butane, as we increase the coefficient of risk term in the objective function from 0% to 20%, or in other words, by spending an extra \$12K, we can put approximately 43K fewer people into the risk due to transportation of Butane railcars, which can be translated to spending every extra \$1 can save almost 4 people.

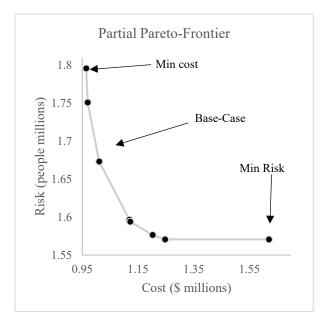


Figure 4-5: (Quasi-) Pareto Solutions, Instance 6, P3, Propane

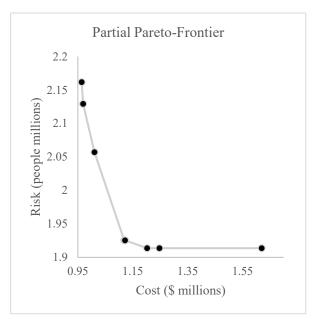


Figure 4-5: (Quasi-) Pareto Solutions, Instance 6, P3, Butane

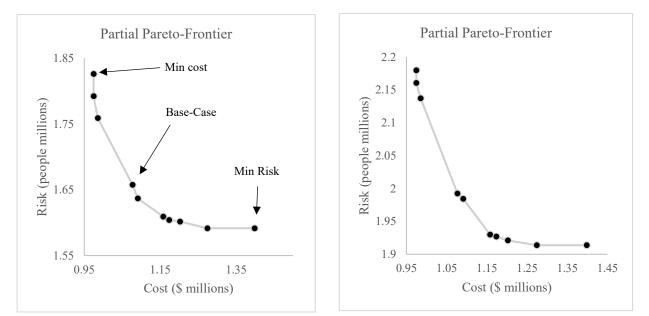


Figure 4-5: (Quasi-) Pareto Solutions, Instance 6, P4, Propane

Figure 4-5: (Quasi-) Pareto Solutions, Instance 6, P4, Butane

The figures, demonstrate a portion of possible Pareto frontier, which could be considered on the course of risk and cost quantification and evaluation of monetary and societal ramifications of Hazmat transportation. Moreover, considering instance 6, if we look at the cost and risk values of P1, Table 4-11, and P3, Table 4-17, we can see that using fewer number of trains, 19 compared with 41 trains in P3, decreases the cost by 59.3% at the expense of increasing the risk due to

transportation of Propane and Butane by 113.75% and 114.5%, respectively. In the same fashion, considering instance 6, if we look at the cost and risk values of P2, Table 4-11, and P4, Table 4-17, one can see that using fewer number of trains, 19 compared with 31 trains in P4, decreases the cost by 69.3% at the expense of increasing the risk due to transportation of Propane and Butane by 113.2% and 113.6%, respectively.

Further, to elaborate more on the parameters setting for various instances, ζ' , ϕ' and P, we need to consider the sparsity of the hypothetical network which provides the decision maker with fewer routing possibilities, hence increasing the risk at yards and on service-legs of the train services; as a result, lower values of the above-mentioned parameters increase the chances of infeasibility. However, for larger instances of the problem with more service-legs and yards, lower values can be set for those parameter which leads to better risk mitigation and lower possibility of infeasibility while increasing the computational effort. However, since this dissertation concentrates more on various modeling approaches that can be taken in modeling the problem under study rather than developing a solution approach using exact algorithms or heuristic methods, focusing on the computational effort in this document has not been given a high priority. Nonetheless, carrying out experiments indicated that those constraints concerning the risk on service-legs and yards, as well as the total risk, as complicating constraints, can be made use of by decision makers and authorities in achieving risk equity and risk mitigation strategy on the course of tactical planning of Hazmats transportation.

