PROCESS INTEGRATION AND OPTIMIZATION WITH RELIABLITY, SAFETY, AND COST ANALYSES

A Dissertation

by

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ABSTRACT

As the global population reached more than 7.7 billion, the needs for better living conditions and industrialization have grown rapidly all over the world. As the result, the consumption of natural resources has risen dramatically. With such increasing demands of resources, such as water and energy, it is significant for us to ensure safe, continuous, and efficient supplies to meet the demands.

During the chemical production, transportation, and material allocation processes, process integration and optimization has been approved to be a useful method and tool for resource conservation and recovery. Unused materials could be recycled, and energy produced could be reapplied to the system. However, a highly integrated and optimized process usually results in a complex system with a large number of connections for materials and energy exchange. A minor incident could cause a decrease in production rate or a complete shutdown of the system. Thus, safety and reliability studies are the key to develop such a complicated production infrastructure.

This work focuses on providing insight and a methodology of combining process safety and reliability analysis with the current process integration and optimization techniques. The approach proposed in this work will include identifying potential issues within an integrated system, quantifying interested process specifications, such as reliability, safety, and cost, developing a systematic approach to include different variables into the existing optimization frameworks, and solving the integration and optimization problems. This work includes three major topics that involve system synthesis, unit operation, and material allocation. First, we developed a systematic approach to analyze unit and system reliability for direct water recycle network and then integrate the reliability analysis into the optimization framework to study its

effect on overall water recycle system design and operation. Besides, we also studied how different pretreatment technologies can improve the reliability of a reverse osmosis water treatment unit. Techno-economic analyses were performed on all pretreatment technologies and were compared to the saving from extended cleaning and replacing schedules of the RO membrane. In addition, we applied data analysis techniques to quantify hazardous material transportation risk and then integrated the data-based safety variable into the supply chain material allocation problem to see how transportation decisions could be differed by different system risk value. The results of this work demonstrate the significance of safety and reliability in an integrated process and how other variables could change based on different requirements for the newly added variables. For future works, it is possible to extend this study by proposing a standard methodology for identifying and quantifying additional variables, such as environmental impacts, and by developing a systematic approach to analyze the effect of these variables on the existing integration and optimization frameworks.

DEDICATION

To my mother Xiangyang Huang and father Xiuling Zhang, for all their unconditional love and support.

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Contributors

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NOMENCLATURE

Subscript:

i	Source in supply and demand model
j	Sink in supply and demand model
b	Containment in water network
fresh, f	Fresh water supply in water network
waste, w	Wastewater treatment in water network
x,y	Interval starting and ending points in time analysis
c	Cleaning schedule in time analysis
r	Replacing schedule in time analysis
t	Transportation mode
d	Distance

Superscript:

pump, tank, pipe	Units in water network
fresh, waste	Fresh supply and waste treatment in water network
alter	Alternative fresh and waste in water network
cold	Cold parallel system in water network

Variable:

F	Supply and demand of sink and source
f	Flowrate
z	Containment concentration
y	Binary Variable
N	Number of connections

A	Availability
MTTF	Mean time to failure
MTTR	Mean time to repair
p	Probability
C	Cost
OC	Operating cost
FC	Fixed cost
d	Distance
DI	Pipeline diameter
AOC	Annualized operating cost
AFC	Annualized fixed cost
AC	Annualized cost
T	Time
V	Storage tank size
DI	Pipeline Diameter
R	Risk
TSC	Total supply chain cost

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1. INTRODUCTION*

Due to the rapid growth of the global population and industrialization, the demands for various resources, such as water and energy, have increased dramatically in recent year. However, the current supplies for these resources will not meet such demands. Water plays a central role in today's world economy and politics. Water scarcity has become one of the major global challenges due to the rapid growth of the population and the increasing trend of industrialization in developing nations. Global freshwater demand will increase by 40% by 2030 (2030 Water Resources Group, 2009). However, in the current situation, standard-quality drinking water cannot be obtained for roughly 10% of the global population (World Water Assessment Programme, 2015). Besides human consumptions, industrial water uses have also increased dramatically in recent years. According to the United Nations World Water Development Report 2015, there will be a four-time increase for industrial water demand from 2000 to 2050. Besides water, the global energy demand and consumption also face great challenges. The U.S. Energy Information Administration predicts a 48% growth in global energy consumption between 2012 and 2040 (Annual Energy Outlook 2016, U.S Energy Information Administration). The listed forecasting data demonstrates the speed of human's demand growth and the speed of natural resource depletion. To meet these increasing demands, one method has been widely used is to directly increase the production of natural resources, which can be especially observed in developing countries, such as China and India. However, such a method is highly not sustainable and will eventually result in damage to the environment and people's quality of life.

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In addition to the direct increase in natural resource production, another approach focuses more on recycle and reuse of existing materials and energy. Process integration and optimization plays a central role in such an approach. According to El-Halwagi (1997), process integration is defined as "a holistic approach to process design, retrofitting, and operation which emphasizes the unity of the process." The process integration method includes many different aspects, such as mass, energy and most recently, property integrations (El-Halwagi, 2006). Decades' research and studies have proven that process integration is the useful method to improve process efficiency. For example, Stijepovic and Linke (2011) have introduced a systematic approach to maximize waste heat recovery across multiple plants based on heat integration and pinch analysis. Heat integration options and a design of the heat exchange network can be then determined based on the optimization of the economic objective. Furthermore, Noureldin and El-Halwagi (2000) have developed a systematic framework to evaluate the pollution prevention target using various mass integration tools. With consideration of direct recycle and interception for targeted materials, such a method can effectively reduce the usages of feedstocks and the operation cost of the process. In addition, Kazantzi and El-Halwagi (2005) have introduced a new technique, the property-based material-reuse pinch diagram that can ensure maximum integration and minimum fresh usage within the process.

In the last two decades, heat, mass and property integrations in the chemical industry have drawn many researchers' attention and have been well studied, as shown above. Many techniques and algorithms have been developed to solve these integration problems. However, highly integrated processes will usually result in more complex systems. A large number of connections between sinks and sources mean high degrees of freedom within the system. The possibility of abnormal behavior in the system could dramatically increase and the effect could be catastrophic.

Even though a process could be highly integrated, these abnormal behaviors could result in production incidents, which will be highly counter-productive. It is significant to ensure a continuous and more efficient production infrastructure. In order to ensure a continuous supply of resources, safety and reliability should be the primary problems to address within an integrated process. Process integration with safety and reliability studies will be the key for the development of such an infrastructure. The purpose of this work is to study the role that safety and reliability play in an integrated system. The work will first focus on using existing methods or developing novel approaches to quantify interested process specifications, such as cost, safety and reliability, in chemical processes. Later, it is significant to develop a systematic approach to combine safety and reliability analysis with the existing process integration techniques. The method will propose a multi-objective optimization framework that can reveal the trade-off between costs (fixed plant cost, operation cost, transportation cost, etc.) or other major process specifications and safety/reliability. The results of this work will provide a more comprehensive and realistic solution for the process integration problems than the existing integration techniques. The ultimate target of this dissertation is to help guide the decision-making process of the management to develop both continuous and efficient supplies of resources that can meet the increasing demands of human society.

In this dissertation, three different projects will be proposed from three different areas in the chemical industry, which are system synthesis, unit operation, and material allocation. First, we developed a systematic approach to analyze unit and system reliability for direct water recycle network and then integrate the reliability analysis into the optimization framework to study its effect on overall water recycle system design and operation. Besides, we also studied how different pretreatment technologies can improve the reliability of a reverse osmosis water treatment unit.

Techno-economic analyses were performed on all pretreatment technologies and were compared to the saving from extended cleaning and replacing schedules of the RO membrane. In addition, we applied data analysis techniques to quantify hazardous material transportation risk and then integrated the data-based safety variable into the supply chain material allocation problem to see how transportation decisions could be differed by different system risk value.

1.1 Dissertation Outline

Section 1 introduces the background and motivation for this work and research project, current problem in natural resource conservation, existing studies in process integration and optimization, research efforts in water-energy nexus and reliability analysis, research efforts in reverse osmosis water treatment, and research efforts in transportation safety.

Section 2 describes the main target and objective of this work, information and data that are available to us, models and frameworks that can be used, major results that need to be obtained.

Section 3 presents the methodologies that have been applied to utilize the information, data, and models available to obtain the results.

Section 4 shows the results from different research projects I have proposed to include reliability and safety analysis in process integration and optimization, which focus on direct water recycle network, unit operation of reverse osmosis water treatment, and supply chain network optimization.

Furthermore, section 5 concludes the overall findings for research projects and the dissertation, as well as the future directions that could be applied to the models and frameworks developed in this work.

Last but not least, section 6 includes additional research work in the area of fixed cost analysis and correlation development for shale-gas monetization projects. The cost calculation has been used throughout the work and other research projects in the area of process optimization and integration.

1.2 Current Studies on Water-Energy Nexus and Reliability Analysis

Recent research has focused on studying more complex integration problems, such as Eco-Industrial parks (EIPs) and Water-Energy Nexus (WEN). Many techniques and tools have been developed for mass integration within EIPs (Topolski et al. 2018; Panu et al. 2019). Studies have also focused on simulation and optimization of water integration and recycle network for multi-plants systems. Lovelady & El-Halwagi (2009) applied the source and sink model in EIPs for optimizing system design and water recycle network. Rubio-Castro et al. (2012) developed a decomposition approach for solving water integration problem within EIPs. Bishnu et al. (2014) studied the effect of multiperiod planning on the optimization of direct water recycle network in eco-industrial parks. Alnouri et al. (2015) considered both off-site centralized and on-site decentralized water treatment units for water integration within EIPs. Fouladi and Linke (2018) proposed an optimization approach to include sustainability analysis in water and energy integration problems within industrial parks. Alnouri et al. (2018 & 2019) introduced the idea of principle pipes to the synthesis of interplant water network for eco-industrial parks and solved the non-linear optimization problem for the optimal economic objective.

However, highly integrated processes, such as industrial cities and eco-industrial parks, usually result in a complex system. A large number of connections between sinks and sources will be made for mass and heat integrations. The possibility of abnormal behavior in the system could dramatically increase due to the system's complexity, and the effect of such behavior could be catastrophic. Production incidents could lead to the decrement in the overall production rate and even a complete shutdown of the entire integrated system. The results will be highly counter-productive and totally against the goal of integrations. In order to ensure a continuous production process, the reliability of the system should be the primary problem to be addressed ahead of integration. Additional methods should be applied to increase the system reliability with relatively low costs.

The concepts and mathematical models for process system reliability have been well-studied in the area of reliability engineering and systems engineering. Bazovsky (2004) and Ebeling (2010) well defined the term reliability and demonstrated the derivation of the reliability function in their books. Henley and Gandhi (1975) compare methods like block diagram and reliability function, as well as fault tree analysis to determine system reliability. In addition to the traditional reliability studies, most recent research has looked into reliability analysis in various processes and systems. Aguilar et al. (2008) constructed an optimization framework for a utility system, which includes reliability analysis. Haghifam et al. (2011) used the Markov process and state-space modeling to evaluate reliability in combined heat and power systems. Terrazas-Moreno et al. (2010) proposed an algorithm to solve the optimization problem considering system reliability and cost for an integrated production site. Ye et al. (2018) studied the effect of parallel units on system reliability and developed an optimization model to determine the optimal design of a reliable chemical process. Similar work in process uncertainty and operability analysis can also be found in Mukherjee and El-Halwagi (2018) and Tian and Pistikopoulos (2018).

Although previous studies have focused on water integration within EIPs and reliability analysis of chemical processes, few of them look into the combination of these two aspects. The above analyses on these two distinct research areas show very different applications in solving process integration and optimization problems, where mass exchange network, EIPs and WEN focus on developing framework and techniques to address optimal material distribution and resource/energy conservation problems under different circumstances such as multi-period and uncertainty, and the process reliability analysis focuses on developing mathematical and statistical models for quantifying system reliability and applying different optimization algorithms to solve various mathematical programming problems. The target for this project is to propose a problem and a novel framework that can be addressed by applying techniques from both research areas and then to fill in the gap between them. In addition, the imbalance between research efforts on water management/water integration and reliability analysis needs to be broken to resolve the concern on system continuity and performance of complex water networks and highly integrated chemical processes raised by the industry. Several challenges will need to be overcome in this work. The complexity of formulating the interactions between chemical plants is one major issue that needs to be addressed. Furthermore, due to the nature of reliability/availability calculations and models, a mixed integer nonlinear programming problem (MINLP) will be formed, and the computational difficulty associated with it is another problem that needs to be solved. Since mass and water integration directly affects the efficiency of an EIP and multi-process systems usually result in a low system reliability value, it is significant to study the impact of reliability on the source and sink integration model and to determine the optimal design and operation strategies for the water recycle/reuse networks within eco-industrial parks.

In this work, a systematic approach is developed to quantify reliability for the source and sink model that is used for direct water recycle network. Three methods to improve system reliability are proposed, which are alternative fresh and waste treatment, parallel units and storage tanks. An optimization framework is modeled to determine the optimal design and operating strategy for the mass exchange system. Two cases and formulations are presented at different computational difficulties, and distinct methods are proposed for solving each of those cases. The framework is first formulated as a single objective MINLP problem while combining reliability analysis within the cost objective. Then we study the multi-objective MINLP problem using the epsilon-constrained method to solve for the Pareto optimal solutions of system reliability and cost. The results illustrate the tradeoff between system reliability and cost, which can guide the decision-making process of the management for a more reliable and cost-efficient direct water recycle network within EIPs.

1.3 Current Studies on Water Treatment and Reverse Osmosis Unit Operation

Freshwater generation, such as seawater desalination and wastewater treatment, have drawn much attention in the area since water and energy are closely related and dependent in both problems. According to Jamaly et al. (2014), more than 15,000 desalination facilities are operating globally to fulfill the freshwater requirement from the growing population. Recent industrial applications have seen an increasing trend in using membrane technologies to achieve freshwater generation and wastewater treatment. One of the most significant and widely used membrane technologies is reverse osmosis (RO). It has been accepted by the industry and applied to newly installed desalination and wastewater management plants due to its advantages in selectivity, energy consumption, cost, and scale over other water treatment technologies. According to El-Halwagi (1992), the RO waste treatment system can be easily applied to fulfill any discharge standards and regulations at a relatively moderate cost. For seawater desalination, RO has significant advantages in fixed cost investment, operating cost and most importantly, energy consumption compared to thermal desalination technologies (Miller, 2003). Furthermore, RO membranes could also be included in small-scale, modular units, which can be easily attached to existing operations and plants.

Although RO has many advantages in terms of cost and energy consumption, it is also important to look at the efficiency and effectiveness of the technology to ensure a reliable and continuous water supply. The reliability of RO units is heavily dependent on the performance of RO membranes. Fouling and scaling on the membranes are the major factors that could block membrane pores, reduce water flux, increase osmotic pressure, and eventually increase the energy consumption of the system. In order to improve RO membrane performance, appropriate pretreatment technologies should be applied before water is fed into the RO system. Studies have shown additional pretreatment steps could improve RO membrane performance by removing solid particles, dissolving organic matters, or more generally, reducing the fouling propensity of water. Pretreatment technologies can be divided into two categories: conventional and non-conventional. According to Greenlee et al. (2009), conventional pretreatment step should include all or some of the following technologies: acid addition (such as sulfuric and hydrochloric acid), coagulation addition (such as ferric chloride, aluminum sulfate, dimethyldiallylammonium chloride, and polyamines), flocculation addition (such as anionic polymers), disinfection (such as ozone, chlorine, chloramine, and potassium permanganate), granular media filtration (such as sand, anthracite and garnet), and cartridge filtration. Non-conventional pretreatment step will require the addition of other membrane separation technologies with larger pore sizes, such as ultrafiltration (UF), microfiltration (MF), and nanofiltration (NF), before the RO unit to exclude large particles (Jamaly et al., 2014). Different seawater or brackish water qualities will require different combinations of pretreatment technologies. Applying all pretreatment technologies is obviously not the ideal solution due to high chemical injection and removal, high energy consumption, and low efficiency in clean water production. It is important to look at different pretreatment technologies and water qualities to determine the optimal combinations.

To improve the efficiency and effectiveness of RO units for a more reliable and continuous water supply, research efforts have also been looking at the optimal design and operation of RO membrane systems. El-Halwagi (1992) developed a systematic synthesis approach for generating the optimal arrangement of reverse osmosis networks including RO units, booster pumps and energy recovery devices, based on different requirements and constraints. Zhu et al. (1997) proposed a synthesis technique under uncertainty for the optimal design of reverse osmosis networks. The advances in RO process and equipment designs have significantly reduced the fixed and operating costs of RO systems (Wilf & Bartels, 2005). Lu et al. (2006) developed a mathematical model to solve for the optimal design of RO desalination system while considering the cleaning and replacing schedules of RO membranes. Jiang et al. (2017) optimized the RO membrane cleaning and replacing schedules to minimize the overall operating cost of the system.

The positive effects of different RO pretreatment technologies on preventing RO membrane fouling and scaling have been well studied. For example, Pearce (2008) evaluates the non-conventional pretreatment technologies (UF and MF) and compares their advantages in costs and energy consumptions. Eran et al. (2008) study the effectiveness of conventional pretreatment technologies (chlorination and coagulation). Brown et al. (2008) construct mathematical models to study the impacts of ozone pretreatment on RO membrane permeability. Greenlee et al. (2009) and Jamaly et al. (2014) conducted comprehensive reviews on various pretreatment technologies and related research of their impacts on the RO system. Mathematical models and optimization frameworks have also been developed to determine the optimal design and operation of reverse osmosis networks. Previous research in those two different areas both contribute to a more effective and efficient RO system. However, both sides fail to look at the potential effects of RO pretreatment technologies on the optimal design and schedule of the RO system. It is important to combine both efforts and build a framework that could choose the optimal pretreatment technology combinations and will result in the best design and operation of the reverse osmosis network with minimum cost.

In this work, a pretreatment network including different pretreatment technologies is constructed. The effects of those technologies on the RO membrane are analyzed and categorized. A mathematical model is developed to represent the time-dependent reliability of the membrane system. An optimization framework is used to solve for the optimal schedule of RO membrane cleaning and replacing. The objective of the problem is to minimize the annualized cost including both pretreatment cost and RO system cost. The problem will show the tradeoff between spending on pretreatment technologies and spending on RO membrane cleaning and replacing. The results will suggest different pretreatment technology combinations under different circumstances with various cleaning and replacing schedules of the RO membrane.

1.4 Current Studies on Hazardous Material Transportation Safety

Transportation of chemicals plays a central role in supply chain management and in multi-plant mass integration through eco-industrial parks (e.g., Chew et al. 2008; El-Halwagi 2017a). Raw materials and final products are transported in a significant amount between suppliers and consumers. It is important to ensure an effective, efficient, and yet reliable transportation pathway. Due to the growing concerns about safety in transportation networks, hazardous material (HazMat) transportation has become one of the main issues that need to be addressed by researchers. From the Bureau of Transportation Statistics at the U.S Department of Transportation (USDOT), the annual shipment of HazMat in 2012 in the USA exceeded 22.6 billion tons (Transportation Statistics Annual Report 2015). With such a significant volume of HazMat being transported every year, the risks and impacts associated with potential accidents cannot be ignored. HazMat transportation accidents are relatively uncommon compared to accidents without HazMat, but the public holds a strong opinion against those HazMat accidents due to potential catastrophic consequences (Meng et al. 2005). The consequences of an accident related to HazMat could be significant due to potential HazMat releases, spills, fires, and explosions. Erkut et al. (2007) summaries the average cost in dollar value for non-HazMat vehicle incidents and HazMat vehicle incidents with different circumstances. HazMat incidents with spill and release cost 58% higher than the non-HazMat ones. With the worst-case scenario, an explosion involving HazMat could cost $2 million on average, which is 518% higher than non-HazMat vehicle incidents. It is sufficient to conclude that HazMat transportation accidents will result in substantial capital losses for companies that could affect supply chain management decisions.

Because of the increasing public anxiety towards the HazMat transportation safety issue in the 1980s, research in this area has emerged and drawn a significant amount of attention (Huang and Fery 2005). Especially in operations research and systems engineering, researchers have put continuous efforts in optimizing the HazMat transportation problem. The majority of the efforts focused on two aspects: (1) the development of routing and scheduling optimization framework to minimize transportation risk, (2) risk assessment techniques under different transportation circumstances. Erkut et al. (2007) provided a comprehensive review of this topic. For the routing optimization problem, Abkowitz and Cheng (1988) proposed one of the very first methods to optimize routing of HazMat transportation with consideration of both transportation cost and risk. Additional factors could also be included in the routing and scheduling optimization framework.

For example, Meng et al. (2005) developed a new routing optimization framework to consider operational time for HazMat transportation problem. They looked into the shortest path algorithm and included time-dependent variables for route choices and schedule arrangements. However, the frameworks usually contain thousands of route and schedule choices for a relatively small area. To include multiple origins and destinations will exponentially increase the complexity of the problem. Adding more transportation modes will result in even more route options, which could make the optimization problem impossible to set up and solve. Besides the routing optimization framework, new risk assessment techniques have been developed to assist the optimization of HazMat transportation problem. Zhang et al. (2000) use the Gaussian plume model to study the effect of HazMat air dispersion and apply geographic information system to evaluate risk values based on the dispersion models. Kang et al. (2014) use the value-at-risk model that is widely applied in the financial industry to quantify risk at a certain confidence level for different route choices. Those assessment techniques provide alternatives to evaluate the risk for HazMat transportation, but they are mainly based on ideal mathematical models and have a weak connection with real-world incidents and data.

