SUSTAINABLE TRANSPORTATION ENERGY INFRASTRUCTURE FOR FUEL CELL VEHICLES

By

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A dissertation submitted to the

Graduate School – New Brunswick

Rutgers, The State University of New Jersey

In partial fulfillment of the requirements

for the degree of

Doctor of Philosophy

Graduate Program in Interdisciplinary

Industrial and System Engineering

And

Civil and Environmental Engineering

Written under the direction of

Professor Mohsen A. Jafari

and approved by

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New Brunswick, New Jersey

OCTOBER, 2015

ABSTRACT OF THE DISSERTATION

Sustainable Transportation Energy Infrastructure for Fuel Cell Vehicles

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Alternative Fuel vehicle (AFV) technology and supporting energy infrastructure will become very important as the United States moves towards oil independence and environmentally sustainable economy. The current vehicle fueling infrastructure is not capable of supporting AFV technologies, and there are substantial economic and technical challenges and barriers that must be overcome in the near future. It is expected that AFV technology will require a massive infrastructure redesign and reinvestment constrained on environmental sustainability, economic efficiency, safety, security, public policy and incentives, and consumer acceptance. Hydrogen has the great potential to become one of the major energy carrier in the future energy system especially for fuel cell vehicles.

The objective of this dissertation is to address and solve these interconnected key problems: (1) how to design and plan a sustainable regional infrastructure for hydrogen fuel supply chain network under uncertain demand; and (2) in what capacity and location the infrastructure will need at the macro and micro levels.

We introduce a multi-period optimization model taking into account the stochasticity and the effect of uncertainty in hydrogen production, storage and usage in macro view (U.S. county level).We develop a spatially aggregated demand model to

estimate the potential demand for fuel cell vehicles based on different household attributes such as income and education among others.

We propose a Geographic Information System (GIS)-based Multi-Criteria Decision Making (MCDM) tool which finds the suitable locations for a hydrogen fueling station by considering factors such as land availability, air quality, and energy source availability. The results are used to choose the optimal locations for the location allocation model by maximizing the customer demand coverage.

We also propose a location allocation model which identifies the optimal locations among suitable locations by maximizing the customer demand coverage based on the capacitated Maximal Covering Location Problem (MCLP). Also, the model captures the hydrogen demand uncertainty and measures the location risk of having hydrogen fuel shortage in future. In this dissertation we also propose a life cycle assessment (LCA) and economic assessment model to compare different waste to energy methods for transportation use.

ACKNOWLEDGMENTS

First and foremost I would like to thank my PhD advisor, Professor Mohsen Jafari for his outstanding guidance and great support during the process of writing this dissertation. It was a great honor working for him in different projects at CAIT at Rutgers University. His mentorship was paramount in providing a well-rounded experience consistent with my long-term career goals. It has been such a relief to know that Professor Jafari is always there for me and acting beyond call of duty to offer me both professional and moral support. I think of him and his family, as family members. I will never forget my first meeting with him 10 years ago. He encouraged me to stay in this country and apply for graduate school. For everything you’ve done for me, Dr. Jafari, I thank you.

I am so grateful to have Professor Monica Mazurek as my co-advisor and as my mentor at Rutgers University. She is one of the smartest and nicest people I’ve ever met and she always supported my research and she helped me shaping my future by her constructive suggestions and her inspiring comments, and also assisted me to choose the best location to live in California.

I am grateful to the members of my PhD committee, Professor Hoang Pham, Professor Trefor Williams for taking the time to review my dissertation and for providing valuable and constructive suggestions and supporting my Interdisciplinary studies.

Among those who guided and/ or accompanied me in this journey, with so much regret, Professor Tayfur Altiok is no longer with us. It was an honor for me to have him as a teacher and a member of my PhD committee and a great friend. I will dearly miss his warm smile.

I also have to thank Departments of Industrial & Systems Engineering, Civil & Environmental Engineering, CAIT and Rutgers Graduate School for their continuous support during my PhD years.

I am very lucky to meet and work with so many brilliant and talented friends, whose support, ideas, and academic suggestions have inspired me in my research career. Thank you all.

I would like to thank the Air & Waste Management Association (A&WMA) for their scholarship award to me in their 105th Annual Conference for my research and studies on sustainability.