Furthermore, our observation shows that weather stability condition can extensively affect the routing decisions. Although Gaussian Plume Model have gained popularity by researchers and have been commonly used in the Hazmat transportation literature, our findings imply that the resultant decisions might be different from what authorities and / or society may be expecting

regarding the routing of Hazmat railcars as the risk term is computed using GPM. That is, while one could expect the priority in routing the Hazmat railcars is to route them through rural / open country rather than routing them through urban areas / population centers, our results suggest that this may not always be the case if we make use of GPM. In other words, if we consider population density is evenly distributed in both urban and rural areas, there are chances that transporting Hazmats through rural areas leads to higher risk since the crosswind and horizontal dispersion of buoyant are way lower in more stable weather conditions which leads to greater dispersion radius of the airborne contaminants, thereby exposing more people to the risk of evacuation, injury or death. For instance, considering our hypothetical network and instance 1, for the order, 1/3, there are two possible routes which traverse through either yards 1-2-3 or through yards 1-2-5-4-3; the former is passing through rural areas and the latter rout is passing through urban areas where the density of population is greater than the first route. However, surprisingly, the optimal route for Hazmat commodities of this order has been the second route which passes through urban areas. Hence, although the concentration of Hazmats decreases by distance from the release spot, and the farther from incident spot the lower the chance of fatality, but Hazmat contaminants will spread farther at the downwind distance where the weather is more stable, which leads to greater number of exposed people.

4.3. Case II: Larger Instance of the Problem

In this subsection, a large instance of the problem is presented and the computational results for P1, P2, P3 (base case) and P4 (base case) are summarized in Table 4-19. The network, Figure 4-6, has 25 nodes which can be origin and / or destination of orders; thus, 600 possible orders have been generated using uniform distribution.

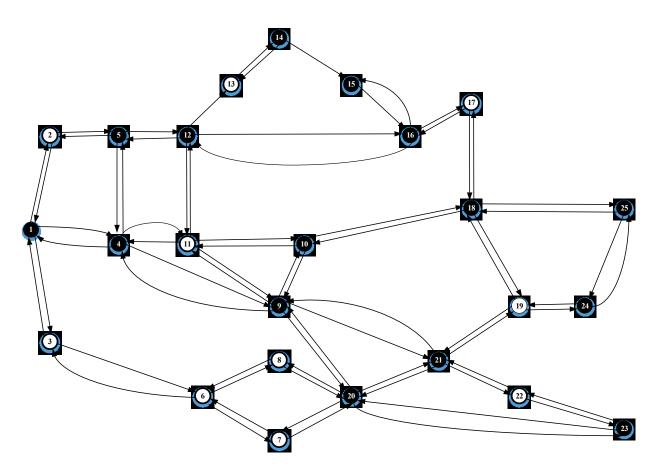


Figure 4-6: Hypothetical Network II, Case II

Train	Itinerary	Train	Itinerary
Service	•	Service	-
1	1-4-11	17	18-17-16-15
2	1-4-9-20	18	18-19-21-9
3	5-2-1-3-6-7	19	20-8-6-3-1
4	5-12-13-14-15-16	20	21-20-7-6-3-1
5	12-5-2-1	21	1-3-6-8-20
6	1-2-5-12-16	22	1-3-6-7-20-21
7	20-9-11-4	23	9-10-18
8	4-5-2-1	24	9-21-22-23
9	4-5-12	25	4-11-9-10-18
10	12-16-17-18	26	16-12-11-9
11	25-18-17-16	27	9-4-1
12	21-19-24-25	28	24-19-21-22-23
13	25-24-19-21-20	29	25-18-10-9-11-12
14	25-24-19-21-22-23	30	20-9-4-1
15	23-20-9	31	23-22-21
16	9-4-5		

Table 4-18: Itinerary of Train Services, Case II
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The black circles represent the yards with classification capability while the white circles represent the transfer yards. Itinerary of 31 trains services are defined in Table 4-18. Looking at the computational result of Case II, we realize that the computational effort increases exponentially with the number of yards, service-legs, and weekly orders. Risk threshold coefficients, $\zeta = 0.20$ and $\phi = 0.20$ are set in this experiment, therefore none of the service-legs and yards can take a risk more that 20% of the total risk around the service-legs and total risk at all yards within the underlying network, thereby assuring equity in spatial distribution of risk. The solutions given in Table 4-19 fall within at most 5% gap to the optimal solution.