In this work, a multi-objective optimization framework is developed to minimize the cost and risk of the HazMat transportation problem. The framework does not consider routing and scheduling as the optimization variables since it is safe to assume companies have their preferences on road choices (the shortest distance) and fixed schedules that cannot be changed in a short period of time. The assumption significantly reduces the complexity of the problem. Besides, instead of using ideal mathematical models, a novel approach developed by Samuel et al. (2009) is applied to quantify transportation risk using historical incident data. The epsilon-constrained method is used to make risk a constraint and transform the framework into a single-objective optimization problem. A Pareto optimal curve is obtained from the optimization framework to guide the decision-making process. The numerical results will suggest different transportation arrangements using different transportation modes within the supply chain network.

2. PROBLEM STATEMENT*

From the discussion in Chapter 1, it can be seen that although process integration and optimization have been proved to be useful approaches for material recycle and energy conservation, and such areas have drawn much attention in the current research, few of them consider reliability and safety during the integration and optimization processes. The target for this dissertation is to fill in the gap between the area of process integration and optimization and the area of reliability and safety engineering. The objective of this work is to develop a systematic framework that can quantify reliability and safety and then integrate the analyses into the current optimization problems and frameworks. The novelty of the problem that is proposed in this work is to study the impact of reliability and safety analyses on the optimization results from both design and operation aspects. The problem is stated and defined as the following:

Given:

- A system that requires process integration and optimization for resource conservation
- A framework that has been developed to represent such a system
- Information on the fixed and operation costs of the system
- Information on either safety or reliability analysis in the system

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By applying the existing information and framework, this work will determine:

- Approaches to quantify system safety or reliability
- Approaches to integrate safety and reliability into the framework
- Designs and operating strategies based on both the cost and safety/reliability of the system

To be more specific, the problem statement and the objective of each research projects that have been proposed in this work will also be listed in the following sections.

2.1 Problem Statement for Reliability Analysis in Direct Water Recycle Network

The problem that will be addressed in this research project is the arrangement of connections between water sources and sinks. The novelty of the problem in this paper is to consider system reliability and its effects on the mass exchange network. The difference between the problem raised in this work than the previous works is that two distinct objectives need to be addressed at the same time and at both design and operation levels. The first objective is to minimize the system overall fixed and operating costs, while the second objective requires the maximum system reliability value. This work will mainly focus on the direct water recycle network within an eco-industrial park. The EIP contains a known number of chemical plants. Processing units that produce wastewater will be treated as water sources, and processing units that require water inputs will be treated as water sinks. The problem is stated and defined as the following:

Given:

- the supply of each water source and the demand of each water sink
- a set of contaminants and their compositions in each water source/maximum allowable compositions for each water sink

- the shortest distance between each source and sink/each source and waste water treatment/fresh water supply and each sink
- the unit costs for fresh water supply and waste water treatment
- the cost of pipeline construction based on flowrate for each connection

In addition to the given information on the source and sink mass exchange model, the newly included reliability objective requires more information for models to quantify unit reliability and methods to improve system reliability:

Given:

- reliability value for each water source and water sink
- the mathematical model to calculate system reliability based on the layout of the mass exchange network
- methods to improve reliability including alternative fresh and waste treatment, parallel unit and storage tank installations
- the cost data for implementing all three reliability improving methods and their effects on system reliability

The objective of this work is to determine the optimal design of the water direct recycle network and the optimal water allocation operating strategy with low cost and high system reliability value. Two different cases are proposed for solving the optimization problem:

- a single-objective MINLP where system reliability is integrated into the system cost objective function
- a multi-objective MINLP that maximizes system reliability and minimizes system cost

By applying existing data and building the optimization framework, this work will determine:

- the mapping between water sources and water sinks for the mass exchange system
- the flowrate for each connection between source and sink/source and waste water treatment/fresh water supply and sink
- the amount of fresh water needed and the amount of water for waste treatment
- storage tanks and parallel units that are needed in the network and the resulted system reliability value
- the operating cost associated with fresh water supply and waste water treatment/the fixed cost associated with storage tank and parallel unit installations

2.2 Problem Statement for Reverse Osmosis Unit Operation

Consider a pretreatment system containing different pretreatment technologies for RO system, as shown in Figure 1. The information regarding each technology is known, such as cost, input water concentration, output water quality, and effect on RO membrane. Different combinations of these technologies can be considered as different pretreatment networks for further analysis.

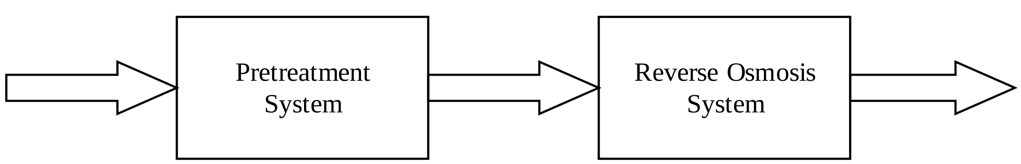

Figure 1 Combination of Pretreatment and RO Systems

The objective of this paper is to determine the optimized combination of both conventional and non-conventional pretreatment technologies on RO membrane for water treatment and to conduct the optimized strategy for cleaning and replacing of the RO membranes. We are given the following information: (1) Information and data on various pretreatment technologies or combinations of technologies, (2) seawater/wastewater compositions, (3) design specifications for the RO membrane, (4) required clean water quantity and quality. By applying existing data and models, the paper should address the following questions: (1) what are the optimized pretreatment system and operating strategy of the RO unit for the lowest unit cost of fresh water produced? (2) what are the optimized pretreatment system and operating strategy for the RO unit to meet a certain freshwater requirement?

2.3 Problem Statement for Hazardous Material Transportation Safety

Consider a set of suppliers (sources) of HazMat and a set of plants (sinks) that use the transported materials. The availability of materials from each source and the demand for each sink is known. The locations of the sources and sinks are also known. Different modes of transportation may be used. The cost of transporting materials between a source and a sink using a specific mode of transportation is known. The risk of transporting materials depends on the mode of transportation, route, and quantity. Historical incident data for a certain HazMat related to each transportation mode are known. Although weather effects are important, they are not considered in this paper. The objective of this paper is to integrate risk factor into the HazMat transportation problem and to construct a framework that can determine the trade-off between transportation cost and risk. Specifically, the following questions will be answered: (1) how to quantify transportation risk and correlate it with traveling distance? (2) How to evaluate the trade-off between transportation cost and risk? (3) What is the optimal transportation strategy under certain conditions and what is the minimum transportation cost associated with such a strategy?

A generic supply chain is assumed for a company with multiple manufacturing plants. These plants require a set of feedstock or material that is classified as HazMat. A set of suppliers is expected to deliver the feedstock to meet each plant's demand. Different modes of transportation such as highway and railroad can be used to achieve such a goal. The overall supply chain network is shown in Figure 2.

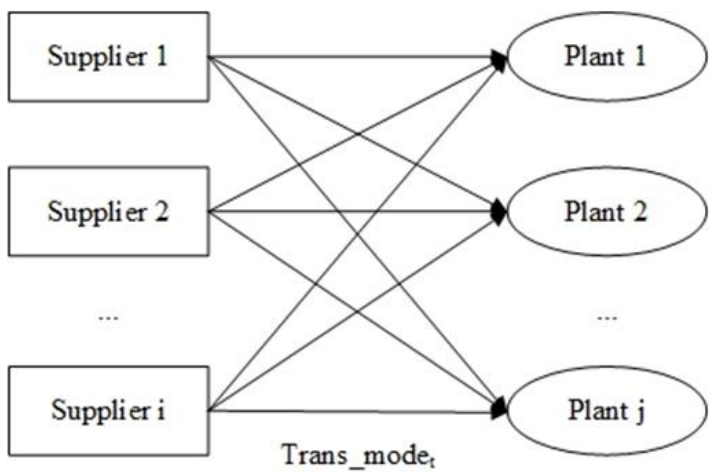

Figure 2 Overall Supply Chain Network for Material Allocation

3. METHODOLOGY*

As discussed in the previous chapter, the objective of this work is to develop a systematic approach for quantifying process reliability and safety, integrating the reliability and safety analyses into existing system optimization frameworks, and studying the effects of those newly added objectives on the overall design and operation of the system with cost consideration. The approach that has been taken in this work involves the following several steps:

1. Identify the targeted process specifications other than the existing ones that should be included in the integration and optimization techniques
2. Data and model acquisition
3. Quantify the targeted process specifications based on the acquired data and model through either existing techniques or developing novel approach and correlations
4. Construct an optimization framework that can combine targeted specifications with the existing integration system
5. Solve the optimization framework and update the design or operation strategy of the integrated process based on the result

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As mentioned before, three different research projects were introduced for three distinct areas including process synthesis, unit operation, and supply chain material allocation. Each research project will follow the same general steps listed above. However, each project will have its own unique approach based on the data collected and model developed. The following section will further discuss the detailed methodologies that have been applied for all three areas.

3.1 Methodology for Reliability Analysis in Direct Water Recycle Network

3.1.1 Sink and Source Representation

The first part of the problem formulation focuses on the sink and source representation for the direct water recycle network that is presented in El-Halwagi et al. (2003) and Bishnu et al. (2014). A set of processing units within EIPs that need to deliver their waste water to water sinks or directly discharge to waste water treatment are considered as water sources. A set of units that will consume waste water from water sources or directly from fresh water supply are considered as water sinks. The connections between sinks and sources represent water flows to meet the supply and demand of the network. The addition demand of sinks that cannot be satisfied by sources will be fulfilled by freshwater. Similar, addition supply of sources that cannot be taken by sinks will be treated elsewhere. No water flow is allowed between freshwater and wastewater treatment. All the flowrates are continuous variables that need to determine by the optimization framework.

A number of sets that will be used in our model are shown in Equations 1-3:

Consider a set of water sources, I, defined as:

$$I = \{i = 1, 2, 3, \dots, N_{source}\} \tag{1}$$

Consider a set of water sinks, J, defined as:

$$J = \{j = 1, 2, 3, \dots, N_{sink}\} \tag{2}$$

Consider a set of contaminants, B, defined as:

$$B = \{b = 1, 2, 3, \dots, N_{contaminant}\} \tag{3}$$

In addition to the set definitions, the supply and demand information is also given. The supply of source i is defined as F_i, and the demand of sink j is defined as F_j. The flowrate for each connection will be defined for mass balance calculations. There will be three kinds of water flows within the network: (1) flow between sources and sinks, (2) flow between sources and waste water treatment, and (3) flow between fresh water supply and sinks. The water flowrate between source i and sink j is defined as $f_{i,j}$. The water flowrate between source i to the wastewater management is defined as $f_{i,w}$. The water flowrate between the fresh water to sink j is defined as $f_{f,j}$.

Based on the definitions, the source and sink mass balance constraints can be modeled as shown in Equations 4-7:

The mass balance around water source i is:

$$F_i = \sum_j f_{i,j} + f_{i,w} \tag{4}$$

where each source i can be split into unlimited number of sub-streams to fulfill the supply constraint.

The mass balance around water sink j is:

$$F_j = \sum_i f_{i,j} + f_{f,j} \tag{5}$$

where each sink j can also take unlimited number of sub-streams to fulfill the demand constraints.

The flow rate of fresh water needed and water sent to waste water treatment can be denoted as F_{fresh} and F_{waste}, where the constraints are formulated as:

$$F_{fresh} = \sum_j f_{f,j} \tag{6}$$

$$F_{waste} = \sum_i f_{i,w} \tag{7}$$

Since the water coming from sources contains contaminants that can have negative impacts on the performance and safety of the downstream water sinks, addition constraints are placed on the composition of impurity b that sink j can take from water inputs:

$$z_{j,b}^{min} \leq z_{j,b} \leq z_{j,b}^{max} \tag{8}$$

where $z_{j,b}^{min}$ and $z_{j,b}^{max}$ are the lower and upper bounds for the impurity composition.

The impurity composition $z_{j,b}$ can be further calculated as the fraction of the total amount of impurity b going into sink j and the total amount water fed into the same sink:

$$z_{j,b} = \frac{\sum_i (f_{i,j} \cdot z_{i,b})}{F_j} \tag{9}$$

where $z_{i,b}$ is the composition of the impurity b in the water stream coming from source i.

Besides the upper and lower limits on impurity concentrations, the flowrate for each connection is also limited to certain range, as shown in Equation 10:

$$\mu \cdot y_{i,j} \leq f_{i,j} \leq U \cdot y_{i,j} \tag{10}$$

where $y_{i,j}$ is the binary variable for representing the existence of a connection between source i and sink j. The lower bound μ ensures that connections with small flowrates will not be allowed in the mapping for economic reasons. The upper bound U, which is a large enough number, will ensure the flowrate goes to zero when the binary variable takes the value of zero. Equation 10 also represent an if-then condition:

$$\begin{cases} if\ y_{i,j} = 0, & then\ f_{i,j} = 0 \\ if\ y_{i,j} = 1, & then\ \mu \leq f_{i,j} \leq U \end{cases} \tag{11}$$

As Equation 12 shows, a maximum constraints is also assigned to the total number of connections in order to avoid an over-complex system with unlimited mapping possibilities between sources and sinks:

$$\sum_i \sum_j y_{i,j} \leq N_c \tag{12}$$

3.1.2 Reliability and Availability Formulation

The second part of the problem formulation includes reliability analysis of the sink and source network and the model and data that have been used to quantify unit and system reliability and availability value. The definition of reliability can be concluded as the probability of a unit that will work properly at a certain point of time under valid conditions (Ebeling, 2010). As a function of time, reliability can be formulated using the constant failure rate model and the exponential distribution function, shown in Equation 13, under the assumption of random failures and events.

$$R(t) = e^{-\lambda \cdot t} \tag{13}$$

where $R(t)$ is the reliability value of the unit at time t, and λ is the constant failure rate.

However, since this work does not propose a dynamic model and time is not considered as a variable in our model, different quantifying methods needs to be used for calculating reliability. The analysis in this work will be based on inherent availability, $A_{inherent}$, instead. Inherent availability is the steady-state availability of a component or a system. The value for inherent availability of a unit is determined by the engineering design and material quality, and it is usually fixed for a specific type of unit under certain operating conditions. Inherent availability can be calculated using Equation 14:

$$A_{Inherent} = \frac{MTTF}{MTTF+MTTR} \tag{14}$$

where MTTF is the mean time to failure of a unit, MTTR is the mean time to repair of a unit.

MTTF and MTTR are determined by historical operating and repair data collected by manufactures and plant operators. The value for MTTF and MTTR of all types of process units can be obtained from various sources, such as Offshore Reliability Data Handbook and research papers and books in the reliability engineering area. Furthermore, inherent availability is commonly used in reliability studies in the area of process systems engineering, as shown in Terrazas-Moreno et al. (2010) and Ye et al. (2018).

Based on the mathematical model for calculating inherent availability and the data obtained from the Offshore Reliability Data Handbook, an availability value will be determined for each source and sink as A_i and A_j based on the assigned MTTF and MTTR data, shown in Equation 15 and 16:

$$A_i = \frac{MTTF_i}{MTTF_i+MTTR_i} \tag{15}$$

$$A_j = \frac{MTTF_j}{MTTF_j + MTTR_j} \tag{16}$$

Equations 15-16 represent the basic formulation for unit reliability and availability analysis in this work. Although each source and sink will have its own reliability value, additional information and models are needed for combining individual unit analysis and calculating the system reliability and availability value. Based on the systematic method proposed by Ebeling (2010), the serial configuration and parallel configuration of a system have different representations, as shown in Equations 17-18 accordingly:

$$A_{serial} = \prod A_{unit} \tag{17}$$

$$A_{parallel} = 1 - \prod (1 - A_{unit}) \tag{18}$$

Each connection between water sources and water sinks will be treated as a sub-system in this work. The serial configuration can be applied for reliability calculation of each connection, shown in Equation 19:

$$A_{i,j} = A_i \cdot A_j \tag{19}$$

Since the mapping of the mass exchange network could not be changed after system installation, multiple water flows coming from each source and going into each sink are not considered as a parallel configuration. The overall system is assumed to be a coagulation of sub-systems (connections) between sources and sinks. So the serial configuration can also be applied for the overall system reliability calculation, shown in Equation 20:

$$A_{system} = \prod_{i,j} A_{i,j} \tag{20}$$

Equations 14-20 summarize the unit and system reliability and availability formulation used in this work. Besides, several methods are proposed to improve the system reliability value and will be discussed in the following section.

3.1.3 Methods to Improve System Availability

The model developed using Equations 14-20 represents the basic setup for the availability analysis in the water recycle network. However, it is necessary to consider redundancy within the system to improve reliability and availability. According to Birolini (2017), the system redundancy is defined as additional methods to ensure the system to work properly and deliver designed function. Besides the basic model, those additional methods and factors should also be included in the analysis as means and optimization variables to improve system reliability and availability values. In this section, different methods to improve system availability are listed. The mathematical models that describe those methods are also constructed and compared with each other.

Three major availability-improving methods are considered and discussed in this work: (1) storage tank (2) parallel system, and (3) alterative fresh/waste treatment. Intermediate storage tanks are used to reduce system downtime by storing water flows from water sources due to failure of water sinks, or by supplying stored water to the sinks due to failure of water sources. Similarly, water flows can go through parallel units to ensure a continuous production process if major components within the system are unavailable and need immediate repairs. If both storage tank and parallel unit are not unavailable, and a failure happens within the system, the only method to ensure a continuous production is to supply more fresh water to the sinks or feed more wastewater from the sources to the treatment.

Figure 3 demonstrates the sub-system with potential storage tanks and parallel units to increase system reliability. The pump unit is specifically included and studied for parallel configuration because of its importance in the water recycle and reuse system, as well as its low availability value. We believe such an important part of the network with relatively low reliability value should be handpicked and integrated into the system reliability analysis. However, any unit and component can be considered for the parallel configuration analysis if needed in the future. The alternative fresh/waste treatment method is not included in the figure because it has already been included in the overall network as fresh and wastewater streams.

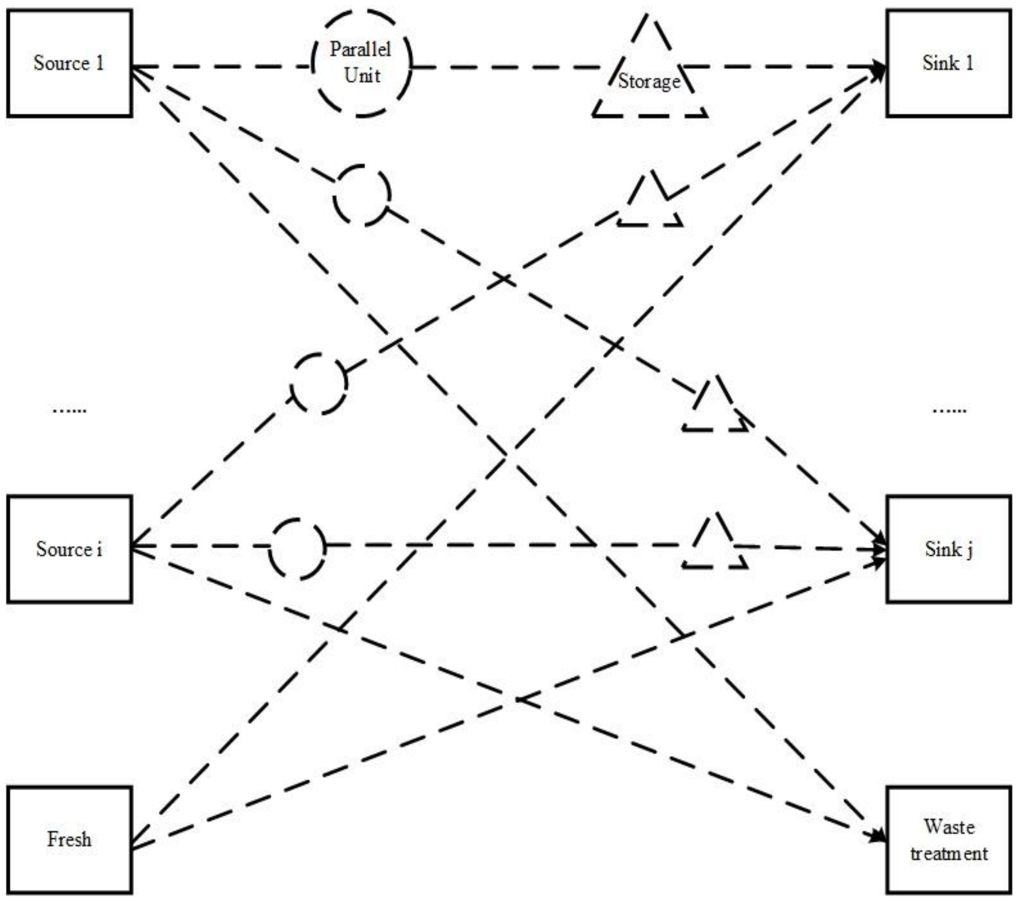


Figure 3 Connection between Sources and Sinks with Improving Methods

Based on the configuration shown in Figure 2, the mathematical formulations for calculating the connection reliability value need to be updated to include the effect of potential storage tanks and parallel units. The parallel pump section will have the system reliability value shown in Equation 21:

$$A_{i,j}^{pump} = 1 - \prod(1 - A^{pump}) \quad (21)$$

where $A_{i,j}^{pump}$ is the availability value of the parallel pump section between source i and sink j, and A^{pump} is the availability value of each individual pump within the subsystem.