I would like to thank my dear friend and colleague, Abolfazl Vaghefi for all his help and support during the process of writing this dissertation.

I can barely find words to express my deep gratitude to my beloved family. I am so blessed and fortunate to have such a wonderful and smart parents who both are my role models. They always supported me to choose a career that I really like to do.

Last but not least, I want to say thank you to the most wonderful, supportive and understanding fiancé, Sahar, without whose continuous love, support and motivation this thesis would not have been completed.

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Chapter 1- Introduction

1.1. Objectives

This dissertation addresses the following research challenges and problems:

- Develop a life cycle assessment (LCA) and economic assessment model (EAM) to compare different waste-to-energy methods for transportation use.
- Create the necessary analytics and a decision support system for efficient and sustainable design of fueling infrastructure for the hydrogen fuel cell vehicles.
- Formulate an approach for optimal planning of a sustainable regional infrastructure for hydrogen fuel supply chain network under uncertain demand.
- Identify and evaluate a number of strategic decisions required to fulfill customers' needs. These decisions include: the number, location, type and capacity of hydrogen production plants and storage facilities, delivery modes and the total production rate of hydrogen in each region, the determination of the total average inventory in each region, and the size and type of delivery flow with uncertain demand over a long time horizon.
- Build a multi-period two-stage stochastic programming model with uncertain demand for hydrogen infrastructure.
- Develop a spatially aggregated demand model to estimate the potential demand for those who are interested in purchasing fuel cell vehicles and eventually consume hydrogen as a fuel based on different household attributes.
- Create a GIS-based Multi-Criteria Decision Making (MCDM) tool to find the suitable locations for locating hydrogen fueling station by considering factors such as land availability, air quality, and energy source availability, among others.
- Develop a methodology to calculate risk from hydrogen road transport that high risk routes can be avoided.

- Formulate a GIS-based location allocation model with uncertain demand which maximizes the coverage of demand at the micro level.

1.2. Motivation

Transportation is the fastest growing energy use sector in the US economy and consumes two-third of U.S petroleum output [1]. With the growth in energy usage by many emerging world economies, the demand for limited resources increasingly is outstripping available supply. Transportation energy consumption has contributed substantially to greenhouse gas (GHG) emissions. According to the Energy Information Administration Annual Report [2], about 33% of total US GHG emissions are generated by the transportation sector, and CO2 accounts for 95% of the GHG emitted from motorized transportation sources. These statistics point to the development of energy sourcing and infrastructure which will enable transitions from conventional vehicles to alternative fuel vehicles such as electric- and fuel- cell vehicles. Utilization of sustainable and green energy sources, such as solar, wind, hydro, geothermal, or biomass are part of future energy options for transportation infrastructure. These are mandatory options for sourcing energy to electricity (secondary energy form) as well as the use of alternative fuels in the overall architecture transportation energy supply [3].Over the last few years, the disposal of municipal solid waste (MSW) has become an increasingly important topic within the sustainability and energy sourcing domain. This holds particularly true in states of New York, New Jersey and Pennsylvania, where many consulting companies as well as universities continue to propose innovative waste disposal alternatives, especially to convert waste-to-energy. With this background in mind, we are motivated to develop a life cycle assessment (LCA) and economic assessment model to compare different waste-to-energy methods for transportation use.

Alternative fuel vehicle (AFV) technology and supporting energy infrastructure will become critical components and infrastructure assets as the U.S. moves toward oil independence and to an environmentally sustainable economy as a whole. The security of our nation clearly depends on how efficiently we can use renewable energy resources. Transit and environmental agencies have key roles to play in reducing energy consumption and GHG emissions that contribute to climate change. Most U.S. transit and environmental agencies already are helping to reduce GHG emissions by operating their current services more efficiently with conventional fuels, but these agencies can further reduce GHG emissions and achieve other important goals by promoting and implementing AFV technologies.

The current energy supply infrastructure is not capable of supporting AFV technologies, and there are substantial economic and technical challenges and barriers that must be overcome in the near future. Energy systems and transportation networks must be linked and optimized. It is expected that AFV technology will require a massive infrastructure redesign and reinvestment constrained on environmental sustainability, economic efficiency, safety, and security. Presently, the attention from industry and academia are on alternative fuel production processes and power train technologies. The infrastructure planning is under investigation only sporadically and on limited basis.