Model	AVG. Run	Cost	Risk (peop	le millions)	No. of Trains	
Variant	Time (S)	(\$ millions)	Propane	Butane	NO. OF TTAILS	
P1	3287	14.5	28.5	33.2	277	
P2	6983	14.7	28	33.0	287	
P3 (Base Case)	89545	16.6	24.7	28.6	361	
P4 (Base Case)	5474	15.8	24.9	28.9	320	

Table 4-19: Computational Results (in percent), Case II

4.3.1. Analysis of the Experiments and Insights – Case II

The main motivations of presenting Case II were first to demonstrate that all model variants can be solved within reasonable time considering the size and complexity of the problem under study. Table B-1 in Appendix B reports on the number of variables and constraints of each of the previously discussed instances. In addition, we would like to compare them with on another and obtain insights and draw conclusion before closing this chapter. As shown in Table 4-19, P1 incurs the least transportation cost amongst all other model variants; however, by spending 2100K more than P1, P3 (Base Case) results in putting 3,800K and 4,600K less people to the risk of transportation while solving P3 (Base Case) is taking approximately 27 times more than solving P1. As clearly shown, the discrepancy between the results of P1 and P2 is negligible while such discrepancy is remarkably significant if we compare their results with those of P3, and P4, respectively. As seen, both multiobjective model variants expose less number of people to the risk due to transportation, compared with single-objective model variants. There is also a trivial discrepancy in terms of cost and risk, between P1 and P2, single objective model variants, which is also the case if two multiobjective model variants are compared with each other. Furthermore, it turns out that the single-objective models, P1 and P2, lead to lower transportation cost while increasing the risk considerably. Moreover, setting a value as an acceptable risk threshold in terms of the total number of people exposed due to the risk of evacuation, injury or fatality, seems to be too controversial to be viable in practice; therefore, all in all, the multiobjective variants of the problem, can be practically made use of to enable the decision makers to make route planning decisions at tactical level while considering interests of main stakeholders. In addition, the results of the experiments reveal that the risk at yards, or so called "not-in-transit" risk is remarkably higher than the risk of carrying Hazmats along service-legs, i.e. "in-transit" risk, which is consistent with the statistics of risk in the literature (see also section 1.1). 1.1Table 4-20 shows that the maximum yard risk is higher than the maximum service-leg risk in each of the model variants.

Table 4-20: Maximum yard risk divided by maximum rail-segment risk

P1	P2	P3	P4
3.41	3.11	4.18	4.25

Overall, conforming with the results of the instances discussed in Case I, results of Case II similarly show that multiobjective models lead us to better results in terms of risk and cost of transportation.

Chapter 5

5. Conclusion, Contributions and Future Research Avenue

This chapter briefly concludes the dissertation, highlighting the main contributions and areas of research to be pursued in future.

5.1. Conclusion

This thesis addressed railway transportation of both Hazardous materials and regular commodities. Inspired by the many lots of real-life applications of toxic inhalation Hazmats, we focused on transportation of dangerous goods which become buoyant in case of accidents resulting in derailment of railcars, rupture and release of Hazmat. Regarding the adverse societal consequences of such incidents, which is indeed intrinsic to transportation of dangerous goods, we made use of a commonly used mathematical air dispersion model, Gaussian Plume Model, to evaluate the risk in terms of the number of people exposed to the risk of evacuation, injury and fatality.