Since the parallel pump unit showing in Figure 2 is optional, a binary variable is needed to assign to Equation 21. Equation 22 demonstrates the if-then condition for the parallel configuration:

$$\begin{cases} if\ y_{i,j}^{pump} = 0,\ \ then\ A_{i,j}^{pump} = A^{pump} \\ if\ y_{i,j}^{pump} = 1,\ \ then\ A_{i,j}^{pump} = 1 - (1 - A^{pump,1}) \cdot (1 - A^{pump,2}) \end{cases} \tag{22}$$

where $y_{i,j}^{pump}$ is the binary variable for the parallel pump unit between source i and sink j.

To reduce the nonlinearity and complexity of the problem, two identical pumps are assumed for the parallel unit system. No split of the water flow is allowed to ensure only one of the parallel pumps is functioning at a certain time. Thus, the availability of the pump section can be further updated using Equation 23:

$$A_{i,j}^{pump} = A^{pump} + (1 - A^{pump}) \cdot A^{pump} \cdot y_{i,j}^{pump} \tag{23}$$

Equation 23 satisfies the if-then condition in Equation 22 and the assumption of identical unit. Similarly, a binary variable will be assigned to the intermediate storage tank, where the if-then condition is the following:

$$\begin{cases} if\ y_{i,j}^{tank} = 0,\ \ then\ A_{i,j} = A_i \cdot A_{i,j}^{pump} \cdot A_j \\ if\ y_{i,j}^{tank} = 1,\ \ then\ A_{i,j} = A'_{i,j} \end{cases} \tag{24}$$

where $y_{i,j}^{tank}$ is the binary variable for the intermediate storage tank between source i and sink j, $A'_{i,j}$ is the connection reliability value after implanting the storage tank. The definition and value of $A'_{i,j}$ will be further discussed.

To model the new availability value, $A'_{i,j}$, of storage tanks, it is necessary to consider the different impacts of storage tanks on source and sink sides. If an incident happens on the sink side, the tank can be used to store water from the sources. Similarly, if an incident happens on the source side, the water stored in the tank can be supply to the sinks. However, under several conditions, these two events will not occur. For example, if an incident happens on the sink side and all storage tanks are full or an incident happens on the source side and there is no stored water in the tank, the continuous process will still be interrupted. So it is significant to consider the water level in the storage tanks to calculate the reliability value. In this study, since time is not considered as a variable, the water level of storage tanks will not be modeled as a continuous variable. Instead, a novel approach is proposed to quantify the condition of storage tanks as probability values. Three different states will be assigned to the storage tanks: (1) storages can fully satisfy sinks and sources, (2) storages can partially satisfy sinks and sources, and (3) storages can not satisfy sinks and sources. The probability value assigned to each state indicates the chance that the tank is at the certain state. Below is the mathematical model for such approach:

$$p_{i,j}^{tank,k} = \begin{cases} p_{i,j}^{tank,1} & State\ 1: storages\ can\ fully\ satisfy\ sinks\ and\ sources \\ p_{i,j}^{tank,2} & State.\ 2: storages\ can\ partially\ satisfy\ sinks\ and\ sources \\ p_{i,j}^{tank,3} & State\ 3: storages\ can\ not\ satisfy\ sinks\ and\ sources \end{cases}$$

The state probability of storage tank should also follow the Equation 25:

$$p_{i,j}^{tank,1} + p_{i,j}^{tank,2} + p_{i,j}^{tank,3} = 1 \qquad (25)$$

The value of the state probability will be determined by the reliability values of source i and sink j that are connected to the storage tank, the water flow, as well as the actually size of the tank.

Furthermore, the updated availability value, $A'_{i,j}$, can be calculated based on the different state probabilities as a weighted sum. When storage tank is at State 1, the reliability value between source i and sink j will be 1 since the needs of both ends can be satisfied whenever an incident happens within the connection. When storage tank is at State 2, the reliability value between source i and sink j will improve fractionally but not up to the value 1. When storage tank is at State 3, the reliability value between source i and sink j will stay the same. The mathematical model corresponds to the assumption is shown in Equation 26:

$$A'_{i,j} = p_{i,j}^{tank,1} \cdot 1 + p_{i,j}^{tank,2} \cdot (1+\delta) \cdot \left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right) + p_{i,j}^{tank,3} \cdot \left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right) \tag{26}$$

where δ is the fractional improvement in the reliability value at State 2.

The updated reliability formulation for connection between source i and sink j with consideration of storage tank can be summarized as Equation 27:

$$A_{i,j} = \left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right) \cdot \left(1 - y_{i,j}^{tank}\right) + A'_{i,j} \cdot y_{i,j}^{tank} \tag{27}$$

The if-then condition can also be applied to the binary variable, $y_{i,j}$ for the system reliability calculation. Since the overall system reliability value is the product of reliability value for each connection, an unmatched connection between source i and sink j should not affect the overall system reliability, thus should take the value of 1. The addition if-then condition is the following:

$$\begin{cases} if\ y_{i,j}\ = 0,\ \ then\ A_{i,j} = 1 \\ if\ y_{i,j} = 1,\ \ then\ A_{i,j} = \left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right) \cdot \left(1 - y_{i,j}^{tank}\right) + A'_{i,j} \cdot y_{i,j}^{tank} \end{cases} \tag{28}$$

So the final reliability formulation for connection between source i and sink j is:

$$A_{i,j} = \left(1 - y_{i,j}\right) + y_{i,j} \cdot \left[\left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right) \cdot \left(1 - y_{i,j}^{tank}\right) + A'_{i,j} \cdot y_{i,j}^{tank}\right] \tag{29}$$

Equations 21 and 29 conclude the reliability and availability formulation for the configuration shown in Figure 2 with consideration of reliability improving methods.

More constraints will be placed on binary variables for the intermediate storage tank and parallel pump unit, as shown in Equation 30-31.

$$y_{i,j} \geq y_{i,j}^{tank} \tag{30}$$

$$y_{i,j} \geq y_{i,j}^{pump} \tag{31}$$

The two equations show the if-then condition that if source i and sink j are not connected for water recycle, there will be no storage tank and parallel unit in between. If source i and sink j are connected, the selections for the two reliability-improving methods become optional and will be the optimization variables determined by the framework.

3.1.4 System Cost Formulation

In addition to the objective of system availability, the system cost is the other objective for this work. The overall cost of the network can be divided into two major components, system operating cost and fixed capital investment. The operating cost for the mass exchange system is assumed to be the sum of fresh water input cost and waste water treatment cost, as shown in Equation 32:

$$OC = F^{fresh} \cdot \gamma^{fresh} + F^{waste} \cdot \gamma^{waste} \tag{32}$$

where OC is the system operating cost, γ^{fresh} and γ^{waste} are unit costs for freshwater and wastewater treatment.

The fixed capital invest includes three major factors, which are the pipeline cost, the pump cost and the storage tank cost:

$$FC = \sum_{i,j} C_{i,j}^{pipeline} + \sum_{i,j} C_{i,j}^{pump} + \sum_{i,j} C_{i,j}^{tank} \tag{33}$$

The pipeline cost can be calculated using Equation 34 from Bishnu et al. (2014):

$$C_{i,j}^{pipeline} = \alpha \cdot \left(DI_{i,j}\right)^{\beta} \cdot d_{i,j} \tag{34}$$

where $C_{i,j}^{pipeline}$ is the pipeline fixed capital investment between source i and sink j, $DI_{i,j}$ is the diameter of the pipeline, $d_{i,j}$ is the shortest distance between source i and sink j, α and β are constant parameters.

The diameter of the pipeline, $DI_{i,j}$ can be determined based on flowrate between source i and sink j and the density of the flow (Bishnu et al., 2014):

$$DI_{i,j} = 0.363 \cdot \left(\left(\frac{f_{i,j}}{\rho}\right)^{0.45} \cdot \rho^{0.13}\right) \tag{35}$$

where ρ is the density of the flow.

The pump cost is assumed to be linearly dependent on the flowrate through the pump. Similarly, the cost of intermediate storage tank is assumed to be linearly dependent on the size of the tank. The correlations are shown in Equations 36 and 37:

$$C_{i,j}^{pump} = \gamma^{pump} \cdot f_{i,j} + \beta^{pump} \tag{36}$$

$$C_{i,j}^{tank} = \gamma^{tank} \cdot V_{i,j}^{tank} + \beta^{tank} \tag{37}$$

where $C_{i,j}^{pump}$ and $C_{i,j}^{tank}$ are the fixed capital investments for pump and tank between source i and sink j, γ^{pump} and γ^{tank} are the variable cost coefficients, $V_{i,j}^{tank}$ is the size of the storage tank within the connection, and β^{pump} and β^{tank} fixed cost coefficients for pump and tank accordingly.

To combine the operating cost with fixed capital investment and to form the overall system cost optimization objective, the annualized operating cost and fixed capital investment are calculated in Equations 38 and 39.

With the assumption of 8000 operating hours per year, the annualized operating cost is determined using Equation 38:

$$AOC = 8000 \cdot OC \tag{38}$$

With the assumption of 10% depreciation rate and 10-year life span of the system, the annualized fixed capital invest is determined using Equation 39:

$$AFC = \frac{FC \cdot (100\% - 10\%)}{10} \tag{39}$$

And the overall system cost will be the sum of annualized operating cost and fixed capital investment:

$$AC = AOC + AFC \tag{40}$$

Equations 32-40 summarize the system cost formulation in the optimization framework.

3.1.5 Preliminary Analysis of Reliability Improving Methods

Three reliability improving methods have been proposed in the previous sections. Before conducting a case study, we performed a preliminary analysis and comparison between different reliability improving methods to compare their costs and effectiveness on the overall system reliability value.

Alternative fresh and waste treatment are used to cover the downtime of the water recycle system when no other sources and sinks are available. For example, when a water source is shut down due to incidents, the demand of the water sinks that are connected to the specific source can be temporarily fulfilled by alternative freshwater inputs. It is also applicable the other side around for water sinks and wastewater treatment. The additional cost associated with this method is the following:

$$C_{i,j}^{alter} = F^{fresh,alter} \cdot \gamma^{fresh} \cdot T^{fresh,alter} + F^{waste,alter} \cdot \gamma^{waste} \cdot T^{waste,alter} \tag{41}$$

where $C_{i,j}^{alter}$ is the total alternative fresh and waste treatment cost between source i and sink j, $F^{fresh,alter}$ is the total amount of alternative fresh required, $F^{waste,alter}$ is the total amount of alternative waste treatment required, $T^{fresh,alter}$ is the total time annually that alternative fresh water input will be applied to sink j, and $T^{waste,alter}$ is the total time annually that alternative wastewater treatment will be applied to source i.

The impact of the alternative fresh and waste treatment can be summarized as the following:

$$A_i^{alter} = \frac{MTTF_i}{MTTF_i + MTTR_i - T^{fresh,alter}} \tag{42}$$

$$A_j^{alter} = \frac{MTTF_j}{MTTF_j + MTTR_j - T^{waste,alter}} \tag{43}$$

The extreme cases are when $T^{fresh,alter}$ equals to $MTTR_i$ and $T^{waste,alter}$ equals to $MTTR_j$. Since the down times for both source i and sink j are covered by the alternative fresh and waste treatment, the reliability values for source i and sink j should equal to 1.

Two additional inequalities should also be included to ensure the availability values of source i and sink j will not exceed 1:

$$T^{fresh,alter} \leq MTTR_i \tag{44}$$

$$T^{waste,alter} \leq MTTR_j \tag{45}$$

The comparison between reliability values of the original connection between source i and sink j and the updated one with alternative fresh and waste treatment is the following:

$$\%change = \left(\frac{A_i^{alter} \cdot A_{i,j}^{pump} \cdot A_j^{alter}}{A_i \cdot A_{i,j}^{pump} \cdot A_j} - 1 \right) \cdot 100\% \tag{46}$$

The parallel systems should be installed for units with low reliability value within the network, which in this work is the pump unit. Having the parallel systems can ensure a continuous process when the original unit breaks down and needs to be repaired. There are three different kinds of redundancy associated with parallel system, which are cold standby, warm standby, and hot standby system. However, in this work, we only consider cold standby parallel system to ensure the full capacity can be reached when the parallel unit is used to recover the downtown of the original unit.

The cost for the cold standby parallel pump system is summarized in Equation 47 as:

$$C_{i,j}^{pump,cold} = \gamma^{pump,cold} \cdot f_{i,j} + \beta^{pump,cold} \tag{47}$$

The reliability value between source i and sink j for the cold standby parallel pump system is summarized in Equation 48:

$$A_{i,j}^{pump,cold} = A^{pump,cold} + (1 - A^{pump,cold}) \cdot A^{pump,cold} \cdot y_{i,j}^{pump,cold} \tag{48}$$

The comparison between reliability values of the original connection between source i and sink j and the updated one with parallel pump is the following:

$$\%change = \left(\frac{A_i \cdot A_{i,j}^{pump,cold} \cdot A_j}{A_i \cdot A_{i,j}^{pump} \cdot A_j} - 1 \right) \cdot 100\% \tag{49}$$

As mentioned in the precious section, the storage tanks are used to reduce system downtime by storing water flows from water sources due to failure of water sinks, or by supplying stored water to the sinks due to failure of water sources. The cost for a storage tank between source i and sink j was summarized in Equation 50:

$$C_{i,j}^{tank} = \gamma^{tank} \cdot V_{i,j}^{tank} + \beta^{tank} \tag{50}$$

The reliability value between source i and sink j was summarized in Equation 51:

$$A'_{i,j} = p_{i,j}^{tank,1} \cdot 1 + p_{i,j}^{tank,2} \cdot (1+\delta) \cdot \left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right) + p_{i,j}^{tank,3} \cdot \left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right) \tag{51}$$

One additional inequality should also be included to ensure the availability values of source i and sink j will be smaller than 1 for the second state:

$$(1+\delta) \cdot \left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right) < 1 \tag{52}$$

The comparison between reliability values of the original connection between source i and sink j and the updated one with storage tank is the following:

$$\%change = \left(\frac{p_{i,j}^{tank,1} \cdot 1 + p_{i,j}^{tank,2} \cdot (1+\delta) \cdot \left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right) + p_{i,j}^{tank,3} \cdot \left(A_i \cdot A_{i,j}^{pump} \cdot A_j\right)}{A_i \cdot A_{i,j}^{pump} \cdot A_j} - 1\right) \cdot 100\% \qquad (53)$$

In addition to the model differences between three reliability improving methods, we use a specific case to observe the actual cost and reliability improvement. We assume a water source and a water sink both with a 60 hr MTTR and 1440 hr MTTF. The availability value associated with the source and the sink is 0.96. The reliability value for the pump unit is assumed to be 0.85. The water flowrate between the source and the sink is assumed to be 10 MT/hr.

For alternative fresh and waste treatment, the unit costs for fresh water and wastewater treatment are assumed to be \$1/MT and \$5/MT accordingly. The annual downtime for both the source and sink is 320 hr. Thus, the annual cost for alternative fresh and waste treatment can be estimated to be \$3,200 and \$16,000, and \$19,200/yr total. The reliability value for connection is increased from 0.783 to 0.85, which is an 8.6% increase.

For the parallel pump unit system, the variable cost coefficient and the fixed cost coefficient are assumed to be \$90000/MT and \$800. One pump is assumed to pressurize the 10 MT/hr water flow. The overall cost is estimated to be \$98,000/yr. With the assumptions of 10-year life span and 10% depreciation rate, the annualized fixed cost is calculated to be \$8,820. The reliability value for the connection is increased from 0.783 to 0.901, which is a 15.1% increase.

For a storage tank system with size 1,000 MT to cover 100 hr repair time, 1 identical tanks with 1000 MT capacity are included in the system. The cost is estimated as \$160,000. With the assumptions of 10-year life span and 10% depreciation rate, the annualized fixed cost is calculated to be \$14,400/yr. The probability values for all three states are assumed to be 0.3, 0.6, and 0.1 accordingly. The δ value is assumed to be 0.25. The updated reliability value between source i and sink j is estimated to be 0.966, which is a 23.8% increase.

Based on the data assumed in this section, the preliminary analysis results are shown in Table 1. The alternative fresh and waste treatment has the highest additional annualized cost, but has the lowest percentage improvement in reliability value between source i and sink j. The storage tank has the second highest additional annualized cost, but the reliability value between source i and sink j increases the most in the three cases. If the coefficient data for the three methods is different, the results of the preliminary analysis will also change.

Table 1 Results from the Preliminary Analysis

Method	Cost (\$/yr)	Reliability Improvement (%)
Alternative fresh and waste	19200	8.6
Parallel System	8820	15.1
Storage Tank	14400	23.8

3.2 Methodology for Reverse Osmosis Unit Operation

The overall structure and boundary of this study is shown below in Figure 4. A stream of input water (either seawater or wastewater) with certain level of containment is fed into the network. A system containing conventional and non-conventional pretreatment technologies, as well as different combinations of both categories is built to determine the optimal pathway to treat the feed water before going into the RO unit. The RO unit will then perform further membrane separation, and permeate water that meets the standards and requirements is collected afterwards. The model developed in this work can be divided into two parts, a RO unit model and a RO membrane fouling model.

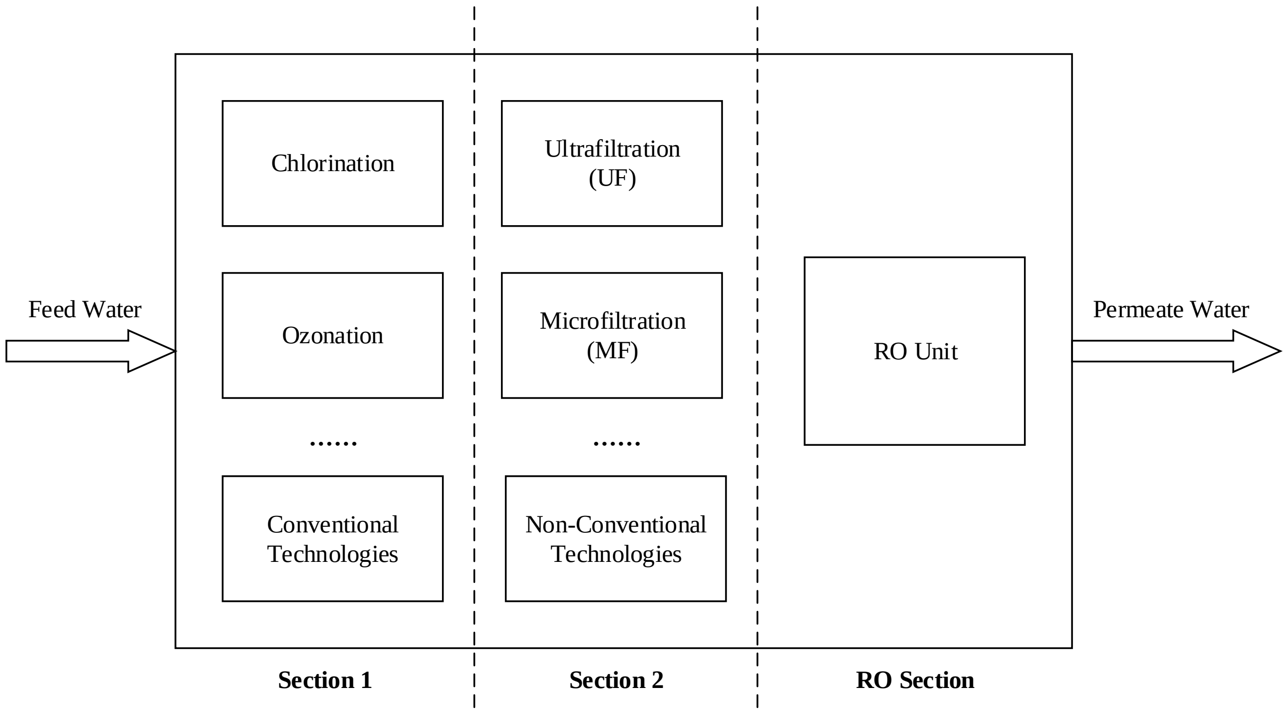


Figure 4 Overall Network Design for RO System

3.2.1 RO Unit Model

The RO unit for water treatment is summarized in Figure 5. Seawater or wastewater is pressurized through a pump and is fed into the RO unit. The membrane separates the water stream into two different outlets, a permeate stream with low contaminant concentrations and a reject stream with high contaminant concentrations. The flowrate, concentration and pressure of those streams are also listed in Figure 5.

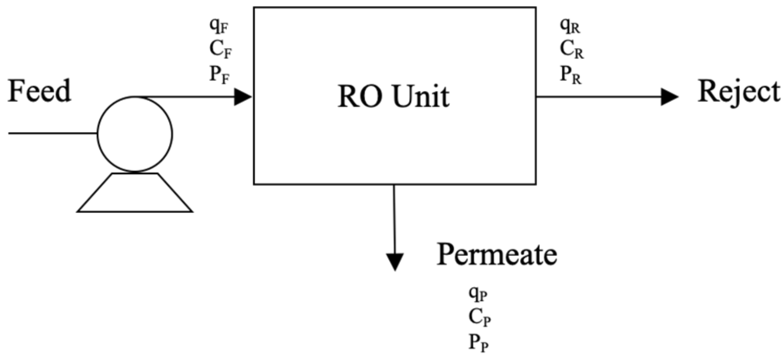


Figure 5 Representation of the RO Unit

The mathematical model associated with the RO unit mass balance is shown below:

$$q_F = q_P + q_R \tag{54}$$

$$q_F \cdot C_F = q_P \cdot C_P + q_R \cdot C_R \tag{55}$$

where q_F is the flow rate of the feed stream, q_P is the flow rate of the permeate stream, q_R is the flow rate of the reject stream, C_F is the concentration of contaminants in the feed stream, C_P is the concentration of contaminants in the permeate stream, C_R is the concentration of contaminants in the reject stream.