Hydrogen has the great potential to become one of the major energy carriers in future energy systems especially for fuel cell vehicles. The transition from the current energy infrastructure to a hydrogen economy in which hydrogen plays a major role as an energy carrier has stimulated the interest of both the technical community and the broader public. The hydrogen economy is centered on the production of molecular hydrogen using coal, natural gas, nuclear energy, or renewable energy such as biomass, wind, solar; the delivery and storage of hydrogen in some fashion; and the end use of hydrogen in fuel cell vehicles [3].

The lack of hydrogen fueling stations is a major barrier to the introduction of fuel cell vehicles. Finding suitable and optimal locations for hydrogen fueling stations are significant issues in the energy infrastructure planning especially in highly populated locations. This is a very important topic in the near future for hydrogen fueling station planning and investment.

With this background in mind, we are motivated to develop the necessary analytics and a decision support system for efficient and sustainable design of refueling infrastructure for the hydrogen fuel cell vehicles.

1.3. Technical Approach

In chapter two, we introduce a life cycle assessment (LCA) and economic assessment model and compare three different municipal solid waste (MSW) treatments of incineration, anaerobic digestion, and plasma gasification options. Together these MSW treatments produce energy outputs in the form of electricity and thermal heat, hydrogen and methane gas for the states of New York, New Jersey and Pennsylvania. For this study SimaPro (7.0 version) software was used for LCA tasks. SimaPro is a LCA tool developed by PRé Consultants (city, state). Also, economic analysis was performed by using different sources and data base based on project proposals and finished projects (should name these). The contribution of this chapter is comparing the three waste-to-energy methods with real data and then assessing feasibility and of implementation these MSW energy conversion methods for facilities operating in New York, New Jersey and Pennsylvania. This is a crucial topic for the near future. Currently, there is some comparison method research available however, this research does not include location related studies. In this dissertation research, we hypothesize the location of the hydrogen refueling infrastructure plays an important role in decision making

In chapter three we formulate the infrastructure problem as a network flow problem with different types of nodes and flow types. The dynamics of the network is partially defined by the demand at some of these nodes. There will be at least two network views employed as part of this study: A macro view encompassing a wider or multistate level. Here the demand will be defined on regional basis and the objective will be to decide on the major infrastructure elements. A micro view will take a closer look at various regions on a county or city level, and will take the demand and supply with finer granularity.

We introduce a multi-period optimization model taking into account the stochasticity and the effect of uncertainty in hydrogen production, storage and usage in macro view (state/regional level). The objective function includes minimization of the total daily social cost of the hydrogen supply chain network with the condition of uncertain demand. The underlying models are stochastic and use a two-stage programming approach for optimization. Uncertainty in demand is assumed for each region. This demand uncertainty can be estimated using a combination of energy economy model, statistical data, and survey results.

There are several factors and key attributes which influence a consumer's choice to buy a fuel cell vehicle. At the same time, consumer preference on the demand side is the most important factor in predicting changes in the auto market. We develop a spatially aggregated demand model to estimate the potential demand for fuel cell vehicles based on different household attributes such as income and education as initial criteria. Vehicle demand at an aggregate level usually focuses on household income, land use, household demographic characteristics for example. The results of this work can be used toward the development of an advanced decision support system that can assist in multi-period planning for such infrastructure.

The contribution of this chapter is developing a new framework to capture all the cost elements in our two-stage multi-period stochastic optimization model such as economy, emission, energy consumption, and risk simultaneously. We then implementing the model with real data for the state of New Jersey and develop a new methodology for estimating future hydrogen demand.

In chapter 4 we propose a Geographic Information System (GIS)-based Multi-Criteria Decision Making (MCDM) tool which finds the suitable locations for hydrogen fueling stations by considering factors such as land availability, air quality, and energy source availability as initial criteria. These results are then used to choose the optimal locations for the location allocation model (Chapter 5) by maximizing the customer demand coverage. We will choose the locations such that all or a high % of estimated customer demand is within a specified impedance cutoff. This study was carried out within the framework of an Analytic Hierarchy Process (AHP) as a multi-criteria decision analysis approach by integrating it with the GIS for choosing the suitable locations. The purpose of integrating the GIS-based location suitability analysis using the multi-criteria AHP approach is that together, the tools provide a unique and effective approach for solving complex problems related to land-use planning.