Looking at the problem from different angles, we developed four novel model variants to investigate the routing decisions, risk and cost minimization under logical, functional and Hazmatrelated constraints. Due to the complexity of the risk function which did not have a closed-form expression, we linearized the risk function by making use of auxiliary decision variables. Since the risk term was a concave-down function, we applied linear regression to prevent underestimating the risk. The linearize risk function, provided us with the opportunity to address the risk equity and risk load of the yards, tracks, and the total risk within underlying network, by setting limits, as a proportion of total risk, on the value of risk at yards and on tracks, as well as by authorities and / or insurance companies. While the model with nonlinear risk term in the constraints would have been a Mixed Integer Quadratically Constrained Problem (MIQCP) which would have made the model computationally expensive, the linearized form was solved within a reasonable time for small-size and medium-size instances of the problem. Moreover, we introduced and incorporated the regulatory restriction on the maximum number of Hazmat railcars to be loaded on each train, into our mathematical model variants. Further, considering the stakeholders' interest regarding bifurcation of flows, we developed model variants for both single-objective and multiobjective models.

Further, our analysis revealed that it the population exposure risk function that has been derived from the Gaussian Plume Model will not necessarily deter the Hazmat traffic classes from being routed from urban areas with less population density, which can be construed as a considerably significant insight into tactical planning problem of Hazmats. We also showed that weather stability conditions can affect the routing decisions significantly. It turns out that routing decisions may contradict the perception of the public and the expectation of the authorities which seeks for routing the Hazmats from rural areas instead of routing them through dense population centers. However, making use of GIS to estimate the density of the population in urban and rural areas can help enhancing the accuracy of our findings.

Further, considering the computational effort, our experiments demonstrated that small and / or medium size of the problem instances can be solved within seconds while the real-life size of the problem can take hours to be solved to optimality due to the large number of integer and binary variables as well as the constraints.

5.2. Main Contributions

Herein, we list the main contributions of this thesis as follows:

- Based on MCP, four novel link-based model variants have been developed. Two of the model variants were single-objective, seeking for the minimization of transportation costs under logical, functional and Hazmat-related constraints enforced by the authorities. Looking at the problem and considering both stakeholder's interest, which is the minimization of risk and cost, two multiobjective model variants have been developed. All model variants were MIP models.
- The risk function which was derived from GPM has been linearized, which enabled us to solve the problem to optimality within a reasonable time.
- Linearizing the complicated risk function enabled us to set limits on the risk at yards, tracks and total risk within underlying network, have been set where the societal risk, in terms of population exposure, have been evaluated using GPM. The first two sets of abovementioned constraints also ensure equity in spatial distribution of risk at yards and on tracks, respectively. Further, setting these constraints using the original nonlinear risk function would make the problem an MIQCP, which would be computationally expensive; as well, the model could not have been solved to optimality even for small instances of the problem.
- We have differentiated between urban areas / population centers with probably more unstable weather conditions, and rural areas / open country with probably more stable weather conditions. Further, through carrying out experiments, we showed that such differences in weather stability condition may indeed affect the routing decisions, which may be different from the expectation of the public or authorities. That is, considering an

evenly distributed population in both urban and rural areas, for two links with the same length, the risk of routing the Hazmats through urban areas may be lower from the risk of routing Hazmats through the link passing through rural areas. Hence, the risk term which have been derived from GPM, may fail in deterring Hazmat railcars from being routed through rural areas with less population density.

 We have considered the regulatory restriction set by Transportation of Dangerous Goods (TDG) of Transportation Canada, which consequently resulted in setting limits on the number of Hazmat railcars that can be loaded on each train.

5.3. Future Research

Immediate extensions of this thesis can revolve around the following directions:

- In this thesis, we assumed that population is evenly distributed in both urban and rural areas which resulted in overestimating risk values. It is recommended to make use of software packages such as ArcView / ArcGIS that has been developed by Esri, to enhance estimating the number of people residing at vicinity of yards and service-legs.
- It would be recommended to investigate the differences between the exact and approximate values of risk. Although we have a compilation of such comparisons, due to the brevity considerations, we decided not to incorporate it into this document.
- The suggested models include a large number of decision and auxiliary variables, as well as including various complicating constraints. Therefore, it would be a good practice if larger instances of the problem could be solved through either exact methods or through making use of heuristics or metaheuristics. For this, one may develop path-based variants of the presented models before implementing either resource-directive, price-directive or partitioning methods to solve the problem within reasonable time.