According to El-Halwagi (2017), the water flux coming out of the RO unit can be modeled as the following:

$$N_{water} = A \cdot (\Delta P - \frac{\pi_F}{C_F} \cdot C_0) \cdot \gamma_{RO} \tag{56}$$

$$\Delta P \approx \frac{P_F + P_R}{2} - P_P \tag{57}$$

$$C_0 \approx \frac{C_F + C_R}{2} \tag{58}$$

where N_{water} is water flux, A is the membrane permeability, ΔP is the pressure difference across the membrane, π_F is the osmotic pressure, C_0 is the average contaminant concentration in the shell side, γ_{RO} is constant parameter determined by the shape and size of the RO unit, P_F is the feed pressure, P_P is the pressure of permeate, P_R is the pressure of reject.

Additional constraints are placed on the permeate flow as Equation 59, 60, 61, and 62.

$$q_P = S \cdot N_{water} \tag{59}$$

$$N_{water} = A \cdot [\Delta P - \frac{\pi_F}{2} \cdot \left(1 + \frac{C_R}{C_F}\right)] \cdot \gamma_{RO} \tag{60}$$

$$q_P = S \cdot A \cdot [\Delta P - \frac{\pi_F}{2} \cdot \left(1 + \frac{C_R}{C_F}\right)] \cdot \gamma_{RO} \tag{61}$$

$$C_P \approx \frac{N_{solute}}{N_{water}} \tag{62}$$

where S is the surface area, N_{solute} is the solute flux.

The model also involves multiple single state RO units in parallel:

$$Q_F = n \cdot q_F \tag{63}$$

$$Q_P = n \cdot q_P \tag{64}$$

$$Q_R = n \cdot q_R \tag{65}$$

$$Q_F = Q_P + Q_R \tag{66}$$

$$Q_F \cdot C_F = Q_P \cdot C_P + Q_R \cdot C_R \tag{67}$$

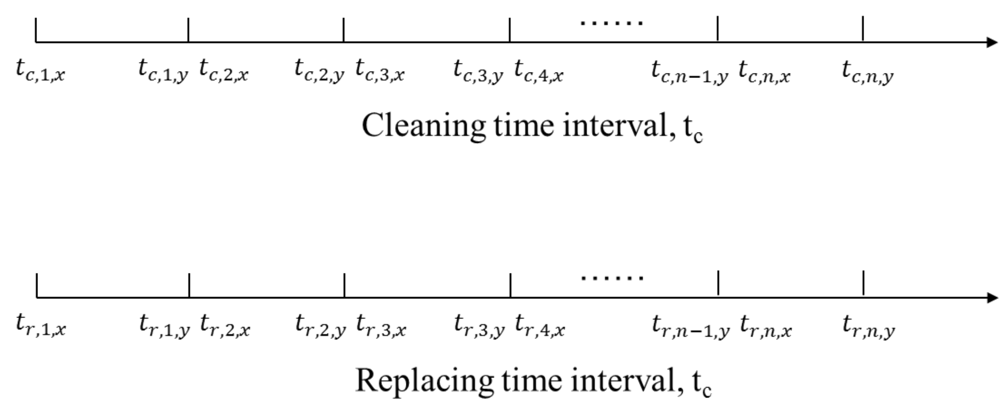
where n is the number of RO units in parallel, Q_F is the total feed flow rate, Q_P is the total permeate flow rate, Q_R is the total reject flow rate.

3.2.2 RO Membrane Fouling Model

In addition to the RO unit model, the optimization framework also includes the RO membrane fouling model that will be presented in this section.

To model the cleaning and replacing strategy for RO membrane with no pretreatment technologies, the technique from Lu et al. (2006) is used and presented in the following section.

First, timelines for both cleaning and replacing are constructed as shown in Figure 6a and 6b.



a.

b.

Figure 6 (a) Timeline for Cleaning Schedule of RO membranes. **(b)** Timeline for Replacing Schedule of RO Membranes

Based on the time intervals for both cleaning and replacing, the mathematic model for RO membrane schedule can be shown as following:

$$t_{c,n,x} = \left(1 - \sigma_{c,n}\right) * t_{c,n-1,y} \tag{68}$$

$$t_{c,n,y} = t_{c,n,x} + \Delta t \tag{69}$$

$$t_{r,n,x} = \left(1 - \sigma_{r,n}\right) * t_{r,n-1,y} \tag{70}$$

$$t_{r,n,y} = t_{r,n,x} + \Delta t \tag{71}$$

$$\sigma_{c,n} \geq \sigma_{r,n} \tag{72}$$

$$A_n = A_0 \cdot (1 - \varphi \cdot t_{r,n}) \cdot exp(-\frac{t_{c,n}}{\tau}) \tag{73}$$

where $t_{c,n,x}$ and $t_{c,n,y}$ are the beginning and ending time for each cleaning interval, $t_{r,n,x}$ and $t_{r,n,y}$ are the beginning and ending time for each replacing interval, Δt is the equally divided time interval for both cleaning and replacing, $\sigma_{c,n}$ and $\sigma_{r,n}$ are binary variables at the beginning of each interval (when cleaning or replacing is taking places, the variables take value 1, if not, 0), A_n is the permeability of the RO membrane after n interval, A_n is the initial permeability of the membrane, φ is the membrane degraded constant, and τ is the membrane decay constant.

By applying Equation 68 to 73 and based on the timelines in Figure 6, the general permeability versus time plot can be constructed as Figure 7:

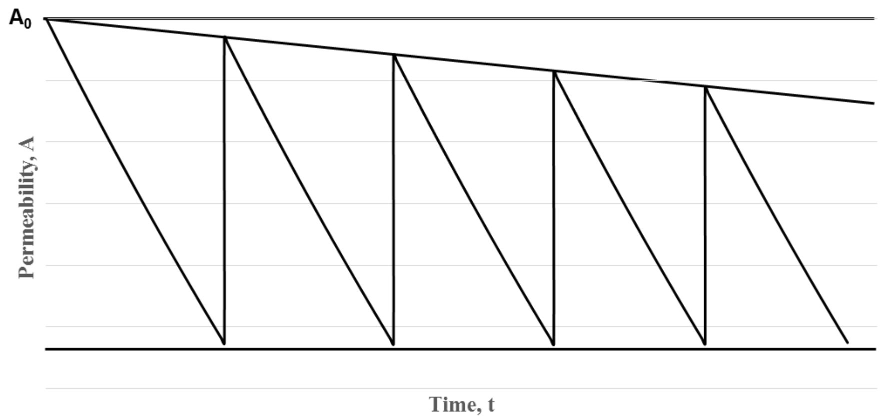


Figure 7 RO Membrane Permeability versus Time Plot

3.2.3 Pretreatment Technologies

A set of pretreatment technologies, G, is defined as:

$$G = [G_1, G_2, G_3, \dots G_n] \tag{74}$$

A binary variable, β_i, is assigned to each technologies so that $\beta_i = 1$ when the system picks technology G_i:

$$COST_{system} = \sum_n \beta_i * COST_i + \varepsilon \tag{75}$$

$$\beta_i \in [0,1] \tag{76}$$

where $COST_{system}$ is the unit cost ($/m^3 permeate water) for the entire pretreatment network, $COST_i$ is the unit cost ($/m^3 permeate water) for individual technologies, ε is the cost deviation from the sum of all individual unit costs when combining these pretreatment technologies.

Different pretreatment technologies that can be applied to the RO system are summarized in Table 2.

Table 2 Potential RO Pretreatment Technologies

Conventional Pretreatment Technologies	**Information**
Disinfection	chlorination, ozonation
Acid addition for pH control	sulfuric acid/hydrochloric acid for pH reduction to increase calcium carbonate solubility
Coagulation addition	small, positively charged molecules
Flocculation addition	high molecular weight and anionic polymers for high SDI feed water
Clarification with floatation	Dissolved Air Flotation (DAF)
Scale inhibitors/Antiscalants	polyacrylates, organophosphonates, sodium hexametaphosphate (SHMP)
Non-Conventional Pretreatment Technologies	**Information**
Microfiltration (MF)	pore sizes 100-5000 nm
Ultrafiltration (UF)	pore sizes 10-100 nm
Nanofiltration (NF)	pore sizes 1-2 nm

3.2.4 Optimization Framework

Additional constraints are placed on stream flowrate, concentration, and membrane permeability.

$$Q_P \geq Q_P^{min} \tag{77}$$

$$C_P \leq C_P^{max} \tag{78}$$

$$q_F^{min} \leq q_F \leq q_F^{max} \tag{79}$$

$$A_n \geq \rho \cdot A_0 \tag{80}$$

$$\sigma_{c,n} \geq \sigma_{r,n} \tag{81}$$

Based on different circumstances, the value of the water flux has to be bigger than a certain value to meet fresh water output quantity requirement:

$$N_w \geq N_0 \tag{82}$$

In addition to water quantity, constraints should also be placed on output water quality.

Based on previous equations, the overall RO membrane cleaning and replacing cost can be concluded as Equation 83:

$$COST_{RO} = COST_c * \frac{T}{\tau} + COST_r * T * \varphi \tag{83}$$

where T is the expected running time for the RO unit.

The objective function for the optimization framework is shown as Equation 83:

$$min\, COST_{total} = COST_{system} + COST_{RO} \tag{84}$$

3.3 Methodology for Hazardous Material Transportation Safety

3.3.1 The Supply-and-Demand Material Allocation Model

The traditional material allocation optimization framework is used in this research. The framework can deal with the allocation problem of a certain commodity from suppliers to plants. The objective of the framework is to minimize the transportation cost while still fulfilling demands of all receiving plants (El-Halwagi 2017b). The total amounts of materials that need to be transported between each supplier and plant are the optimization variables. The transportation cost of HazMat c from supplier i to plant j using transportation mode t is calculated by the product of HazMat replenishment rate, the distance between supplier i and plant j, and the unit cost of transportation mode t. The total shipping cost (TSC) for the supply chain network is shown in Equation 85.

$$TSC \ = \ \sum_{c \in C} \sum_{i_c \in I} \sum_{j_c \in J} \sum_{t_c \in T} (f_{i_c,j_c,t})(S_t)\,(D_{i_c,j_c,t}) \tag{85}$$

where TSC is the total shipping cost, $\mathrm{f}_{\mathrm{i}_c,\mathrm{j}_c,t}$ is the replenishment rate of material c between supplier i and plant j using mode t, S_t is the unit cost of transportation mode t, and $D_{i_c,j_c,t}$ is the travel distance between supplier i and plant j using mode t.

In addition to the traditional material allocation problem, the objective of the work looks to include the risk associated with each shipment in the framework since the materials being transported are hazardous. Based on the USDOT guidelines, the risk is determined by the factor of accident probability and accident consequences (Harwood et al., 1993). Two questions arise while dealing with HazMat transportation: how is the risk associated with the company's supply chain network and how much risk is the company willing to accept. To address these questions, this paper considers the transportation risk adhered with the HazMat supply chain network by relating the risk with the possibility of an incident happening within a certain distance traveled, considering the amount of HazMat being transported. The overall risk for the same network in the economic object function is calculated using Equation 86 as shown below.

$$R = \sum_{c \in C} \sum_{i_c \in I} \sum_{j_c \in J} \sum_{t_c \in T} (V_t)(N_{i_c,j_c,t})(P_{ic,jc,t}) \tag{86}$$

where V_t is the value loss per accident for transportation mode t, $\mathrm{N}_{\mathrm{i}_c,\mathrm{j}_c,t}$ is the number of trips made between supplier i and plant j using transportation mode t, $P_{ic,jc,t}$ is the possibility of an accident happen between supplier i and plant j using transportation mode t. It is worth noting that Equations

67 and 68 may be formulated to include the impact of uncertainty such as uncertain transportation costs, energy prices, and risks.

The number of trips made is determined by the replenishment rate for material c and the capacity of transportation mode t per trip, which is shown in Equation 87. The possibility of an accident is correlated with the distance travelled based on historical data and will be explained in the case study.

$$N_{i_c,j_c,t} = f_{i_c,j_c,t}/M_t \tag{87}$$

where M_t is the maximum capacity of transportation mode t per trip.

The demand of material c at plant j is equal to the sum of the replenishment of the material c sent to the plant j.

$$D_{j,c} = \sum_{i_c \in I} \sum_{t_c \in T} (f_{i_c,j_c,t}) \tag{88}$$

The total supply of material c from supplier i to all plants in the network should not exceed its supply capacity of material c.

$$S_{i,c} \geq \sum_{j_c \in J} \sum_{t_c \in T} (f_{i_c,j_c,t}) \tag{89}$$

3.3.2 The Epsilon-Constraint Method for Multi-Objective Optimization

The ε-constraint method is used to convert the multi-objective optimization problem into a single-objective optimization problem with additional inequality constraints. The two-objective optimization framework in our case was transformed by changing risk as a constraint and assigning an upper bound, ε, to it. The optimization problem is solved at each epsilon value, and the minimum TSC value is determined at each point to form a Pareto-optimum curve. With the constraints on demand and supply as shown in Equation 88 and 89, the ε-constraint method framework is shown in Equation 90.

$$\min_{f} \quad TSC\,(f)$$

$$s.t. \quad R \leq \varepsilon \tag{90}$$

$$D_{j,c}(f)$$

$$S_{i,c}(f)$$

The linear model as shown in Equation 90 is applied to Lingo and solved for the amount of HazMat, f, transported between each supplier and plant. Each supplier was defined as a source, as well as each plant was defined as a destination.

3.3.3 Risk Quantification

According to the definition of the risk function, as shown in Equation 68, the possibility of an incident happen between suppliers and consumers is necessary for quantifying risk in the optimization framework. Samuel et al. (2009) proposed an approach to correlate transportation incident frequency with distance from origin to incident location. The method is used in our case study with additional technique on transforming incident frequency to incident probability. Detailed procedures and results from the approach are shown in this section.

The historical HazMat incident data used in this study was retrieved from the database of the Pipeline and Hazardous Materials Safety Administration of USDOT (PHMSA – HazMat Incident Report Search website). The database includes incidents involving fatalities, major injuries, evacuations and facility shut down that are reported to USDOT under the US Code of

Federal Regulations (CFR) 171.15 (Samuel et al., 2009). The data obtained from the database contains comprehensive information on each incident, such as the location of the incident, postal code of the incident, mode of transportation, transportation phase, the location of the origin, postal code of the origin, packaging type, the total amount of material loss and many other factors. The dataset was further processed to target the desired types of incidents (for example: certain transportation modes/transportation phase).

Since the data set obtained from USDOT does not include any information on transportation route and distance between incident locations and the origins, Geocoding and Haversine Formula are necessary techniques to convert existing information into desired data (Samuel et al., 2009). The major idea behind geocoding is to translate zip codes of incident locations to longitude and latitude data based on a complete database of U.S. postal codes and their coordinates. Furthermore, Haversine Formula is applied to calculate the great circle distance between two locations on a sphere using the longitude and latitude data, as shown in Equation 91 (Samuel et al., 2009):

$$distance = r * arctan\sqrt{\frac{(cos\beta_2 sin(\alpha_2-\alpha_1))^2+(cos\beta_1 sin\beta_2-sin\beta_1 cos\beta_2 cos(\alpha_2-\alpha_1))^2}{sin\beta_1 sin\beta_2+cos\beta_1 cos\beta_2 cos(\alpha_2-\alpha_1)}} \tag{91}$$

where r is the radius of Earth when we assume a perfect sphere (6378 km), α_1 is the longitudes of the origin locations, α_2 is the longitudes of the incident locations, β_1 is the latitudes of the origin locations, and β_2 is the latitudes of the incident locations.

The process is comprehensively explained by Samuel et al. (2009), and is presented in Figure 8.

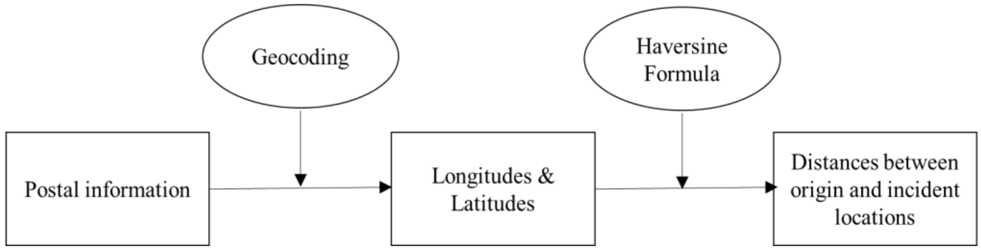


Figure 8 Method to Calculate Distances between Origins and Incident Locations

After obtaining the distances between incident locations and origins, it is possible to construct an incident frequency plot based on the distance data. The plot will provide an insight on the correlation between incident frequency and distance travelled. According to Samuel et al. (2009), the frequency distribution presents a bimodal trend, which is proven and demonstrated by the case study in this paper as well. Due to lack of statistical models to present the bimodal correlation, empirical probability estimation was used to determine the probability of an incident happened at a certain traveling distance. It is assumed that each incident is equally distributed and has the same probability value. The value is determined using Equation 92:

$$P_{incident,c,t} = \frac{1}{N_{\,incident,c,t}} \tag{92}$$

where $P_{incident,c}$ is the probability of a single incident for HazMat c using transportation mode t when we assume all incidents are equally distributed, $N_{incident,c}$ is the total number of incidents happened for HazMat c using transportation mode t.

The cumulative probability at a certain distance d, is the sum of probability values of all incidents happened before the distance d, as shown in Equation 93:

$$P_{incident,c,t,d} = \sum_d P_{incident,c,t} \tag{93}$$

The value we obtained from Equation 75 represents the distribution of incidents happened for HazMat c using transportation mode t over travelling distance d. It can be treated as a conditional probability when we know an incident must happen at certain maximum distances. In order to apply such probability values to the Equation 86, we need to calculate the overall probability using Equation 94 as shown below:

$$P(c_{t,d}) = P(c_{t,d}|c_t) * P(c_t) \tag{94}$$

where $P\left(c_{t,d}\right)$ is the overall probability of an incident for transporting HazMat c using mode t at distance d, $P\left(c_{t,d}\middle|c_t\right)$ is the cumulative probability calculated from Equation 94, $P(c_t)$ is the general probability of an incident for transporting HazMat c using mode t.

According to Harwood et al. (1993), the risk is determined by the factor of accident probability and accident consequences. The model is common in calculating transportation risk and has been used in many studies, such as Kazantzi et al. (2011). The risk function we presented in Equation 86 uses the same model with modifications based on our study. Since we correlated risk with distance travelled, a fixed risk value can be calculated for one shipment between certain sources and sinks with known distances. It is necessary to include the number of shipment between sources and sinks to determine the overall risk. In addition, the values of accident consequences can be largely varied between studies. For example, Kazantzi et al. (2011) calculate the number of population that can be affected by a certain HazMat incident as the consequences. In this study, based on the framework and data availability, the total amount of HazMat released from the incident is used as the consequence. It will be further explained in the case study when the data is presented. All probability and risk calculations and the correlation will also be demonstrated in the following case study section.

4. RESULTS AND DISCUSSION*

From the methodology section, the systematic approach that has been developed used existing data and models to quantify safety and reliability variables and to integrate the safety and reliability analyses as additional objectives in the existing optimization framework. In this section, the results that were obtained using the systematic approach in this work will be presented and discussed. The major target is to use those results to guide the decision making process of the management to achieve better performances and economic metrics. The major findings include the following options:

- Data-based or model-based correlations for safety and reliability analyses
- Novel integration and optimization frameworks for multi-objective programming problems
- Optimal or Pareto optimal results for system designs and operation strategies

As mentioned in the previous section, although the general methodology was proposed, each research project toke its own approach based on the data and model availability. The altered approaches in different projects will give distinct results including multiple integration and optimization solutions. The following sub-section will summarize the findings of the three research projects that have been proposed.

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4.1 Results and Discussion for Reliability Analysis in Direct Water Recycle Network

4.1.1 Optimization Cases

Based on the formulation explained in the previous section, it results in a mixed integer, non-linear programming problem. As mentioned in the problem statement, two distinct MINLP optimization cases will be considered for the water recycle network problem: (1) a single-objective MINLP where system reliability is integrated into the system cost objective function, and (2) a multi-objective MINLP that maximizes system reliability and minimizes system cost. Case 1 considers system availability value as a factor in the overall cost objective function. The result of Case 1 constitutes one design and operation strategy for the network, which associates with one cost value. To further understand the result, sensitive analysis is performed on different constants to demonstrate their effects on the optimization result. Case 2 uses the epsilon constraint method, which transfers the cost objective to a constraint, and solves for the Pareto optimal solutions. The result of Case 2 consists multiple optimal solutions with different system reliability and cost values for guiding the future decision-making process. Both Case 1 and 2 involve the combinatorial optimization problem for the selection of parallel pump unit and storage tank in between each connection. The optimization frameworks that are developed for both cases are presented in detail and further explanations in the following subsections.

Case One: Single Objective Framework

To consider system availability value as a factor in the overall system cost objective, it is important to understand how availability affects the mass exchange network. When the water recycle network becomes unavailable, the supply of sources can not be used to fulfill the demand of sinks. All supply will be forced into waste water treatment, and all demand will be fulfilled by fresh water input. So the unavailable time or system down time will be treated as an additional cost factor in the cost objective function. The system down time is calculated as a fraction of the overall operating time (assumed 8000 hours per year) using the following equation:

$$T_{system}^{down} = (1 - A_{system}) \cdot 8000 \tag{95}$$

where T_{system}^{down} is the annual system down time for the network, and $1 - A_{system}$ is the fraction of time that the system will not be available during the operation.