Also, in chapter 4 we introduce a methodology to calculate hydrogen road transport risk so it can identify which routes have higher hydrogen transport risk than others. There can be many different causes for a truck accident and cargo release, but they can be divided into two most important categories, i.e. crash- initiated releases and non-crash initiated releases. The crash-initiated releases with a truck represent a great potential for substantial damage, injury, and large releases of hydrogen. These include a collision between two vehicles, collisions with fixed objects, and overturn. In this model we only consider the crash- initiated release for risk calculation in hydrogen delivery. In order to calculate overall hydrogen transportation risk we need to calculate the probability of hydrogen release and then, design the consequence model for different accident scenarios.

The contribution of this chapter 4 is developing (GIS)-based Multi-Criteria Decision Making (MCDM) tool which finds the suitable locations for hydrogen fueling station. Unfortunately, our search of the published literature found no papers related to alternative fueling stations, especially hydrogen. This is a very important topic in the near future for hydrogen fueling station investment and planning. Also, the other unique contribution is implementing this tool for the state of New Jersey with the real data. This can be used in different regions of the U.S. as long as data is available for the data layers within GIS applications.

In chapter 5 we propose a location allocation model which chooses the optimal locations among suitable locations (from chapter 4) by maximizing the customer demand coverage so it will choose locations such that all or the greatest amount of estimated customer demand is within a specified impedance cutoff. Also, the model captures the hydrogen demand uncertainty and measures the risk of having hydrogen fuel shortage in future. The model is based on the capacitated Maximal Covering Location Problem (MCLP) and in order to measure the risk of having hydrogen fuel shortage in the future, the Geometric Brownian Motion (GBM) will be used to model the uncertainty of the demand.

The contribution of this chapter 5 is utilizing the results from chapter 4 and then finding the optimal locations for hydrogen fueling station among suitable locations at the micro level. There is much published research focused on choosing optimal locations (mathematically) for hydrogen fueling stations, but there are not necessary suitable locations for constructing hydrogen fueling stations.

Chapter 2- Waste to Energy in Transportation

2.1. Introduction

Over the last few years, the disposal of municipal solid waste (MSW) has become an increasingly important topic within the sustainability arena. This holds particularly true in states of New York, New Jersey and Pennsylvania with large metropolitan areas of high population density. Here burgeoning green energy companies, utilities, waste-management operators, as well as universities continue to propose innovative waste disposal alternatives, especially to convert it to energy. On a small scale these waste-to-energy operations are demonstrating the feasibility of energy recovery and conversion technologies.

Transportation energy consumption has contributed substantially to greenhouse gas (GHG) emissions (about 33% of total U.S. GHG emissions are generated by the transportation sector)[1] so it's time to make decisions toward switching from conventional vehicles to alternative fuel vehicles such as electric vehicle and fuel cell vehicles.

In this chapter three MSW to energy processes were studied: incineration, plasma gasification and anaerobic digestion where their combined outputs are electricity and thermal heat, hydrogen, and methane gas. In this study the objective was to perform and LCA and economic assessments for these processes and to choose the best strategy for the states of NY, NJ and PA. In reality, there is no a single technology that can solve the waste management problem [4]. Integrated waste management system is commonly applied method in many developed countries. Integrated waste management system offers the flexibility of waste treatment option based on different waste fractions such as plastic, glass, organic waste or combustible waste. Energy and resource recovery also are important and these can be recovered through integrated waste management systems [5]. There are different system analysis tools [6] that are available at the present time for decision makers. Systems analysis is analysis of a system which instead of considering separate parts of a large system a more holistic approach is taken [6]. According to [7] systems analysis tools can be divided into procedural and analytical tools which procedural tools focus on improving the procedures leading to decision making, while analytical tools provide information that may be used for communication, comparing different alternatives, etc.

LCA which was used in this study is an analytical tool assessing potential impacts from products using life cycle perspective, including impacts from raw material acquisition, production, use and waste management as well as transportation [6].