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Appendices

In this section, we will provide the reader with more illustrations and details.

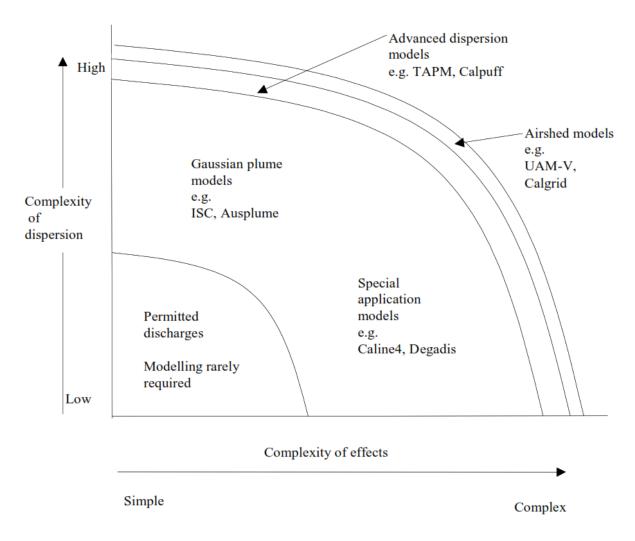




Figure A-1: Complexity of Air Pollutant Dispersion Models

Source: National Institute of Water and Atmospheric Research (2004)

Surface windspeed ms ⁻¹	Day time s (flux densit	un y in W m ⁻²)		Night time (cloud amount in oktas		
	Strong (>590)	Moderate (300–590)	Weak (<290)	8	4–7	0–3
<2	A	A–B	B	D	G	G
2–3	A–B	B	C	D	E	F
3-5	B	B–C	C	D		E
5-6	C	C–D	D	D		D
>6	C	D	D	D		D

Figure A-2: Pasquill-Gifford Stability Classes

Source: Air Pollution, Jeremy Colls (2002)

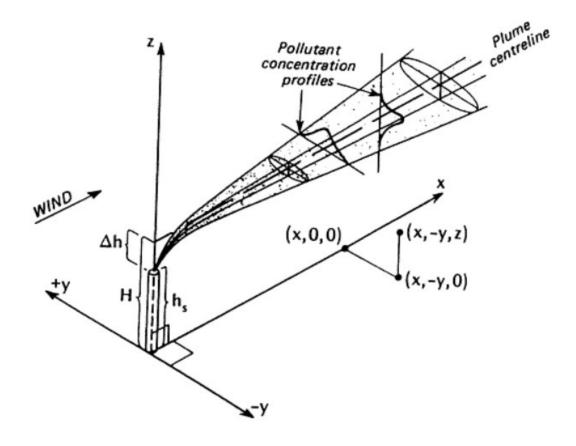


Figure A-3: Dispersion Geometry Specification - Cartesian Coordinate System Source: Air Pollution, Jeremy Colls (2002)

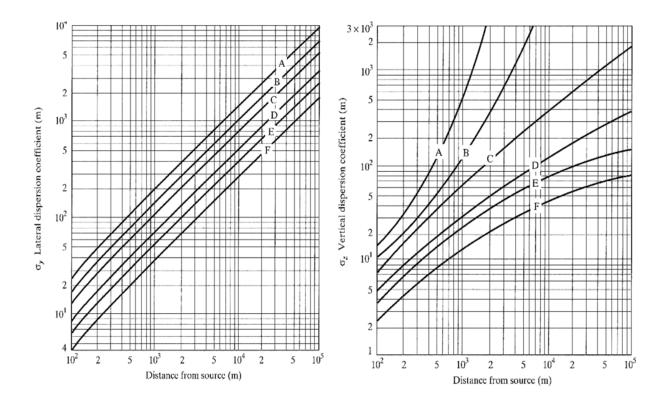
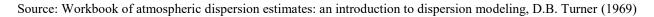