The additional cost factor associated with the system down time can be calculated using Equation 95, where all water coming from sources during the down time is fed into waste water treatment and all sinks are using fresh water input at the same time:

$$C_{system}^{down} = T_{system}^{down} \cdot (\gamma^{waste} \cdot \sum_i F_i + \gamma^{fresh} \cdot \sum_j F_j) \tag{96}$$

The updated overall cost objective function is shown below:

$$AC = A_{system} \cdot 8000 \cdot OC + C_{system}^{down} + AFC \tag{97}$$

where the system is functional during normal time, so the other fraction of total operating time, $A_{system} \cdot 8000$, can still be applied to the regular hourly operating cost of the system.

The optimization framework for Case 1 minimizes AC from Equation 97, and includes constraints from Equations 4-10, 12, 15-16, 20, 23, 25-26, 29-40, 95-96.

Case Two: Multi Objective Framework

The second case evaluates system availability and system cost spontaneously at the same time forming a multi-objective MINLP problem. Similar to the epsilon constrain method applied in Zhang et al. (2018), the cost function from Equation 40 is transformed to a constraint using Equation 98:

$$AOC + AFC \leq \varepsilon \tag{98}$$

The optimization problem is solved at each epsilon value for the maximal system availability to form a Pareto optimal curve between system cost and availability. Each point on the curve is an optimal result associated with a design and operation strategy for the direct water recycle network.

The system availability function from Equation 20 is also reformed as demonstrated in Equation 99:

$$\ln(A_{system}) = \sum_{i,j} \ln(A_{i,j}) \tag{99}$$

Since the variable A_{system} is always greater than zero, and the natural logarithm function is monotonically increasing, maximizing A_{system} is the same as maximizing the natural log of the variable, $\ln(A_{system})$. The optimization framework for Case 2 maximizes $\ln(A_{system})$ from Equation 99, and includes constraints from Equations 4-10, 12, 15-16, 23, 25-26, 29-39, 98.

4.1.2 Case Study

A case study for a direct water recycle network with three sources and four sinks is considered for all three optimization cases in this section. The supplies and demands for the network are summarized in Table 3. The distances between each sink and each source are summarized in Table 4. The impurity concentrations for sources and sinks are summarized in Table 5. Table 6 includes the availability constants for all sources and sinks. The coefficients that are used in the calculations are shown in Table 7. All models are solved using GAMS 26.1.0 and commercial solver BARON (Tawarmalani and Sahinidis, 2005 & Sahinidis and Tawarmalani, 2017).

Table 3 Supply and Demand Data for Sources and Sinks

Source	**Supply (MT/h)**
1	30
2	38
3	32
Sink	**Demand (MT/h)**
1	31
2	23
3	27
4	29

Table 4 Shortest Distance between Sources and Sinks

Distance (km)	**Sink 1**	**Sink 2**	**Sink 3**	**Sink 4**	**Waste**
Source 1	10	8	7	5.5	2.5
Source 2	6.6	7.5	8.2	9	3
Source 3	4.5	7.5	3.6	6.6	2.8
Fresh	10	8.6	7.2	7.4	N/A

Table 5 Impurity Concentration Limits for Sources and Sinks

	Impurity limits (weight%)
Source 1	4
Source 2	3
Source 3	2
Sink 1	[0, 4]
Sink 2	[0, 5]
Sink 3	[0, 3]
Sink 4	[0, 6]

Table 6 MTTF and MTTR Data for Sources and Sinks

	Source 1	Source 2	Source 3	Sink 1	Sink 2	Sink 3	Sink 4	Pump
MTTF (h)	2940	1440	940	2940	1140	1140	1440	
MTTR (h)	60	60	60	60	60	60	60	
$A_{inherent}$	0.98	0.96	0.94	0.98	0.95	0.95	0.96	0.85

Table 7 Coefficients Used in the Model

Constant	**Value**	**Unit**
μ	1	
U	100	
NC	8	
γ^{fresh}	1	$/MT
γ^{waste}	5	$/MT
γ^{pump}	90000	$/MT
β^{pump}	800	$
γ^{tank}	60	$/MT
β^{tank}	100000	$
α	3114.86	
β	1.0532	
ρ	1000	kg/m^3

4.1.3 Results from Optimization Case One

The single objective MINLP problem proposed in the optimization case 1 was solved and the results are summarized in Figure 9. The result only shows one unique system design and water relocation and recycling strategy. The annualized cost of the system is $657182.3. The annualized fixed capital investment is $234115.6. The operating cost is $74282.2 per year. The penalty associated system downtime is $348784.5 per year. The system availability value is 0.929.

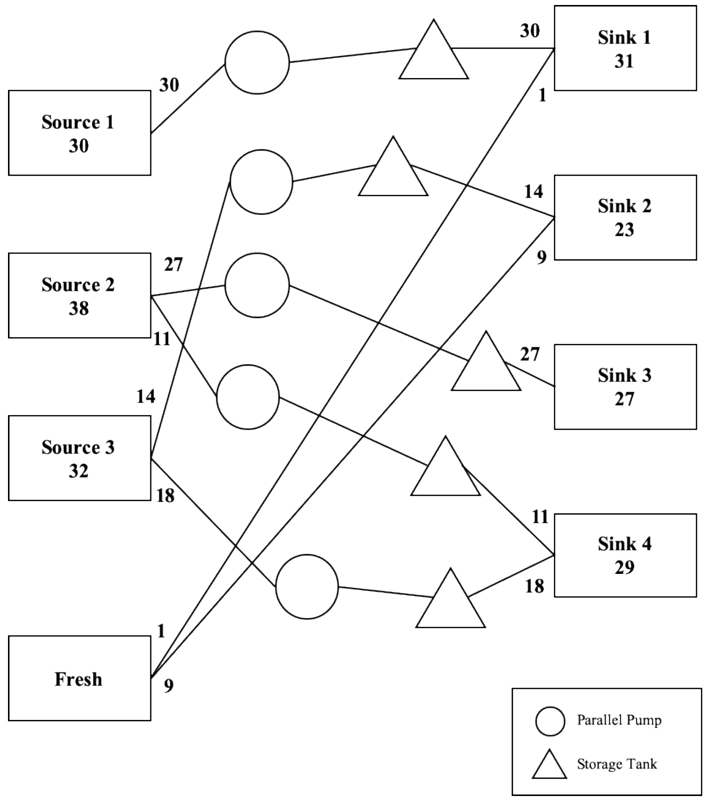


Figure 9 System Design and Assignment with A=0.929

To further understand the model and the problem, sensitivity analyses will need to be performed on different constants to study their effects on the optimization results. The first sensitivity analysis assumes that the costs of fresh water and waste treatment decrease dramatically, which could happen in regions with abundant water resources. The freshwater input is \$0.1/MT and the waste treatment is \$0.5/MT, which are both 10% of the original prices. The results are summarized in Figure 10. The annualized cost of the system is \$178927.3. The annualized fixed capital investment is \$33175.8. The operating cost is \$12805.2 per year. The additional cost due to system down time is \$132946.3 per year. The system availability value is 0.728. Due to the light penalty on system shutdown, the framework will a low availability value with low annualized capital cost.

Similarly, the second sensitivity analysis assumes that the annualized fixed cost increases dramatically due to material and human factor. The fixed cost is assumed to be 5 times of the current value. The results are summarized in Figure 11. The annualized cost of the system is $1,486,086.8. The annualized fixed capital investment is $832352.7. The operating cost is $70437.8 per year. The additional cost due to system down time is $583296.3 per year. The system availability value is 0.880. Due to the heavy cost of installing storage tanks and parallel pump units, the framework will ensure a low system availability value with less improving method installed.

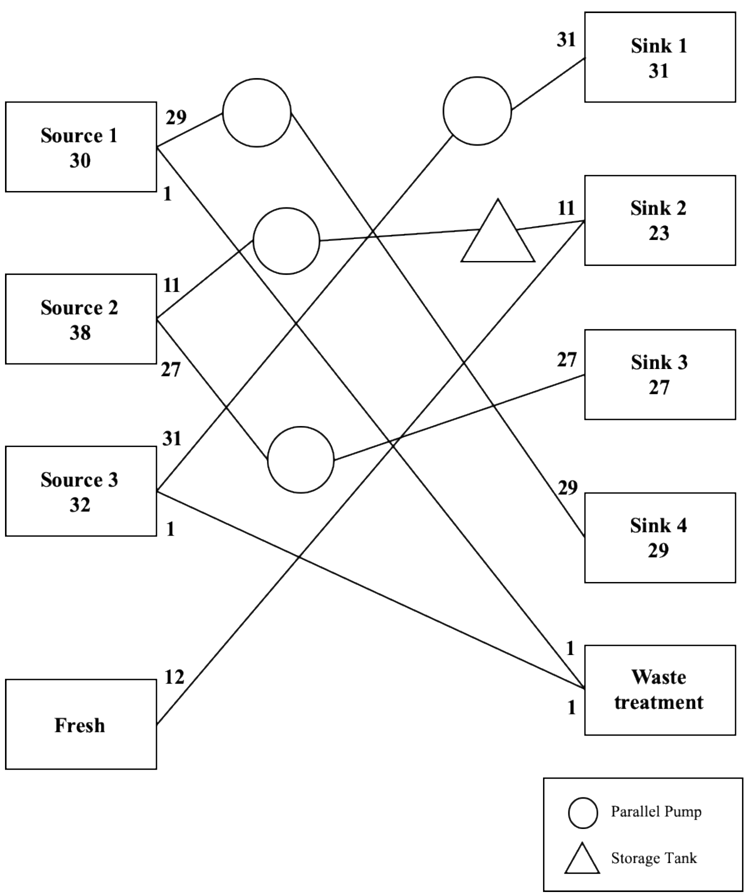


Figure 10 System Design and Assignment with A=0.728

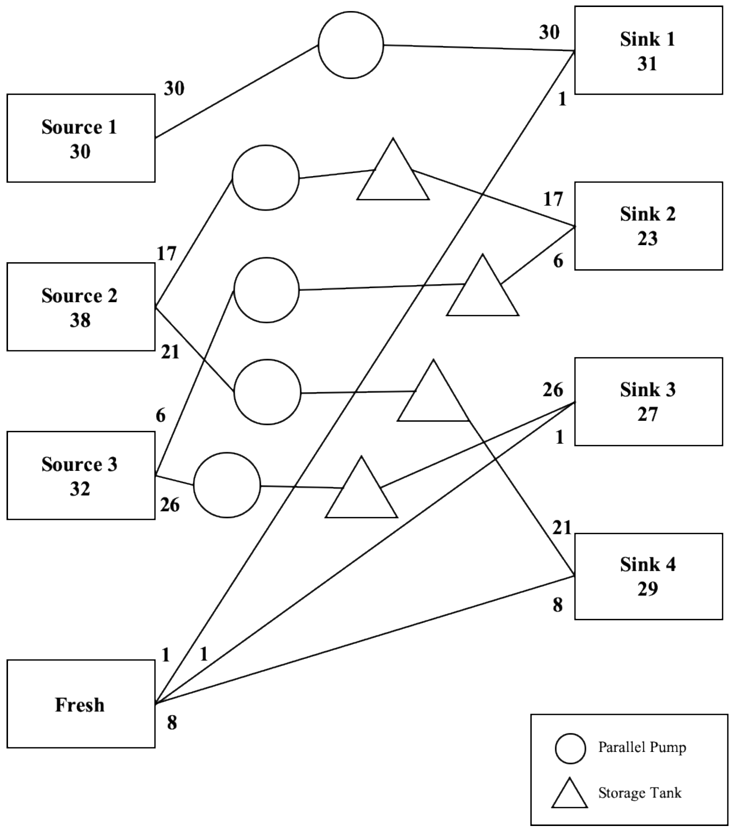


Figure 11 System Design and Assignment with A=0.880

4.1.4 Results from Optimization Case Two

The multi-objective MINLP problem proposed in the optimization case 2 was solved by changing system cost objective function to a constraint and obtaining the optimal system availability value using Equation 98. The second case will result in a Pareto optimal curve, as shown in Figure 12, which shows the tradeoff between systems annualized cost and system availability value.

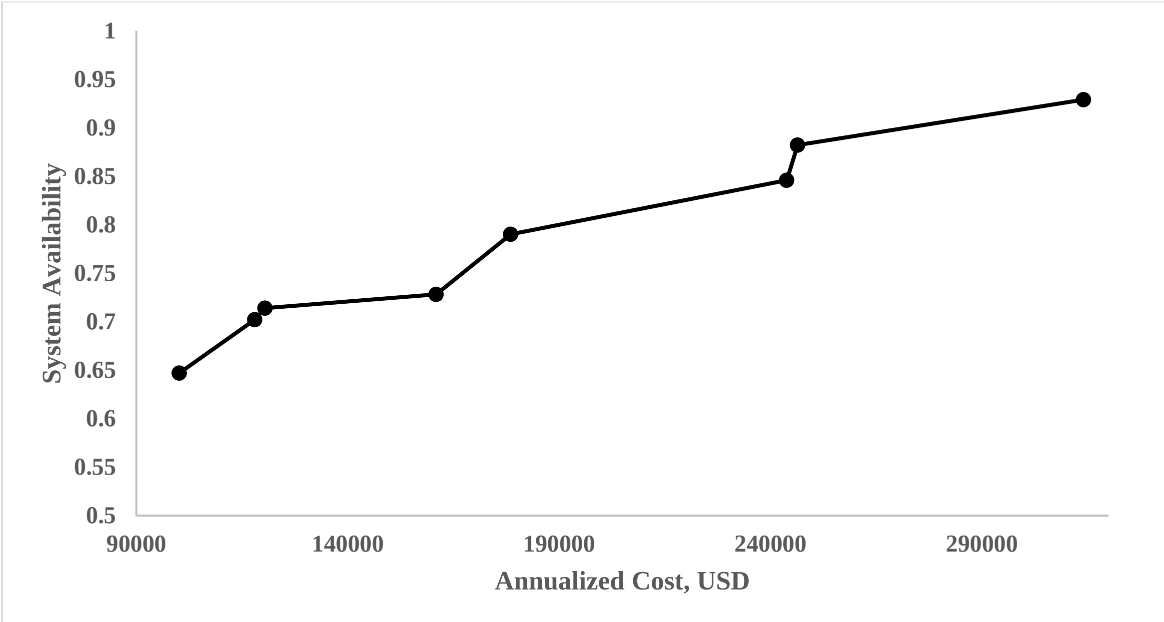


Figure 12 Pareto-Optimal Curve from Optimization Case Two results

The Pareto optimal curve shows a stepwise increasing trend, which follows the logic that higher system availability value requires more investment (both fixed and operational costs) in the system. The results also show a roughly 2:1 ratio for the annualized fixed cost and operating cost, where both cost factors contribute a significant part to the overall system cost. To be more specific, a connection between sources and sinks with high availability values could result in a higher operating cost, but the optimization framework will favor that solution if the epsilon value on the annualized cost constraint is also high. Similarly, storage tanks and parallel pumps can be installed for all connections to increase the fixed cost dramatically, where the point with the highest availability value in the graph has three times of the system cost of the point with the lowest availability value. However, the very large investment can be paid off if the cost to cover system downtime is also very high considering the system downtime for the point with the lowest availability value is 5 times of the downtime for the point with the highest availability value. Each point on the Pareto curve is an optimal solution associated with a distinct network design and a distinct water allocation strategy. The different installation plans of storage tanks and parallel units, as well as the different assignments between the sources and sinks result in the stepwise shape, where optimization results from different assignments will be shown as examples in the following part.

For the system availability equals to 0.882, the annualized cost of the water recycle network is $246447. The design of the system is shown in Figure 13 for water flow assignments, storage tank and parallel pump installations. The result shows that the storage tank between source 1 and sink 1 is not installed. This is due to the limitation on the overall system cost. From the preliminary analysis, the cost for storage tank installation is higher than the cost for parallel pump system. Furthermore, the source 1 and sink 1 have the highest unit availability values and the flowrate between them is the highest in the network, which will result in the highest tank cost, so in order to meet the upper bound value epsilon and not to sacrifice too much on the system availability value, the optimization framework decided to only remove the storage tank between source 1 and sink 1.

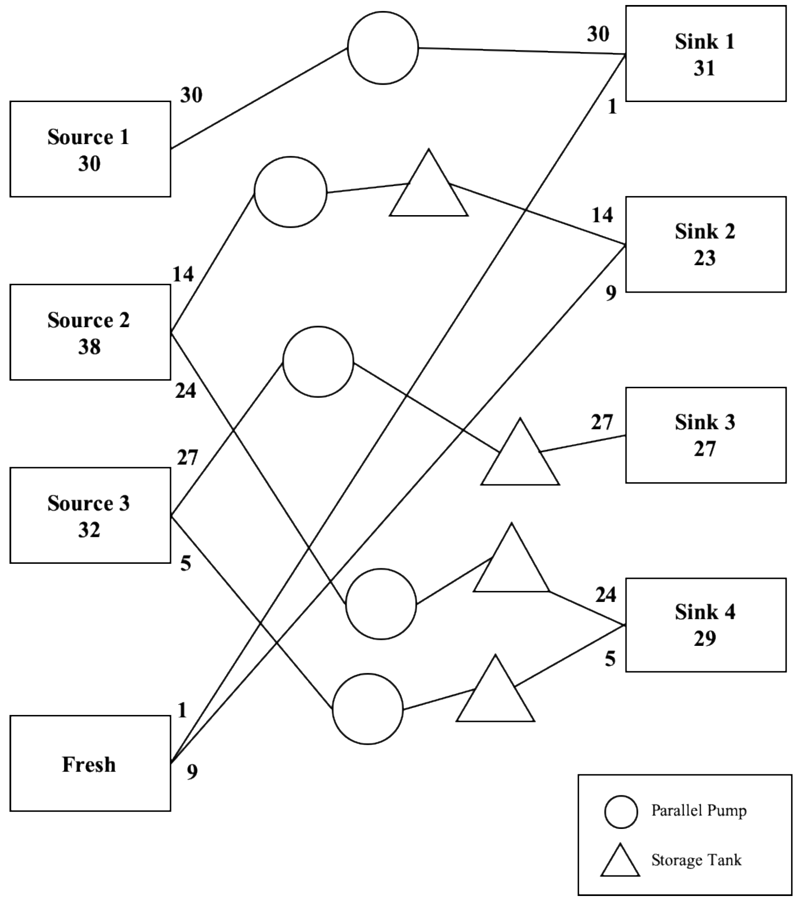


Figure 13 System Design and Assignment with A=0.882

For the system availability equals to 0.849, the annualized cost of the water recycle network is \$243900. The design of the system is shown in Figure 14 for water flow assignments, storage tank and parallel pump installations. Similarly, to further reduce cost to meet the updated epsilon value and still maximize the system availability, the framework decided to remove the storage tank between source 2 and sink 1, where source 2 has the second highest availability value and the flowrate between source 2 and sink 1 is the highest.

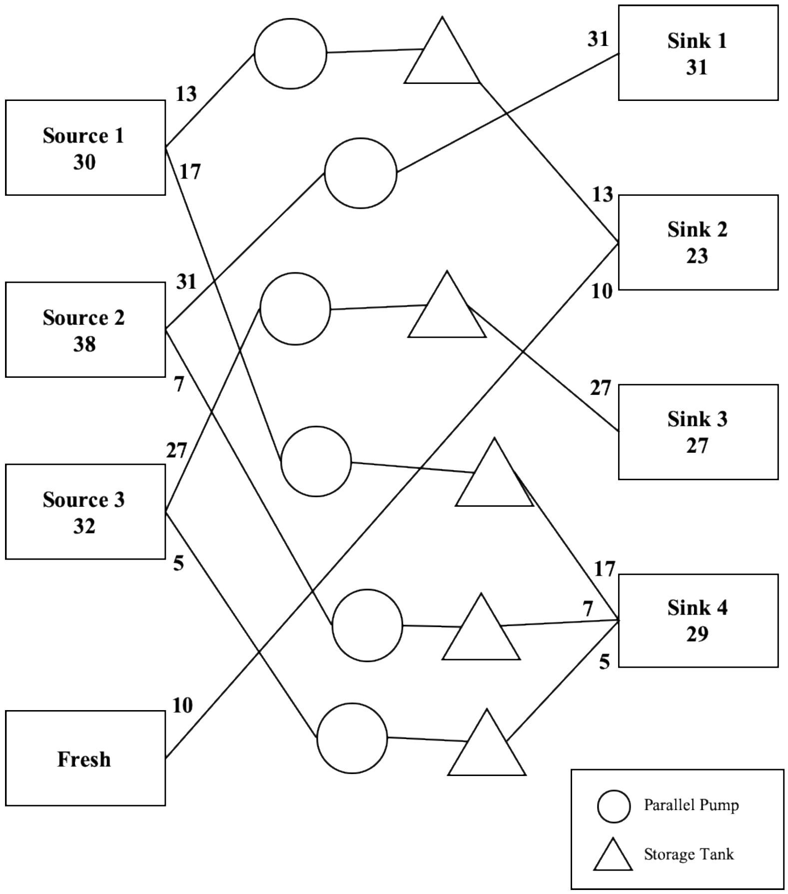


Figure 14 System Design and Assignment with A=0.849

For the system availability equals to 0.728, the annualized cost of the water recycle network is $160947. The design of the system is shown in Figure 15 for water flow assignments, storage tank and parallel pump installations. Due to the further decrease in the epsilon value, the network in Figure 14 only has two storage tanks installed. Source 1, 2 and sink 1, 2 have the highest unit availability values on the both ends, and the flowrates between them are also relatively high. In result, the framework decided to remove the storage tanks between them to further reduce the network cost and still maximize the system availability value under the epsilon constraint.