A technology or management strategy can be analyzed in terms of impact or risk from the environmental, social, or and economic points of view [5]. The LCA approach is a tool commonly applied to analyze the environmental burden for waste management technology. LCA has been applied to energy production systems as well [8].

In this chapter, LCA analysis was performed by using SimaPro software (version 7) [9] and the economic assessment were performed manually based (using Microsoft Excel) on using different sources and databases from project proposals and finished real projects especially from Northeast.

In addition, CML 2 (Centre for Environmental Studies, University of Leiden) baseline (2000) [10] method and Eco-indicator 99(E) [11] were used for life cycle inventory analysis. This study was done primarily to assess three different waste to energy options and to analyze which one of those options would achieve better impacts on transportation energy infrastructure NY, NJ and PA. Results and conclusions from this study would help inform decision-making processes aimed at evaluating the environmental and economic performance of the technologies. Figure 1 shows the steps for this waste-to-energy optimization model as: (1) define process; (2) goal and scope; (3) life cycle data inventory; (4) life cycle assessment; (5) economic assessment; (6) life cycle interpretation; and (7) conclusion.

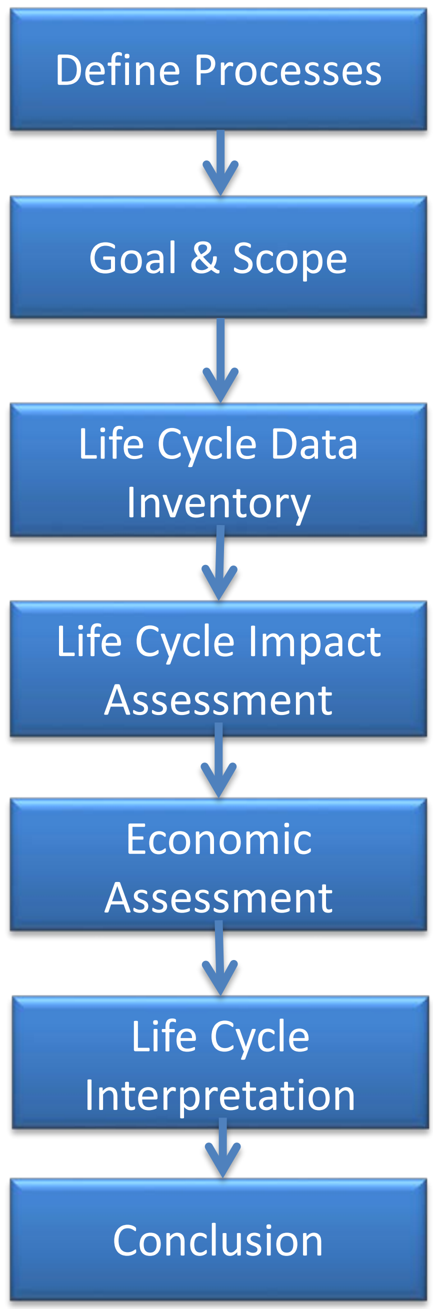
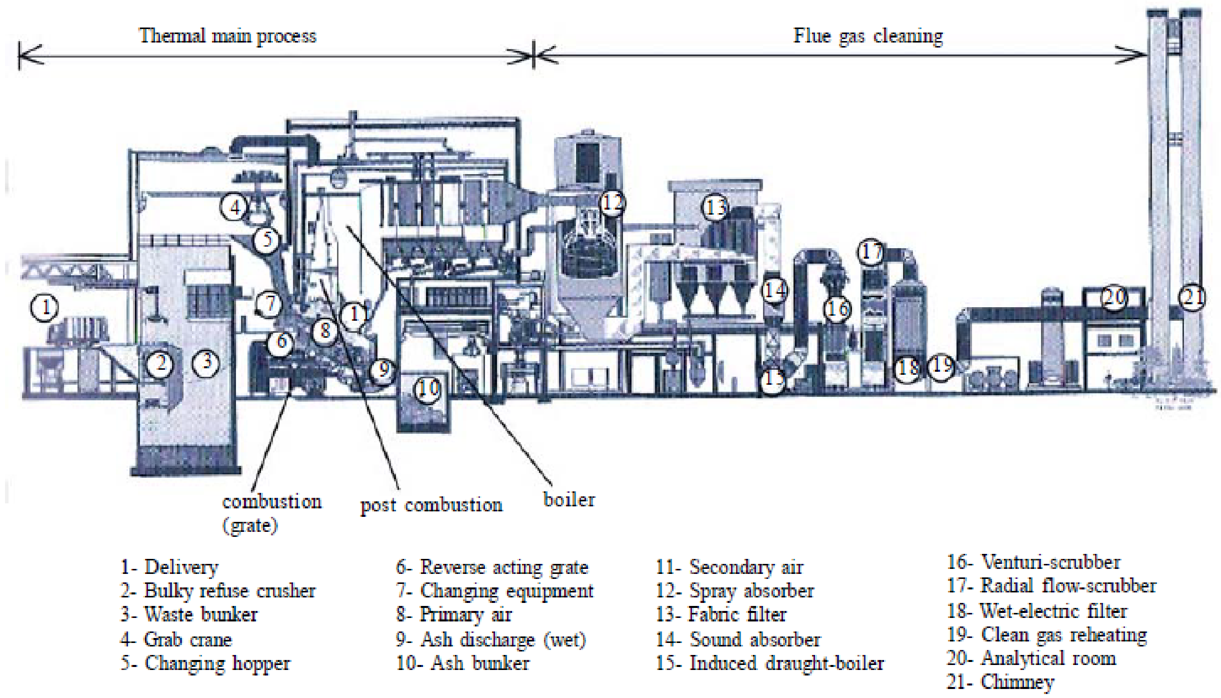