Figure A-4: Variation of Crosswind and Vertical Standard Deviations



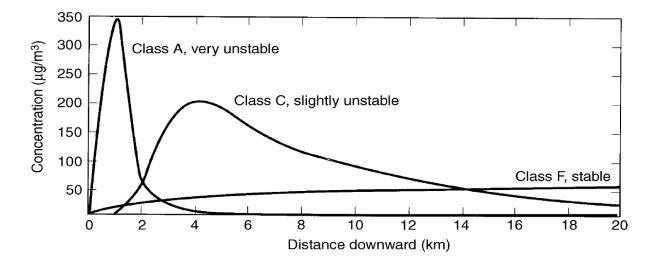


Figure A-5: Ground Level Concentration

Source: Introduction to environmental engineering and science, Master G.M., Ela W.P. (2008)

Pasquill $\sigma_{y}(m)$ $\sigma_{z}(m)$

Urban dispersion parameters (for distances between 100 and 10,000 m)

A-B	$0.32x(1 + 0.0004x)^{-0.5}$	$0.24x(1 + 0.001x)^{0.5}$
С	$0.22x(1 + 0.0004x)^{-0.5}$	0.20 <i>x</i>
D	$0.16x(1 + 0.0004x)^{-0.5}$	$0.14x(1 + 0.0003x)^{-0.5}$
E-F	$0.11x(1 + 0.0004x)^{-0.5}$	$0.08x(1 + 0.00015x)^{-0.5}$

Rural dispersion parameters (for distances between 100 and 10,000 m)

c) ^{-0.5}
c) ^{-0.5}
c) ^{-1.0}
$(3x)^{-1.0}$

Figure A-6: Brigg's Sigma (1973): Open Country and Urban Areas

Source: Mathematical Air Pollution Models, Ti	rabassi (2009)

Class			$x < 600 {\rm m}$		$x > 600 \mathrm{m}$	
	а	b	с	d	с	d
A-B	1.42	0.74	0.09	1.18	0.07	1.22
С	1.26	0.73	0.09	1.11	0.17	1.01
D	1.13	0.71	0.08	1.08	1.07	0.68
E-F	0.99	0.65	0.08	0.96	1.01	0.55

Figure A-7: McElory and Pooler (1968): Dispersion Coefficients

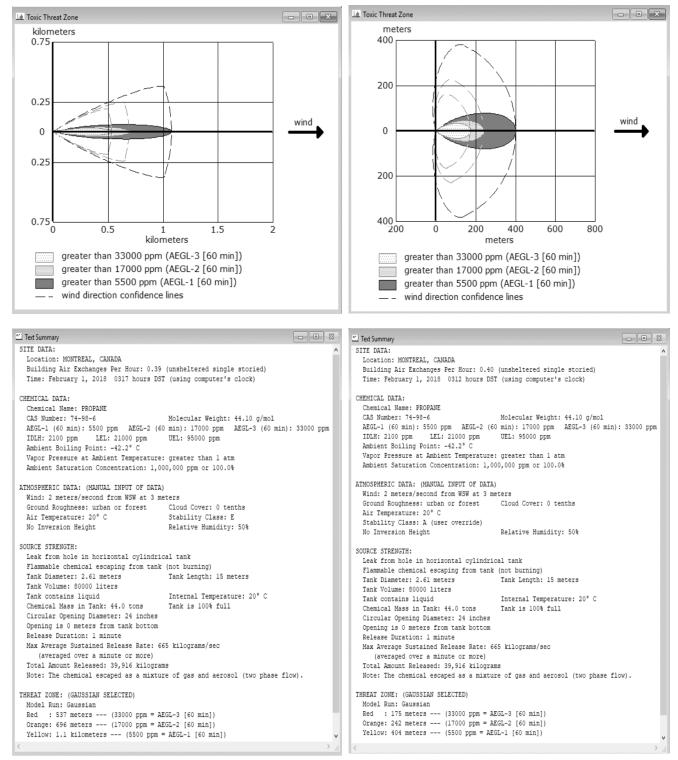
Class	a	b	с	d
A-B	0.40	0.91	0.41	0.91
С	0.36	0.86	0.33	0.86
D	0.32	0.78	0.22	0.78
E-F	0.31	0.71	0.06	0.71