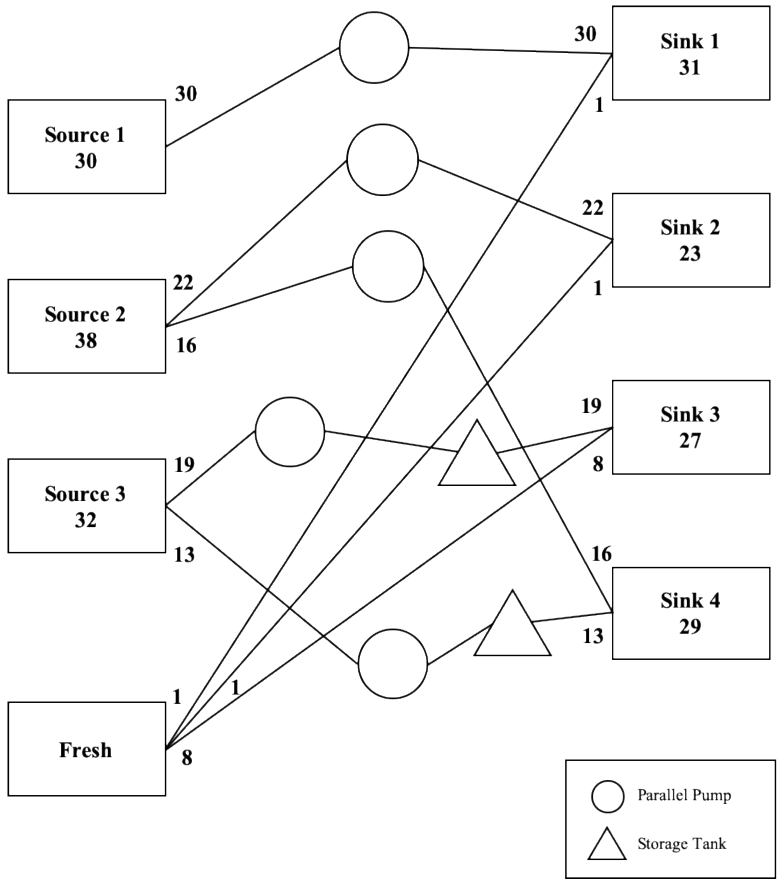


Figure 15 System Design and Assignment with A=0.728

From all three examples, we can observe the different system designs and assignments that result in a stepwise Pareto optimal curve. Furthermore, the Pareto optimal curve also shows how the system availability value changes when reliability improving methods are applied. The trend of the curve follows the logic that a water recycle network with higher cost (additional reliability improving methods) will also have a higher system availability value. While the upper bound epsilon value for the overall system annualized cost decreases, the total investment that can be spent on the three reliability improving methods, as well as the fresh and the waste treatment for the network decreases. So, it can be observed that in the second optimization case, although all three listed networks are optimized results, the installations of storage tanks and parallel pumps are different. The network from Figure 14 only has 2 storage tanks installed compared to 4 and 5 from Figure 12 and 13, that is also why the overall cost for the network in Figure 14 is around 34% lower than the cost for the networks in Figure 12 and 13. From the preliminary analysis, the parallel system has lower cost that the storage tank and has relatively high impact on the availability of the system based on the data in this work, so the optimization framework always decides to remove storage tanks first to meet the epsilon upper bound for the cost of the network. From the results in both optimization case 1 and 2, the parallel pump system has always been considered for each connection between sources and sinks. The removal of the parallel system will happen while we place very low epsilon value on the overall system cost, which will also result in a very low system availability value.

4.2 Results and Discussion for Reverse Osmosis Unit Operation

In order to demonstrate the optimization framework and the synthesis of the optimal pretreatment network, a shortcut method is presented instead of a full rigorous model. The shortcut method will contain most kinds of combinations for pretreatment technologies, so it will be a good representation of the full model. In the case study, six scenarios of the pretreatment system will be considered: (1) UF only, (2) Ozonation only, (3) Chlorination only, (4) a base case of no pretreatment technology. Figure 15 demonstrates the shortcut method used in the case study:

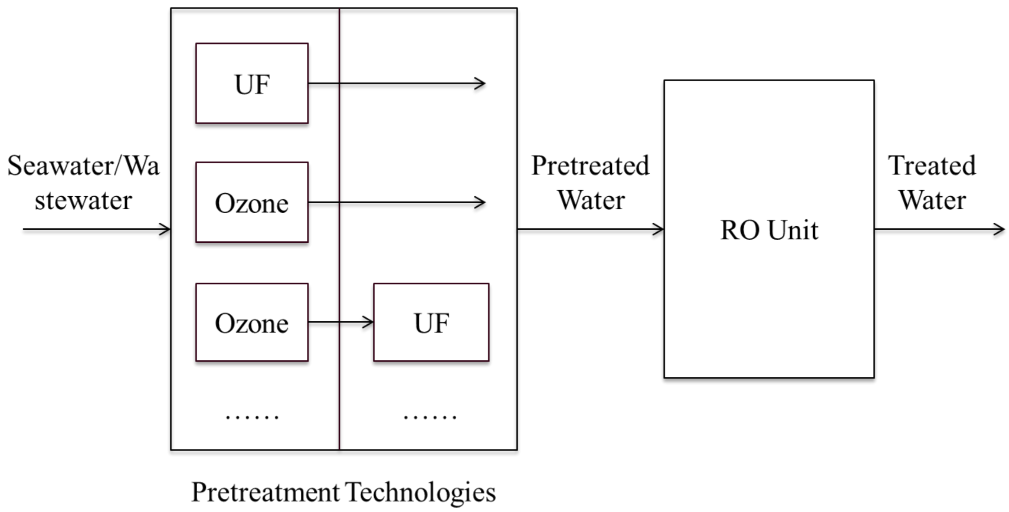


Figure 16 Pretreatment Networks for the Shortcut Method

The base case scenario has the following information: (a) RO membrane cleaning frequency 2-3 months (1440-2160 hr), (b) RO membrane lifetime 6 year (52560 hr).

For scenario (1), the data on UF pretreatment is shown below: (a) RO membrane cleaning frequency 6-12 months (4320-8640 hr), (b) RO membrane lifetime 8 years (70080 hr), (c) total cost is \$0.048-0.057/m^3 based on a 40,000 m^2/d water production rate. In the case without backwash, the UF permeability can be correlated using Equation 100:

$$P = 180 * exp(-\frac{t}{136.1}) \tag{100}$$

The result shows a 20% saving in total cost, and is confirmed by an industrial scale plant operation at Wangtan power plant.

For scenario (2), the optimal ozone dose is tested to be 0.3 mg/L, and the water flux can be modeled using Equation 101 (Brown et al., 2008):

$$N_w = 23.4 * t^{-0.0377} \tag{101}$$

For scenario (3), chlorination requires 10-50 mg/L of FeCl3 to be continuously fed to the system. The cleaning and replacing cost for RO membrane after the pretreatment is estimated to be \$0.05/m^3.

4.3 Results and Discussion for Hazardous Material Transportation Safety

4.3.1 Methanol

This case study is based on the methanol transportation in the United States. Methanol is a widely used feedstock in the chemical industry. According to Jordan & Associates (2013), the annual domestic methanol production is roughly 1.3 million metric tons, which is about 21% of overall US methanol demand. Also, according to the International Chemical Safety Cards (ICSC) issued by The National Institute for Occupational Safety and Health (NIOSH) from Centers for Disease Control and Prevention website, methanol is a highly flammable and explosive liquid. It has a large flammability limit ranges from 7.5% to 36%. A mixture of methanol and air is explosive, and methanol as a pure component is also highly toxic to human for all kinds of contacts.

There are several major distribution hubs in the United States for imported methanol: Houston Ship Channel, Port of New Orleans, Port of Wilmington, North Carolina, Port of New York, US West Coast Ports (Seattle, San Francisco, and Los Angeles) and Midwest (Gebauer & Jordan, 2002). In this case study, it is assumed that a major chemical manufacturing corporation has four facilities that utilize methanol as inbound material. The location and annual demand for each plant are listed in Table 8. Three suppliers are considered, and their locations are determined by the major distribution hubs of imported methanol in the U.S. The location and annual capacity of each supplier are summarized in Table 9.

Table 8 Plant Locations and Annual Demands of Methanol

Plant	Location	Annual Demand (kton/yr)
1	Newark, NJ	280
2	Baton Rouge, LA	320
3	Clinton, IA	190
4	La Porte, TX	350

Table 9 Supplier Locations and Annual Capacities of Methanol

Supplier	Location	Annual Capacity (kton/yr)
1	Baytown, TX	300
2	New Orleans, LA	480
3	Wilmington, NC	360

Although methanol can be distributed by pipeline or water (the Mississippi River and the Atlantic Coast Seaports), these two transportation modes are less common, and few incident data can be found. This paper only addresses two major transportation methods, which are highway and railroad. Distances between plants and suppliers are summarized in Table 10 for the highway and Table 11 for the railroad.

Table 10 Distance between Suppliers and Plants for Highway Transportation

Distance (mile)	Plant 1	Plant 2	Plant 3	Plant 4
Supplier 1	1600	250	1100	10
Supplier 2	1300	80	960	340
Supplier 3	590	950	1100	1200

Table 11 Distance between Suppliers and Plants for Railroad Transportation

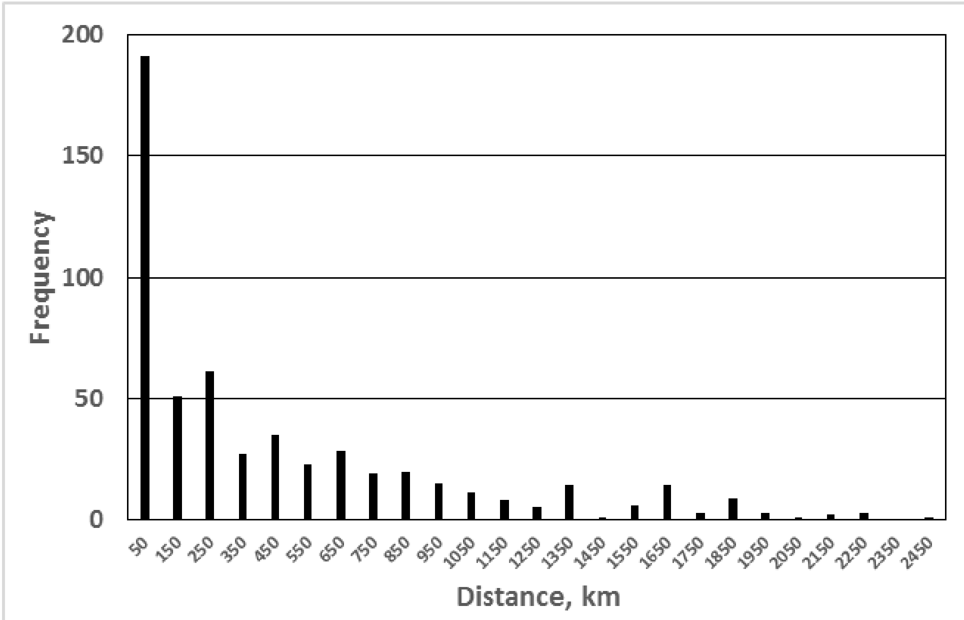
Distance (mile)	Plant 1	Plant 2	Plant 3	Plant 4
Supplier 1	1780	300	1170	10
Supplier 2	1420	90	1130	380
Supplier 3	640	1030	1350	1350

4.3.2 Correlation between HazMat Transportation Distance and Incident Probability

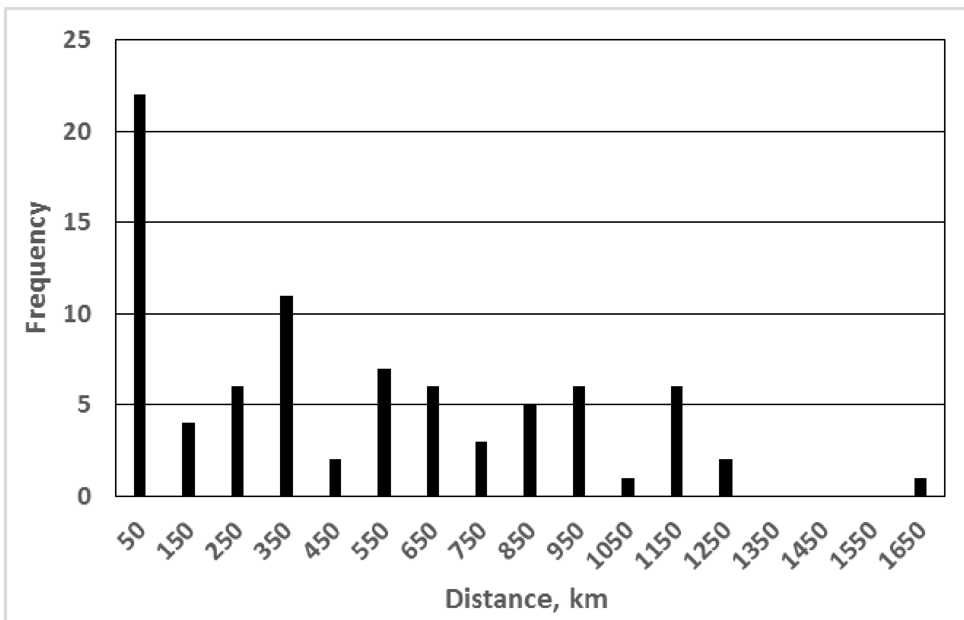
Based on the previous risk quantification section, 10-year data (from 2004 to 2014) of methanol transportation incidents was obtained from the USDOT database of the Pipeline and Hazardous Materials Safety Administration. The data was further processed: (1) transportation modes are limited to highway and railroad, (2) transportation phases include only “in transition”, where loading and unloading incident data was eliminated. 678 incident data points, which include 588 highway incidents and 90 railroad incidents, were the final dataset for the case study.

Postal information of the origins and incident locations was retrieved from the dataset. The techniques in Section 3.3.3 were applied to transform the existing information into distances between the two locations. The incident frequency plots were constructed for both highway and railroad as shown in Figure 17a and 17b. Both plots present the distribution of the number of HazMat transportation incidents as a function of distance. Due to the high volume of incidents at a short distance, the frequency was then plotted against the natural logarithm of distance travelled, as shown in Figure 18a and 18b for highway and railroad. Both correlations present a bimodal trend, which proves the statement mentioned in Section 3.3.3 for empirical probability estimation.

Following Equation 8 and 9, the cumulative probability of a HazMat incident was calculated and then plotted against the corresponding travelling distance, as shown in Figure 19a and 19b for highway and railroad. The plots demonstrate logarithmic trends, so that the cumulative probability was then plotted against the natural logarithm of distance, as shown in Figure 20a and 20b for highway and railroad. Two linear segments can be observed from both figures. Each segment was analyzed individually, as shown in Figure 21a and 21b for highway, and 22a and 22b for railroad.

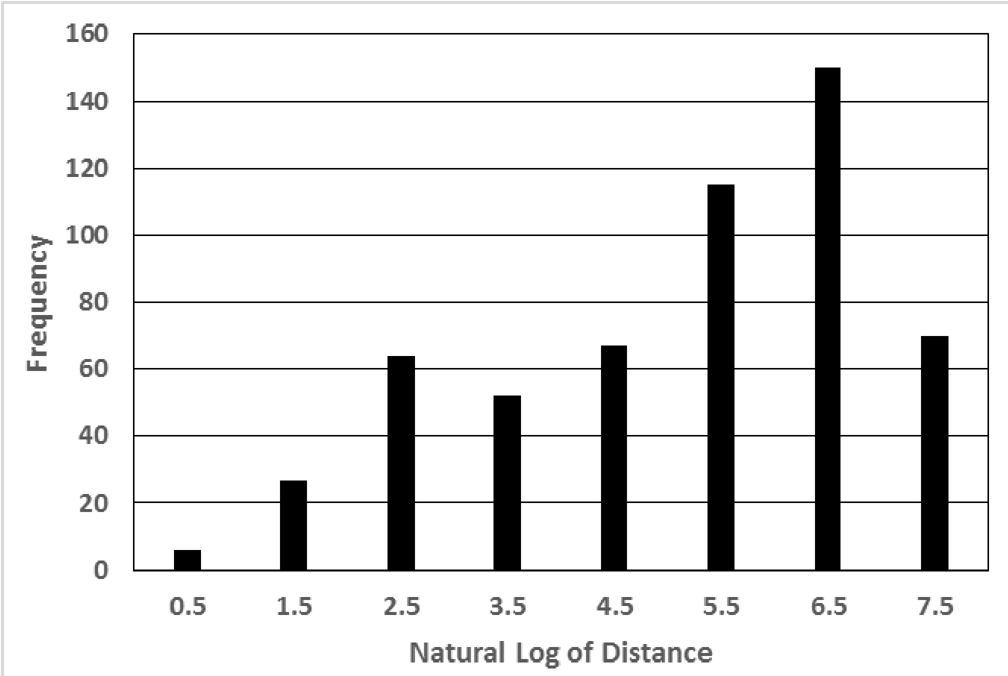


a.



b.

Figure 17 (a) Frequency of Methanol Highway Incidents by Distance. **(b)** Frequency of Methanol Railroad Incidents by Distance

a.


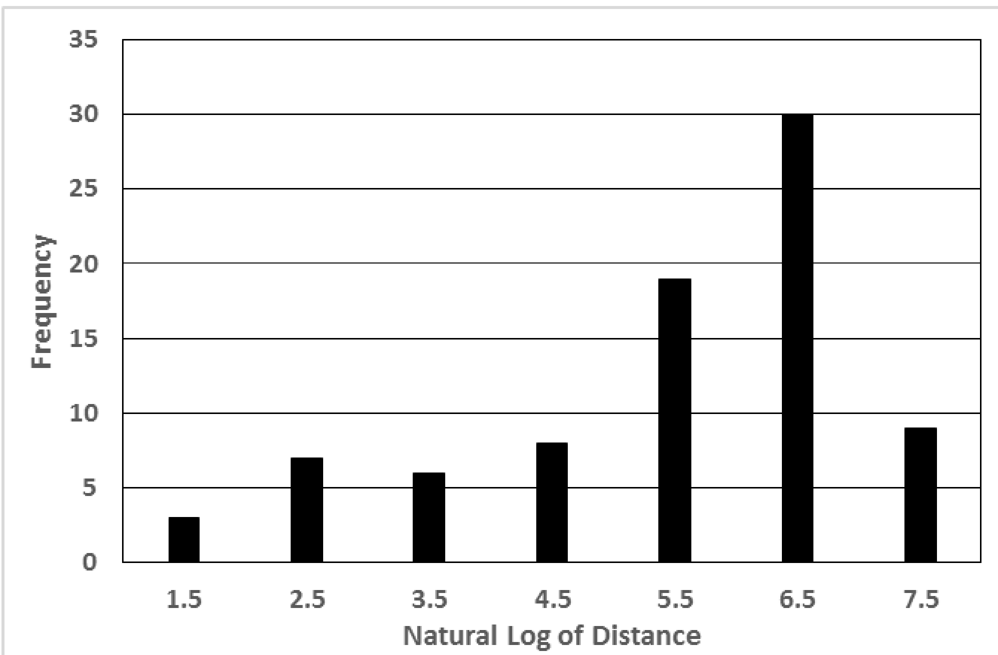
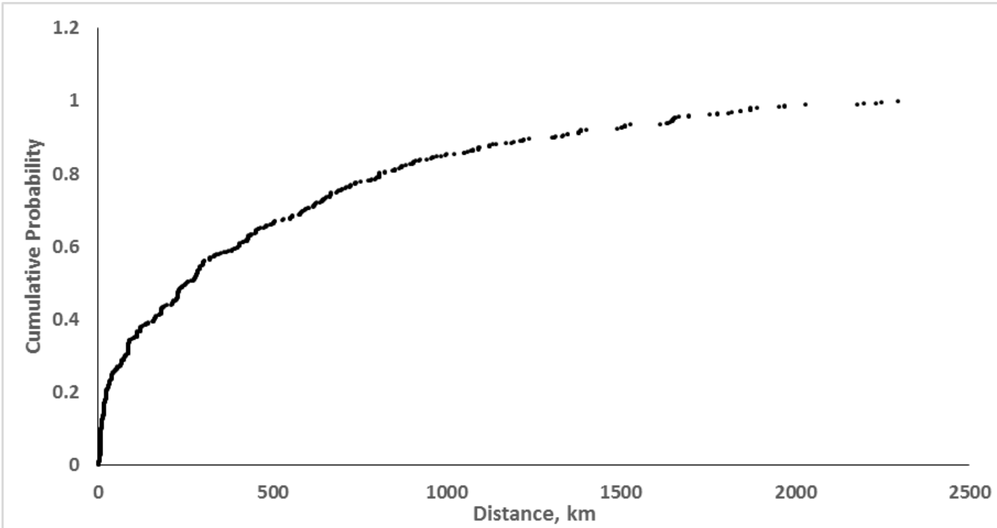
b.


Figure 18 (a) Frequency of Methanol Highway Incidents by the Logarithm of Distance. **(b)** Frequency of Methanol Railroad Incidents by the Logarithm of Distance

a. 