Figure 1. Steps for LCA and Economic Assesmenst

Brief descriptions of the three waste-to-energy technologies are given bellow:

2.1.1. Incineration

Incineration is a thermal waste treatment process where unprocessed municipal solid waste can be used as feedstock. The incineration process takes place in the presence of sufficient quantity of air to oxidize the feedstock (fuel). Waste is combusted at 850ºC. In this stage the waste is converted to carbon dioxide, water and non-combustible materials with solid residue state called incinerator bottom ash (IBA) that always contains a small amount of residual carbon [12,13].



] **Figure 2.** Schematic diagram of MSW combustion plant

Figure 2 shows the schematic diagram of MSW combustion plant where wastes are delivered as feed stock to the pre-combustion location (grate). During post combustion, gas and slug or ashes are produced. Then, in the next phases flue gas is cleaned by a water absorber or different filtering methods. Finally, the clean gas is emitted through the chimney to the atmosphere. Thermal conversation of waste to energy is now a very much applied technology for waste management system due to the generation of heat and energy (electricity) from the waste stream [5]. Based on available data [14] there are 10 facilities in NY, 5 facilities in NJ and 6 facilities in PA now operating as waste-to-energy processing plants.

2.1.2. Plasma Gasification

Plasma gasification is a process to convert solid waste, especially organic waste, into a mixture of hydrogen and carbon monoxide, or syngas. Using suitable temperature and pressure conditions, the syngas product is generated and can be burnt for heat or power generation to produce electricity for charging electric vehicles or for hydrogen to fuel cell vehicles. Figure 3 shows a plasma gasification processing plant in Ottawa, Canada [14]. The plant is a private waste conversion and energy generation company (Plasco).

The waste conversion process begins with any materials with high reclamation value being removed from the waste stream and collected for recycling. Once these high value products are removed, the municipal solid waste (MSW) is shredded and any remaining materials are removed and sent for recycling.