Figure A-8: Singers and Smith (1986): Dispersion Coefficients

 $\sigma_y = ax^b$ $\sigma_z = cx^d$

Class			0.5 < x <	5 km	$5 < x < 50 \mathrm{km}$	
	a	b	с	d	с	d
A	0.3658	0.9031	0.00025	2.125	0.00025	2.125
В	0.2751	0.9031	0.0019	1.6021	0.0019	1.602
С	0.2089	0.9031	0.20	0.8543	0.5742	0.716
D	0.1474	0.9031	0.30	0.6532	0.9605	0.541
E	0.1046	0.9031	0.40	0.6021	2.1250	0.398
F	0.0722	0.9031	0.20	0.6020	2.1820	0.331

Figure A-9: Tadmor and Gur (1969): Dispersion Coefficients



Appendix B. Input Data for Computational Experiments

Figure B-2: Toxic Threat Zone - Propane, PG: E, Urban

Figure B-1: Toxic Threat Zone - Propane, PG: A, Urban

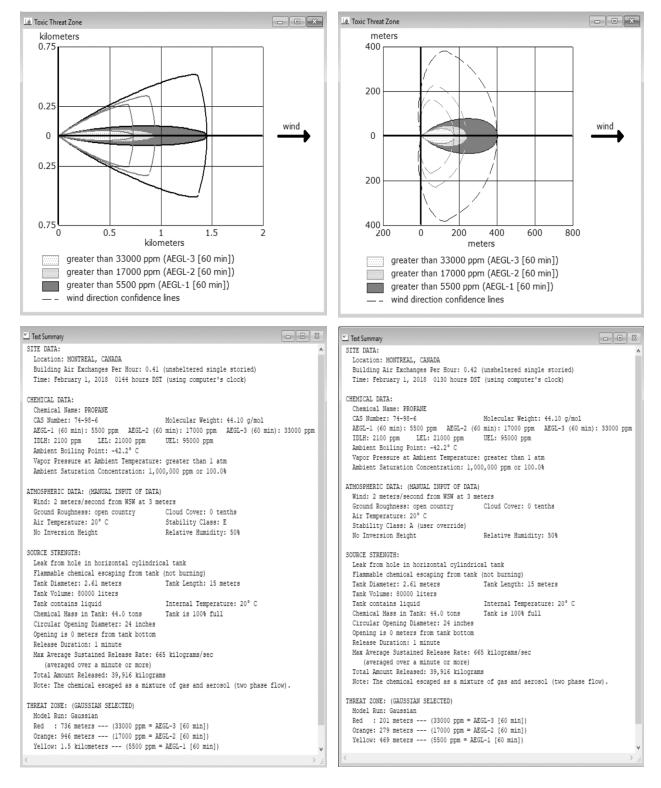


Figure B-4: Toxic Threat Zone – Propane, PG: E, Rural

Figure B-3: Toxic Threat Zone - Propane, PG: A, Rural

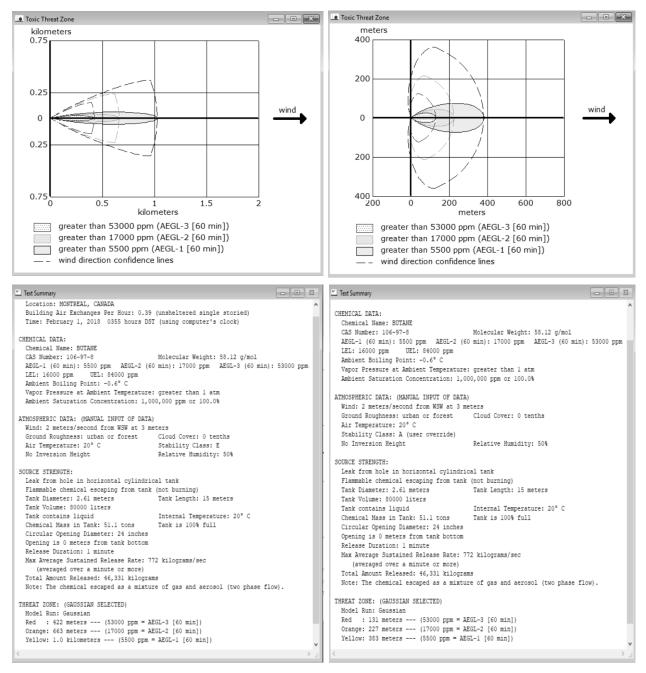


Figure B-6: Toxic Threat Zone – Butane, PG: E, Urban

Figure B-5: Toxic Threat Zone - Butane, PG: A, Urban

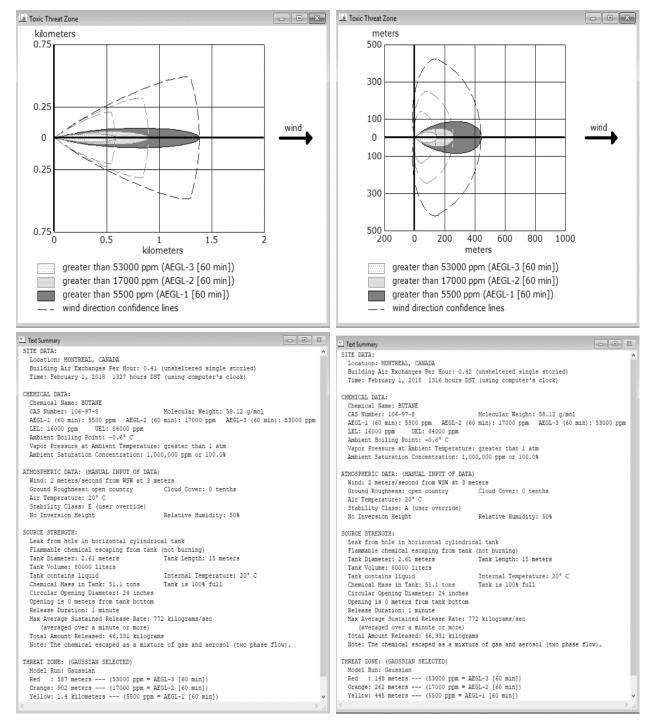