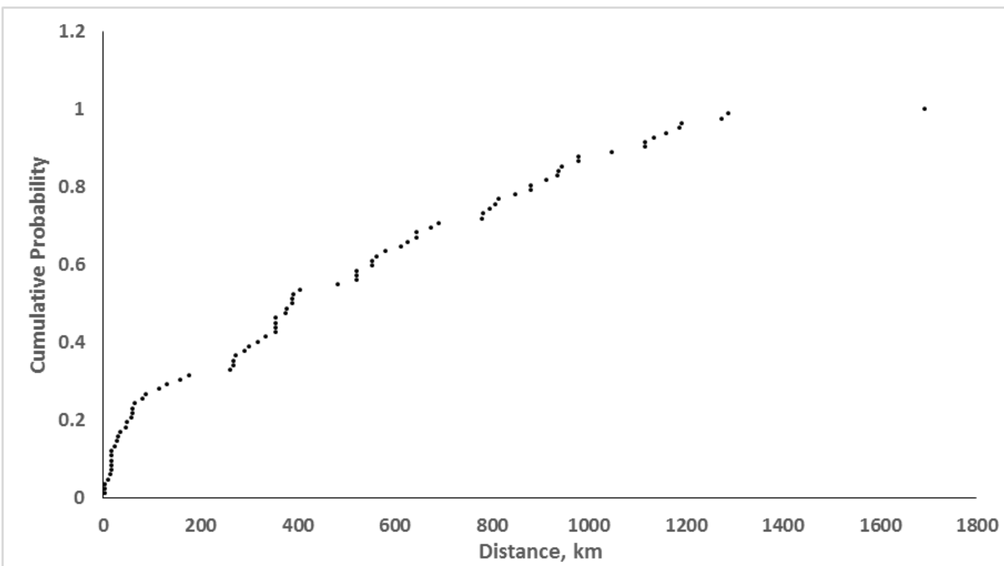
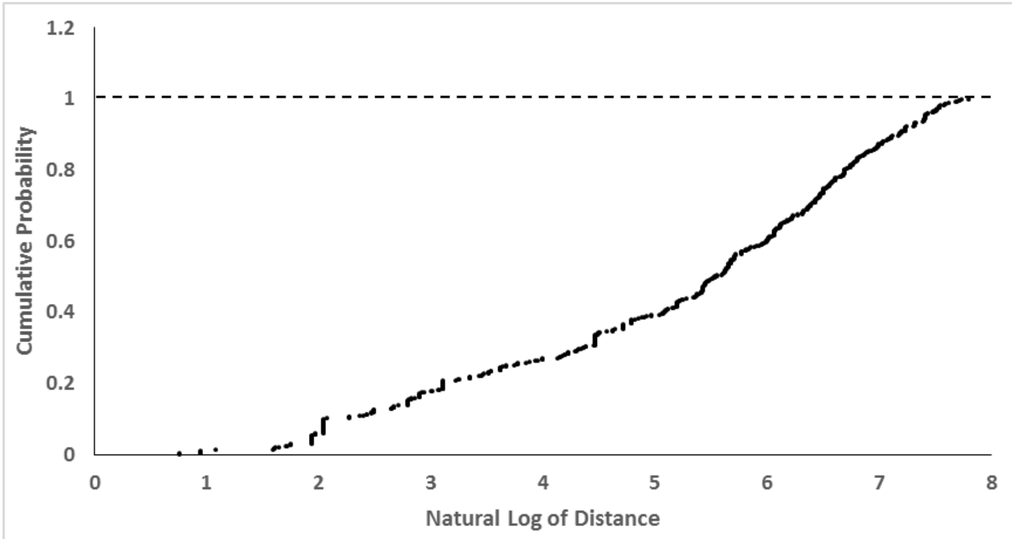
b. 

Figure 19 (a) Cumulative Probability as a Function of Distance for Methanol Highway Incidents. **(b)** Cumulative Probability as a Function of Distance for Methanol Railroad Incidents

a.


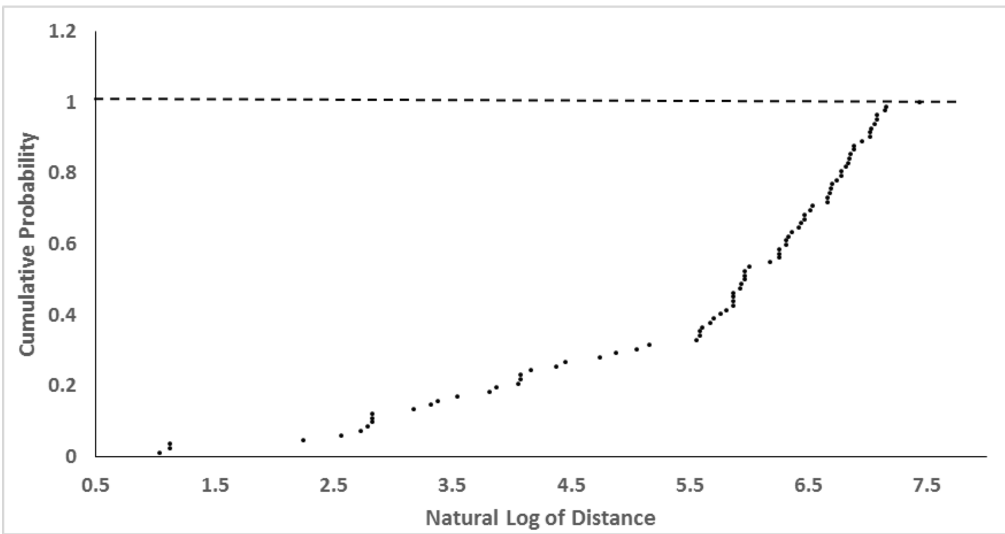
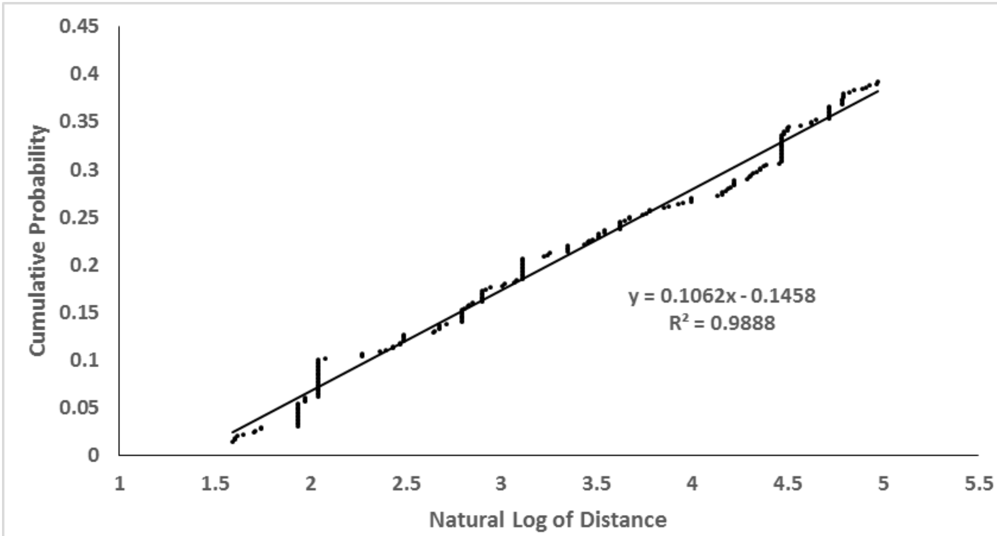
b.


Figure 20 (a) Cumulative Probability as a Function of the Natural Logarithm of Distance for Methanol Highway Incidents. **(b)** Cumulative Probability as a Function of the Natural Logarithm of Distance for Methanol Railroad Incidents

a.



b.

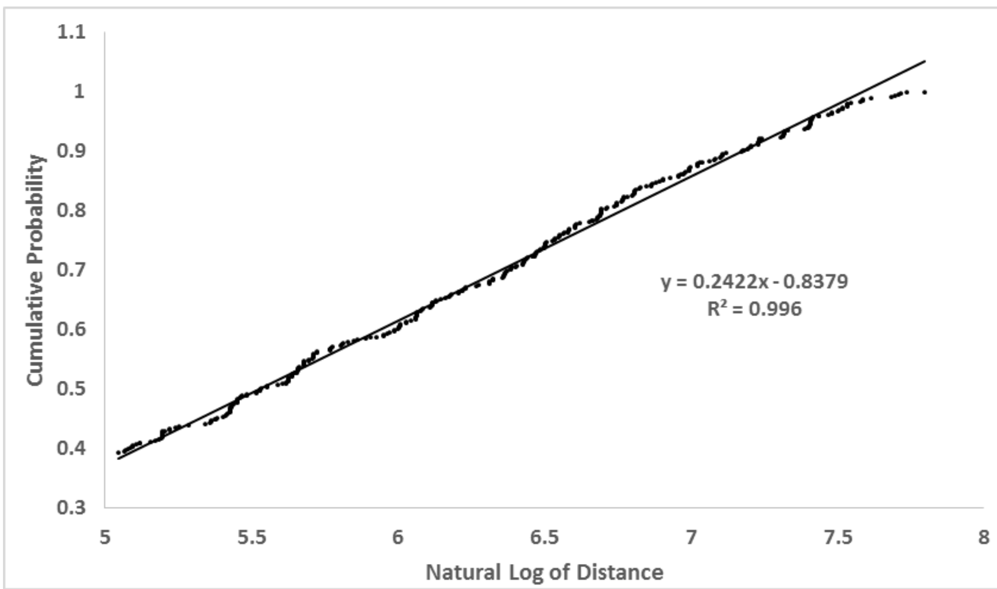
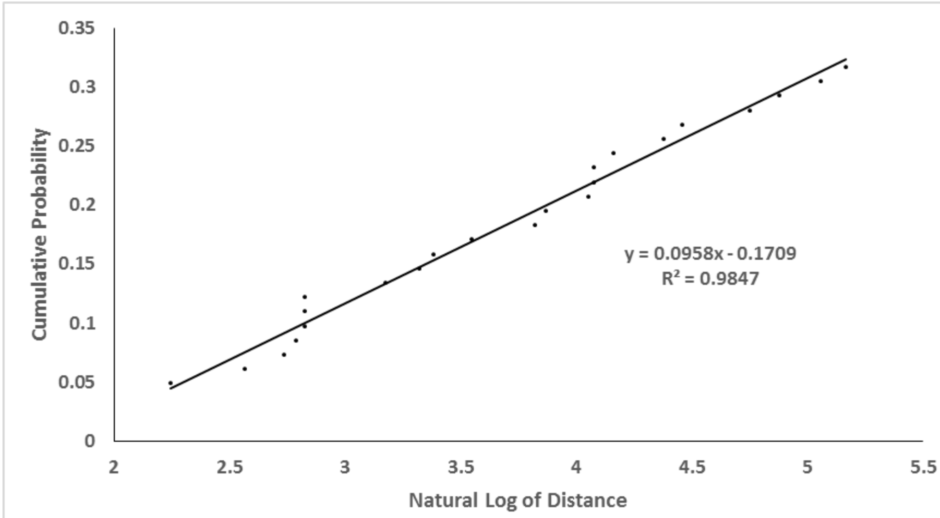


Figure 21 (a) Cumulative Probability as a Function of the Natural Logarithm of Distance between 1.5 and 5 for Methanol Highway Incidents. **(b)** Cumulative Probability as a Function of the Natural Logarithm of Distance between 5 and 8 for Methanol Highway Incidents

a.



b.

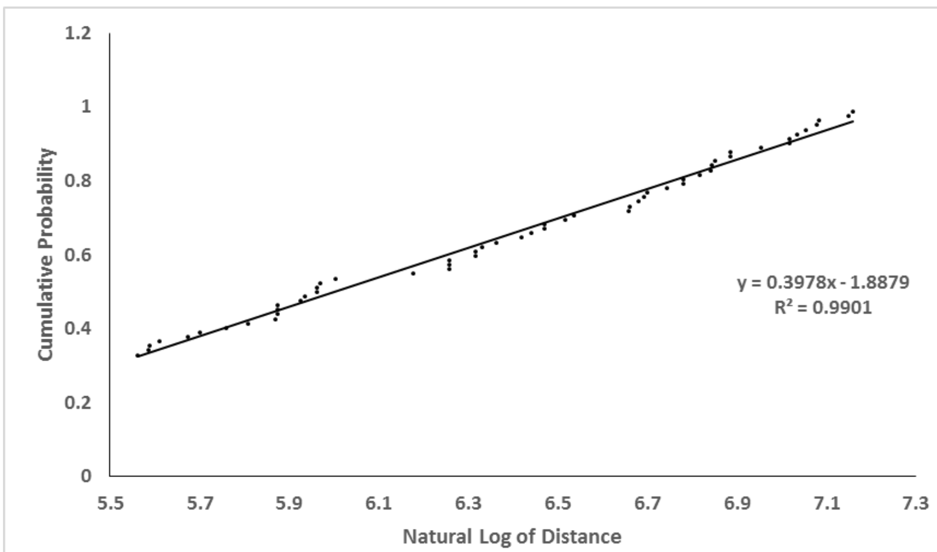


Figure 22 (a) Cumulative Probability as a Function of the Natural Logarithm of Distance between 2 and 5.5 for Methanol Railroad Incidents. **(b)** Cumulative Probability as a Function of the Natural Logarithm of Distance between 5.5 and 7.3 for Methanol Railroad Incidents

4.3.3 Risk Calculation

To calculate the overall probability of methanol transportation incidents using Equation 10, the general incident rates for transportation using highway and railroad are shown in Table 12. In this case study, general incident rates of highway and railroad are used to represent the incident rates of transporting methanol using these two modes. Although general incident rates could be lower than the specified rate for HazMat, the fraction between highway and railroad can still be well presented since transporting HazMat will not affect the inherent risk within different transportation modes. Once more applicable data is available, a more accurate incident rate of transporting methanol using each mode can be calculated. The general incident rates per statistical data were obtained from National Highway Traffic Safety Administration website and Federal Railroad Administration – Office of Safety Analysis (2012), as shown in Table 12.

Table 12 General Accident Rate for Different Transportation Modes

Transportation mode	**Highway**	**Railroad**
General accident rate (per mile)	1.24*10^-6	2.44*10^-6

Although the total loss for each incident in dollar value is included in the dataset, a large number of data points do not have that information. However, the amount of methanol released in each incident is recorded for all data points. Due to the data availability, the value loss or the consequence for each incident shown in Equation 2 is determined as the amount of methanol released.

Additional data and information that was used to calculate risk and total cost are summarized in Table 13.

Table 13 Information on Different Transportation Modes

Transportation mode	Highway	Railroad
Cost (cents per mt mile)	34.6	6.1
Average capacity (metric ton)	24	100

4.3.4 Pareto-Optimal Solutions

To determine the optimal transportation mode, the framework uses both highway and railroad data to calculate the minimum cost considering certain maximum acceptable risk factor. The risk factor is calculated using Equation 2, where accident consequences are the average amount of methanol releases for each transportation mode derived from the incident dataset. The risk factor range is determined from 0.7 to 1.6 in the case study. Sufficient risk factor values are considered to not only cover the whole range but also present the detailed trend between the risk factor and minimum cost. The values of the factors were then plotted against the minimum transportation costs as shown in Figure 23. At lower risk factor value, the minimum transportation cost is higher, which is logical since more money is needed to obtain a relatively safer transportation. Three examples of transportation arrangements using highway and railroad with risk factor value 0.8, 1.0 and 1.2 and corresponding transportation cost $4.65 million, $3.12 million and $1.71 million were shown below in Figure 24, 25 and 26.

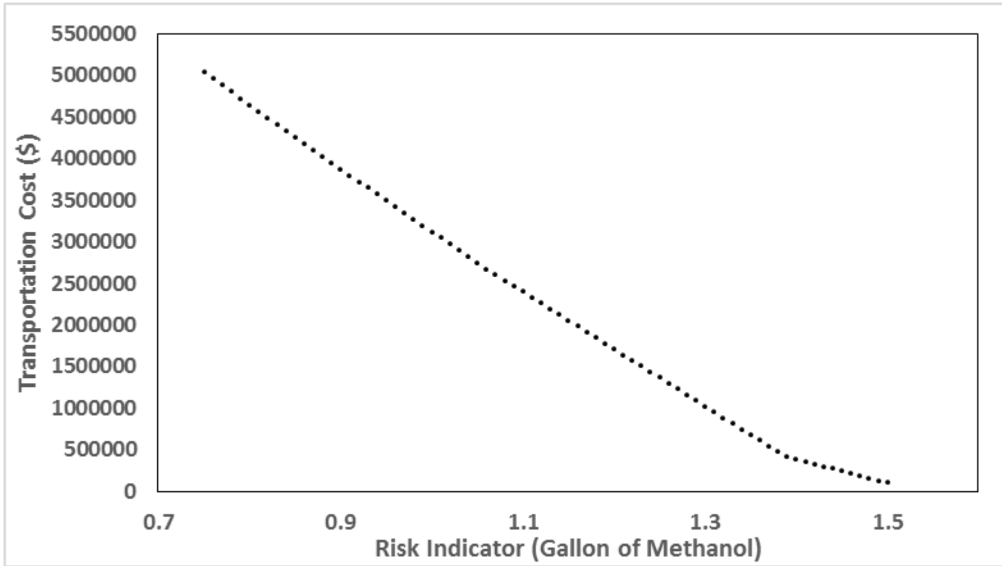


Figure 23 Pareto-Optimal Curve of Risk Indicator versus Minimum Transportation Cost

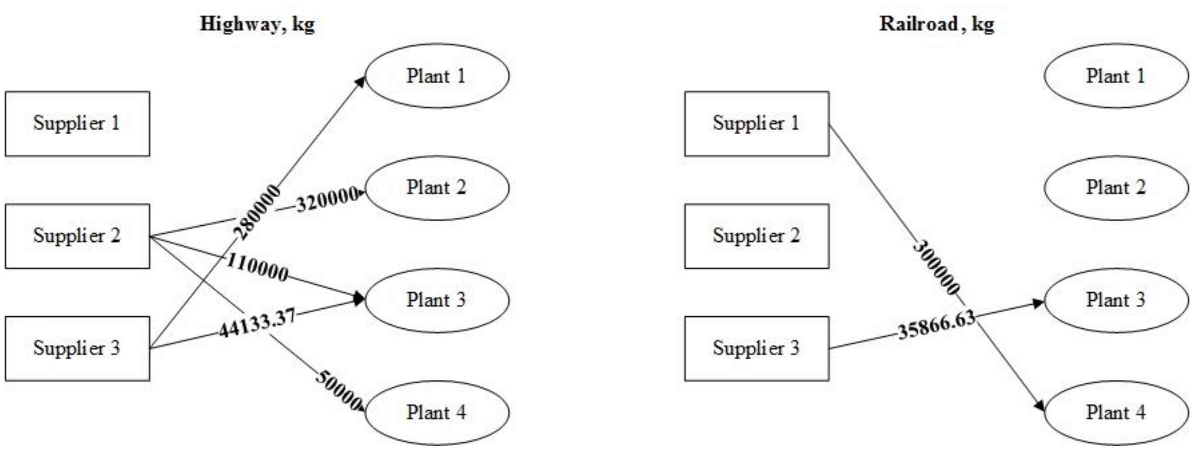


Figure 24 Transportation Arrangement for Risk=0.8 with Cost=$4.65 million

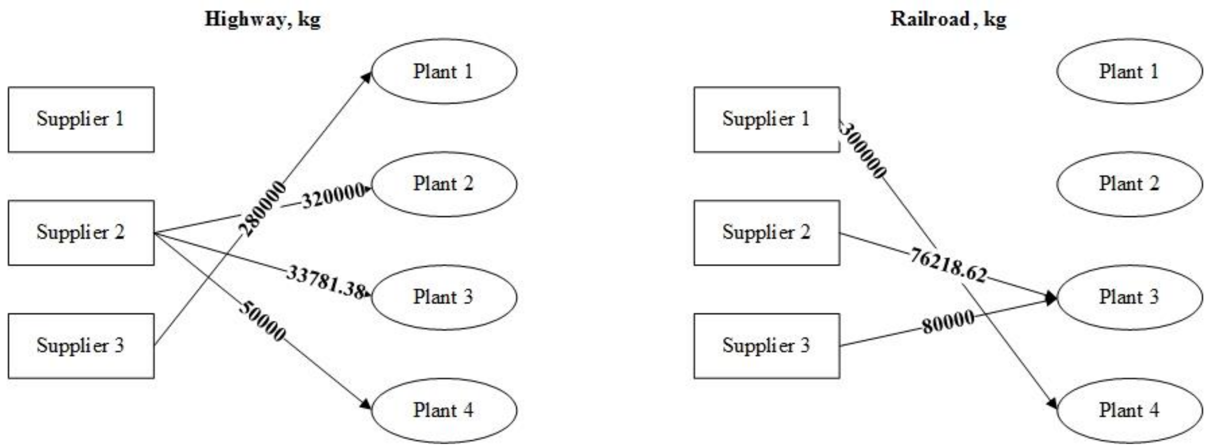


Figure 25 Transportation Arrangement for Risk=1.0 with Cost=$3.12 million

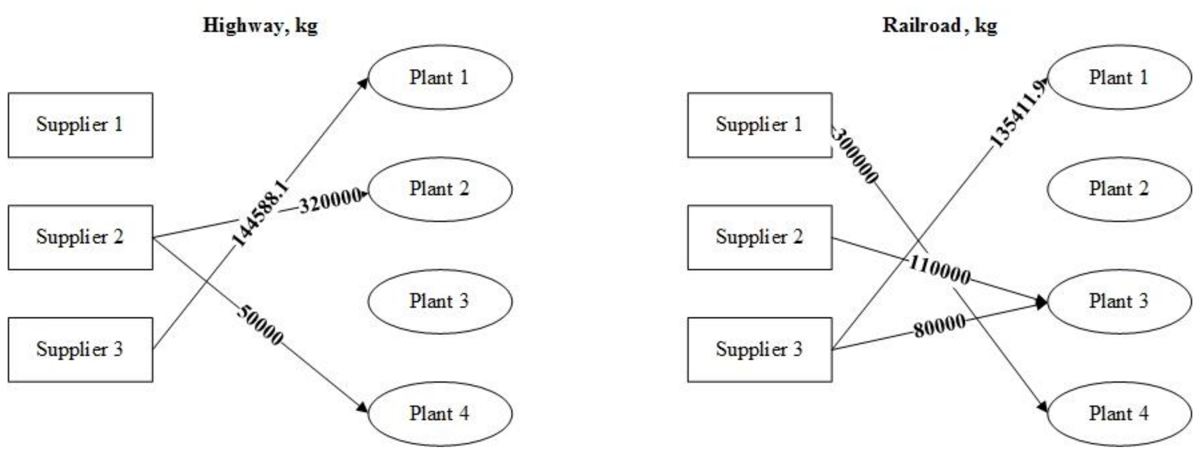


Figure 26 Transportation Arrangement for Risk=1.2 with Cost=$1.71 million

5. ESTIMATE THE CAPITAL COST OF SHALE-GAS MONETIZATION PROJECTS*

With the significant growth in developing shale-gas monetization technologies, there is a critical need for quickly estimating the cost of proposed technologies and manufacturing pathways. The substantial discoveries of shale gas reserves in the U.S. have spurred a boom in production and monetization to chemicals and fuels. The U.S. production of shale gas has jumped from about 2 trillion cubic feet in 2007 to about 15 trillion cubic feet in 2015 (Al-Douri el. al, 2017). This increase is expected to continue. Some estimates predict a cumulative production of 459 trillion cubic feet of shale gas from 2014 to 2040 (Staub, 2015).

With shale gas gaining an advantage as a competitive feedstock in the U.S., a concomitant growth in the chemical industry is taking place. The American Chemistry Council reports that by April 2016, 264 shale-gas-dependent projects have been announced with estimated capital investments totaling $164 billion (American Chemistry Council, 2016). About half of these projects have already been completed or are in the construction and implementation phases.

Shale gas monetization refers to the physical and/or chemical transformation of shale gas constituents into value-added products. A wide variety of chemicals and fuels can be produced from shale gas (Alfadala and El-Halwagi, 2017; Marano, 2015; Siirola, 2014). In addition to the conventional manufacturing chemistries and production routes, there are significant opportunities

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for the creation of novel pathways and technologies. There is a critical need to quickly assess the economic viability of these new and emerging alternatives before detailed design and cost estimates are carried out. This article develops and explains an order-of-magnitude correlation for estimating the capital investment of a shale-gas monetization plant.

Technology developers and process engineers can use this correlation, along with other preliminary cost-estimation techniques, to help make technology selection and design decisions prior to chartering laborious and costly techno-economic studies.

5.1 Capital Cost Estimation Methods

The fixed capital investment (FCI) or capital expenditure (CAPEX) of a plant refers to the money required to design, procure, deliver, and install the process equipment, ancillary units, piping, instrumentation and controls, civil and electrical work, and service facilities needed to ready the process for operation. The total capital investment (TCI) of a plant is the sum of the FCI and the working capital investment (WCI) that is necessary to cover the operating expenses up to the start of operation. There are several approaches for estimating the TCI of a project (El-Halwagi, 2017):

- Manufacturer's quotation
- Computer-aided tools
- Capacity ratios (*e.g.,* six-tenths factor rule)
- Cost indices (*e.g., Chemical Engineering* Plant Cost Index [CEPCI])
- Factors based on equipment cost (*e.g.,* Lang method, Hand's factors)

• Empirical correlations.

The accuracy of each method varies depending on the available information and level of project definition.

The Association for the Advancement of Cost Engineering-International (AACE-International) recommends five levels (or classes) of cost estimates. The least-detailed level is referred to as an "order-of-magnitude estimate" and is given a Class Level 5. Such an estimate is based on very little information (0–2% of project definition) and is used mostly for preliminary and rapid assessment of the economic viability of a proposed project. The accuracy of a Class Level 5 estimate is typically on the order of ±30–50%. The most-detailed level (*i.e.*, check estimate, contractor's estimate, or Class Level 1 estimate) is based on almost full detailing of the project and is used to issue bids and tenders. Its accuracy is on the order of ±5–10%.

A commonly used approach for an order-of-magnitude estimate is to use information from similar processes/technologies. In this context, correlations based on the type of industry, plant capacity, and number of functional units are particularly useful (Zevnik and Buchanan, 1963; Wislon, 1971; Bridgwater and Mumford, 1979; Gerrard, 2000). We adopted this approach to develop an order-of-magnitude cost estimation method for rapidly predicting the capital investment required for a proposed shale gas monetization process. Coupling this order-of-magnitude cost estimate with other sustainability criteria and performance targets can allow preliminary assessment of the sustainability of a gas monetization project (El-Halwagi, 2017).

5.2 Data Collection and Correlation Development

Economic data for 50 gas conversion plants were collected and analyzed. We processed the data to create a consistent basis for cost correlation.

Capital investment data were updated to March 2016 via the CEPCI according to the following formula:

$$FCI_{Time\ B} = FCI_{Time\ A} * \frac{CEPCI_{Time\ B}}{CEPCI_{Time\ A}} \tag{102}$$

We assumed that:

$$FCI = 0.85*TCI \tag{103}$$

For some plants, the data were given for the inside batter limit (ISBL) which refers to the major process equipment and ancillary equipment. For such cases, it is necessary to include the capital expenditure of the outside battery limit (OSBL), which corresponds to the additional infrastructure for utilities, tank farms, workshops, etc. The ISBL and OSBL capital expenditures were related through the following assumption (The Chemical Engineering Plant Cost Index):

$$OBSL\ CAPEX = 0.4*ISBL\ CAPEX \tag{104}$$

We assumed that FCI is related to ISBL CAPEX through:

$$FCI = 2.1*ISBL\ CAPEX \tag{105}$$

We also assumed that the annual on-stream operation was 8,000 hours and that the plant throughput is based on final products. The processed data are shown in Table 14.

Table 14 Economic Data for Fifty Gas Conversion Plants

Process	Relevant Technology and/or Company	Capacity (10^5 MTPA)	FCI (MM$, 2016)
Ethylene Production via Cracking of Ethane-Propane (Steam-Cracking)	Intratec Solutions	15.42	2077.03
Ethylene: Ethane and Ethane/Propane mix	Linde AG	15	2383.68
Ethylene Glycol Production	OMEGA catalytic process by Shell Global Solutions	6.8	502.14
		6	404.91
Hydrogen Production from Natural Gas	Intratec Solutions	4.08	439.32
Hydrogen Production from Natural Gas	CB&I	0.78	139.19
Propane Dehydrogenation: Oxydehydrogenation	The STAR process	4.08	320.03
Propylene Production via Propane Dehydrogenation	Oleflex process by UOP	5	361.83
		4.5	351.23
Propylene Production via Propane Dehydrogenation	CATOFIN by CB&I	5.35	399.27
		5	338.07
D,L-Methionine Production via the Carbonate Process	Evonik Industries AG	1.35	306.8
		5.26	589.13
Hydrogen Cyanide Production	Andrussow process	0.23	62.79
Methanol-to-Olefins Process	UOP	5.44	327.83
		7.1	337.08
		6	298.74
Methanol-to-Propylene Technology	Lurgi GmbH, JGC Corp., and Mitsubishi Cemical	5.08	294
		5.68	322.08
Polypropylene Production via Gas-Phase Process: Stirred-bed Reactor	Lummus Novolen Technology	2.72	197.29
Polypropylene Production via Gas-Phase Process	Unipol	3.63	242.87
		5	323.58
Ethylene Production via Ethanol Dehydration	BP Chemicals	1.9	184.53
Propylene Production via Metathesis	Olefins Conversion Technology by CB&I	3.17	187.32
		3.5	131.08
		3	243.01

Table 14 Continued

Process	Relevant Technology and/or Company	Capacity (10^5 MTPA)	FCI (MM$, 2016)
Dimethyl Ether (DME) Process	Lurgi	15	474.48
Linear Low-Density Polyethylene (LLPDE) Production Using a Gas-Phase Process	Univation Technologies' Uipol and Ineos Technologies' Innovene G	4.5	293.77
Acrylic Acid Production via Propylene Oxidation	Lurgi GmbH and Nippon Kayaku	1.5	334.22
Methanol Production from Natural Gas	Air Liquide Global E&C Solutions, Toyo Engineering Corp, KBR, Inc., and Johnson Matthey and Haldor Topsoe A/S	17	793.98
		15	743.34
Ethane to Ethylene/Polyethylene	Qatar Chemical Co. Ltd.	5	1024.32
		6.95	1073.9
Linear Alkyl Benzene Plant	Qatar Petroleum	1	307.3
Methanol, Acetic Acid, and Vinyl Acetate Monomer from Natural Gas	Lurgi mega methanol process by Acetex Corp.	25.75	1024.32
Ethanol-to-Ethylene Plant	Braskem	2	229.65
Low-Density Polyethylene	Borealis	3.5	406.43
Polypropylene	ExxonMobil	2.72	173.18
Acrylic Acid Complex	BASF	1.6	430.38
Acrylic Acid Plant	American Acryl	1.2	203.74
Ethylene Production	Dow	15	1700
Natural Gas to Petrochemical	Eurochem Technologies Corp.	8	1138.42
Propylene / Polypropylene	Uhde	3.5	588.89
Propane Dehydrogenation to Propylene	Grupa Azoty	4	361.38
Ethane Cracker	Sasol	9.07	1552.64
Gas-Based Petrochemical Complex	Riopol	6.15	971.82
Hydrogen-based Ammonia Production,	Yara, BASF	7.5	530.48
Ammonia from Natural Gas	KBR	6.57	610.69
Ethylene from Ethane	Steam cracking	8.3	837.18

A particularly useful correlation form for cost functions combines the number of process steps or processing complexity and the capacity ratio with an economy-of-scale exponent (El-Halwagi, 2017; Zevnik and Buchanan, 1963; Wislon, 1971; Bridgwater and Mumford, 1979; Gerrard, 2000). We adopted this approach through the following expression:

$$FCI = a*N*F^b \tag{106}$$

where FCI is in $ (March 2016), an unknown parameter, N is the number of major processing steps or functional units, F is the plant capacity (in metric ton per annum or MTPA), and b is the economy-of-scale exponent (also an unknown parameter which is less than one). Both a and b will be determined through regression analysis of the economic data. A major processing step or a functional unit is "a significant step in a process and includes all equipment and ancillaries necessary for operation of that unit" (Gerrard, 2000). Examples of a functional unit include a reaction system, a separation train, a utility system, etc. Regular blowers, pumps, heat exchangers, storage tanks, and flash units do not count as major processing steps, because they are typically part of a larger functional unit.

To determine the unknown parameters a and b in Equation 107, the equation was transformed into following form:

$$\log\left(\frac{FCI}{N}\right) = b * \log(F) + \log(a) \tag{107}$$

Table 14 summarizes the key data of the gas processing plants. A log-log plot was generated for the compiled data (Figure 27). Using linear regression of the log-log data, the values of a and b were determined to be 17,000 and 0.65, respectively, and the empirical correlation is expressed as:

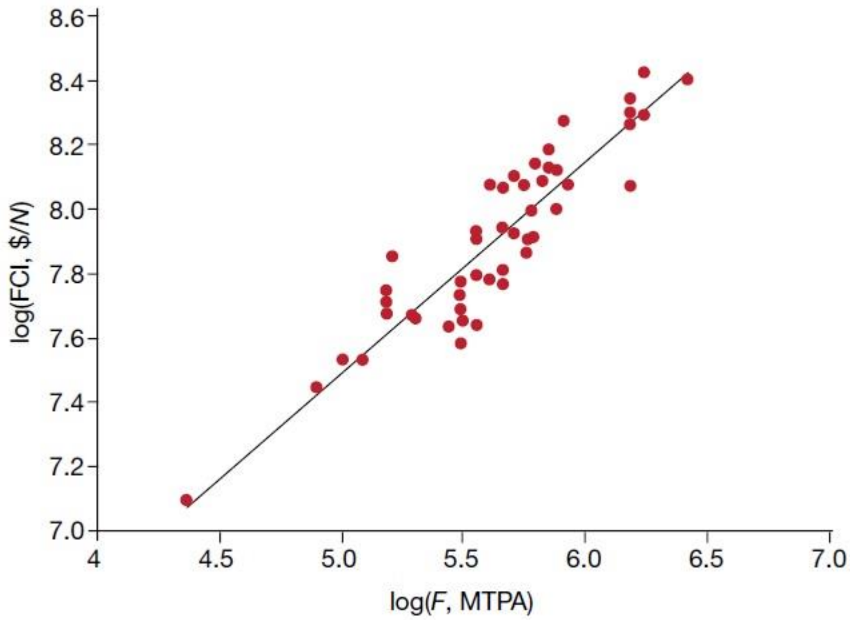

Figure 27 A Log-Log Plot of the Fixed Capital Investment (FCI)

$$FCI\ (in\ \$) = 17{,}000 * N * (F\ in\ MTPA)^{0.65} \tag{108}$$

The valid capacity range is from 22,800 to 2,575,000 MTPA.

By calculating the percentage error between real and estimated FCIs, the accuracy of this empirical correlation is as follows:

• 95% confidence limits: 9.99% and –4.45%

• Standard deviation: 26.04%

For technologies involving extreme pressures or temperatures or specialized materials of construction, the cost can be adjusted using pressure, factor, and materials factors (El-Halwagi, 2017; The Chemical Engineering Plant Cost Index).

5.3 Application of the Correlation

To illustrate the use of the cost correlation we developed, let us consider a process for converting shale gas to methanol. The flowsheet involves six major processing steps: oxygen separation, partial oxidation (reforming) of shale gas, separation (of syngas and CO_2), methanol synthesis, methanol separation, and utilities. The plant capacity is 1,650,000 MTPA.

Using Equation (108),

$$FCI = 17{,}000*6*(1{,}650{,}000)^{0.65}$$

$$= \$1{,}122\ MM$$

The 2016-updated FCI reported by Ehlinger et al. (2014) is $1,242 MM. Although the correlation result underestimates the reported cost by $120 MM (about a -10% error), it is important to recall that such a discrepancy is acceptable for order–of-magnitude (or Class Level 5) estimates which are intended for rapid and preliminary assessments.

5.4 Conclusions

The proposed correlation may be used as one of the order-of-magnitude estimates needed in conceptual design and preliminary screening of alternatives for shale gas monetization projects. The overall accuracy of the correlation is within the expected range of ±30–50% expected for Class Level 5 estimates. Because of the relatively simple inputs needed in the correlation, it is consistent with nature of initial process engineering work where only few details are available. Similar to other methods for order-of-magnitude cost estimation, it must be used with caution.

6. CONCLUSIONS AND FUTURE WORK*

In the result and discussion section, it can be seen that safety and reliability have significant impacts on the designs and operations of process synthesis, unit operation, and supply chain network material allocation problems. The cost of different systems also varies a lot at different safety and reliability values. In this section, we will conclude the major findings in this work and discuss potential future directions for further application and analysis.

This work proposed an insight and a systematic methodology for performing safety and reliability analyses for different systems including process synthesis, unit operation, and supply chain network material allocation problems. The safety and reliability analyses were included in the process integration and optimization frameworks. The objective is to see how safety and reliability variables can affect the design and operation of the systems, and to compare the tradeoff between system cost and the additional objective. Data-based and model-based frameworks were also designed in this work to represent various integration and optimization problems. The methodology that has been taken in this work can be divided into five general steps. First, the targeted process specifications other than the cost variable were identified to be included in the integration and optimization framework. Second, data and model were acquired based on availability. Third, the targeted process specifications were quantified based on the acquired data and model through either existing techniques or developing novel approach and correlations.

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Besides, an optimization framework that can combine targeted specifications with the existing integration system was constructed. In addition, the optimization framework was solved and the design or operation strategy of the integrated process were updated based on the result. The results that have been obtained in this work also include three different aspects. The results first include data-based or model-based correlations for safety and reliability analyses. Novel integration and optimization frameworks for multi-objective programming problems were also discovered. Then, the optimal or Pareto optimal results for system designs and operation strategies were obtained. The future directions for this work can be concluded for several different areas. First of all, additional process specifications can be further studied and analyzed, such as environmental impact for material allocation and energy analysis for water-energy nexus. Furthermore, novel mathematical and statistical models can be applied for stochastic optimization. Machine learning algorithms can be applied for historical incident data analysis and Markov Chain technique can be used for system reliability analysis.

The listed three research projects have their own conclusion and future work, and are presented in the following sections.

6.1 Conclusions and Future Work for Reliability Analysis in Direct Water Recycle Network

This work proposed a systematic method to perform reliability analysis for direct water recycle network within eco-industrial parks. The reliability analysis was integrated into the source and sink model for mass exchange network. The target is to compare how system cost and system reliability can affect the overall design and assignment of the network. In addition to the mathematical model to represent the network, different methods to improve system reliability were included as optimization variables. First, an optimization framework for source-and-sink model was proposed for the direct water recycle network. Then, unit and system reliability analyses with different mathematical models were studied. Instead of the time-depended reliability variable, the inherent availability value was chosen for this work. Each source and sink were assigned with an availability value. Three different reliability improving methods were proposed, which are storage tank, parallel unit, and alternative fresh and waste treatment. The system analysis was applied to calculate the overall network availability value. Due to the natural of reliability calculation, a mixed integer, nonlinear programming problem was formed. Both system cost and system reliability acted as objectives in this work. Furthermore, the MINLP problem was solved for two different cases: (1) the single objective MINLP for one optimal water network design, and (2) the multi-objective MINLP that results in a Pareto optimal curve to show the tradeoff between system cost and system availability. The single objective problem was formulated by integrating the system availability value into the cost function considering the system downtime and unavailability. The multi-objective problem was solved by applying the epsilon constraint method, where the cost objective was transformed into a constraint and an upper bound, epsilon, was assigned to it. The resulted Pareto optimal curve showed the tradeoff between system cost and system availability value, which could guide the decision-making process for choosing the desired direct water recycle network with optimal annual investment and system availability. The results from both cases show the positive impacts of installing additional storage tanks and parallel units on the overall system availability value. If the saving in improving system availability value and reducing system downtime is larger than the spending on additional equipment, it is important to consider those reliability improving methods when designing a direct water recycle network within an EIP.

Future work may focus on transforming the storage size into a variable and then integrating it into the optimization framework. In this work, the storage tank sizing problem was considered and solved during calculating the probability values for different states of the tank. The idea of having a storage tank is to cover the repair time of the system, so the size of the tank can be considered as a continuous variable in the optimization model and further integrated into the calculation of mean time to repair, as shown in Equation 102. This formulation creates a fractional mathematical programming problem. Novel algorithms and methods can be applied to solve such a complex and computational difficult optimization problem.

$$MTTR' = MTTR - \frac{V_{i,j}^{tank}}{f_{i,j}} \tag{109}$$

A centralized water treatment unit may also be included in the network, as shown in Alnouri et al. (2015), to maximize the total amount of water for recycling.

6.2 Conclusions and Future Work for Reverse Osmosis Unit Operation

This work proposed a methodology to study the effect of pretreatment technologies on RO unit membrane permeability and the cleaning and replacing schedules. A mathematical model was developed to represent RO unit and RO membrane fouling. Information and data on different combinations of pretreatment technologies were collected and were used to model development and optimization case study. The major impact of those pretreatment technologies on the RO unit is to increase the membrane permeability by reducing fouling effect. An optimization framework was developed to minimize the system cost including operation cost for pretreatment technologies and RO unit cleaning/replacing, as well as the fixed cost by implementing the additional technologies. The fouling parameters and time factors in the membrane permeability equation will affect the overall optimization results. The results show that although applying pretreatment technologies will result in additional cost, the money saved due to increased membrane permeability and longer cleaning and replacing schedule is significant. The saving on the total annualized cost could be around 20%.

This work only considers multiple single-stage RO system. For future directions, it is possible to consider modeling multi-stage RO system that could lead to better performance and higher purity in the permeate flow. In addition, heat and energy integration could be performed on the system to further reduce the operating cost.

6.3 Conclusions and Future Work for Hazardous Material Transportation Safety

An optimization approach has been developed to integrate risk into the design of a supply chain network. A systematic approach has been proposed for extracting data from historical information and for the derivation of risk factors. By applying the concept of the risk factor, the risk value is used as a constraint in the traditional allocation problem. By solving the linear problem, both risk and cost for transporting hazardous materials can be determined and correlated for further decision-making. The trade-off between risk and cost was established using the ε-constraint method. The optimization method provides a framework to integrate more factors into the traditional transportation or material allocation problem and to aid in the decision-making process for optimizing supply chains and eco-industrial parks. It is hoped that with the messages identified in this work, that there will be an increasing attention to documenting and analyzing transportation incidents and data and to including risk as an essential metric in optimization transportation networks.

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