Figure B-8: Toxic Threat Zone - Butane, PG: E, Rural

Figure B-7: Toxic Threat Zone - Butane, PG: A, Rural

Instance	Model	No. of Integer	No. of Binary	No. Other	No. of
Instance	Variant	Variables	Variables	Variables	Constraints
	P1	172	1512	2016	4161
1	P2	4	1568	2016	4147
1	Р3	172	1512	2016	4158
	P4	4	1568	2016	4144
	P1	215	1890	5127	5127
2	P2	-	1960	5085	2520
Z	P3	215	1890	5127	5124
	P4	5	1960	5085	2517
	P1	1265	1890	2520	6282
3	P2	5	2310	2520	5610
3	P3	1265	1890	2520	6279
	P4	5	2310	2520	5607
	P1	1518	2268	3024	7458
4	P2	6	2772	3024	6618
4	P3	1518	2268	3024	7455
	P4	6	2772	3024	6615
	P1	8825	1890	2520	14598
5	P2	5	4830	2520	9390
3	Р3	8825	1890	2520	14595
	P4	5	4830	2520	9387
	P1	17650	3780	5040	28038
6	P2	10	9660	5040	16950
0	P3	17650	3780	5040	28035
	P4	10	9660	5040	16947
	P1	3850231	52452	69936	402530
Case II	P2	31	1335852	69936	1500244
Case II	P3	3850231	52452	69936	4025227
	P4	31	1335852	69936	1500241

Table B-1: Number of Variables and Constraints - Case II