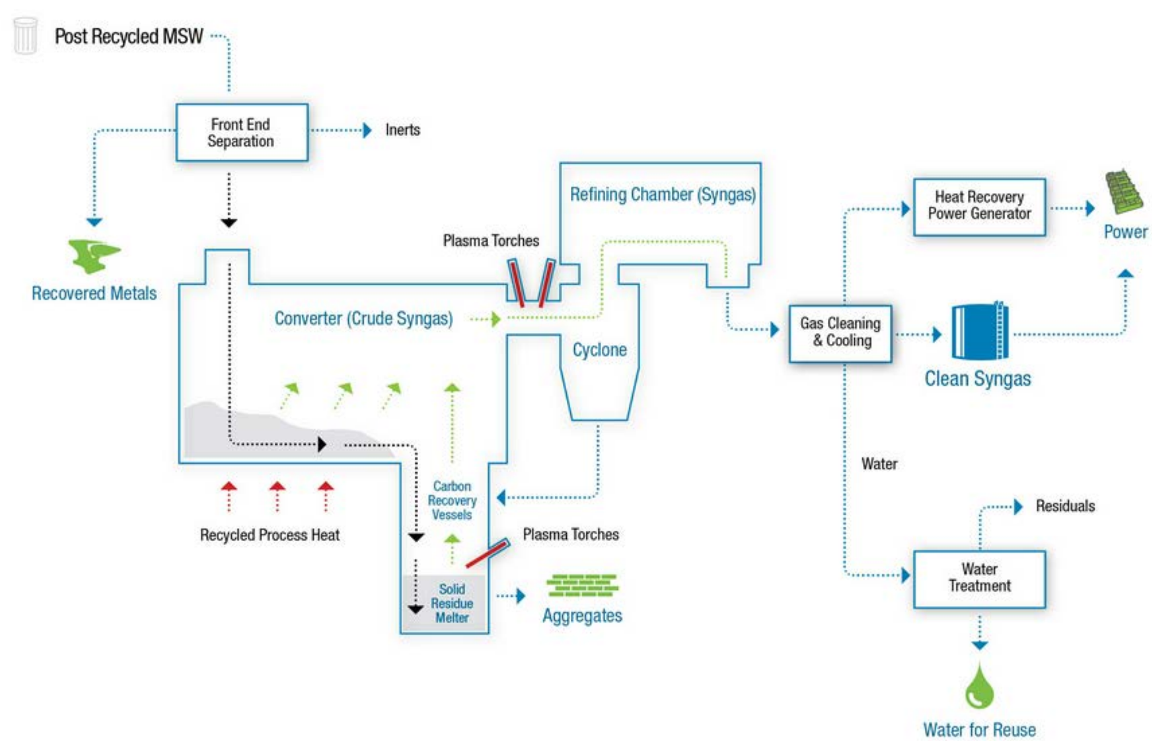


Figure 3. Plasma gasification process in Ottawa, Canada (Plasco) [14].

The MSW stream enters the conversion chamber where the waste is converted into a crude synthetic gas using recycled heat. The crude syngas that is produced flows to the refinement chamber where plasma torches are used to refine the gas [14].

After refining, the syngas is sent through a Gas Quality Control Suite to remove sulfur, remove acid gases and segregate heavy metals found in the waste stream. The output is a clean, energetic syngas created from the conversion of waste [14].

The syngas can be used to fuel internal combustion engines that efficiently can generate electricity and hydrogen. Waste heat recovered from the engines is combined with waste heat recovered from cooling the syngas in a Heat Recovery Steam Generation (HRSG) unit to produce steam. The steam can either be used to generate additional electricity using a turbine (combined cycle generation), or it can be used for industrial processes or district heating (cogeneration) [14].

The solid residue from the conversion chamber enters a separate high temperature Carbon Recovery Vessel (CRV) equipped with a plasma torch where the solids are melted. Plasma heat is used to stabilize the solids and convert any remaining volatile compounds and fixed carbon into crude syngas. This additional crude syngas is fed back into the conversion chamber. Any remaining solids are then melted into a liquid slag and cooled into small slag pellets. The slag pellets are an inert vitrified residue sold as construction aggregate. Leachability tests have been conducted on slag emerging from the process and have confirmed that the slag does not leach and is non-toxic [14].

The entire process is monitored continuously by a proprietary control system that ensures sufficient syngas stability to fuel internal combustion engines regardless of the variations in the energy content of the MSW [14].

The schematic diagram and a picture of the thermal plasma gasification/H2 recovery systems also are shown in Figure 4. The process consists of two sub systems: a thermal plasma gasification system, which converts the organic components of the feed waste into syngas, and an H2 recovery system, which converts the syngas generated by the thermal plasma gasification of paper mill waste (PMW) into high purity H2 (>99.99%) using water gas shift (WGS) and pressure swing adsorption (PSA) steps.

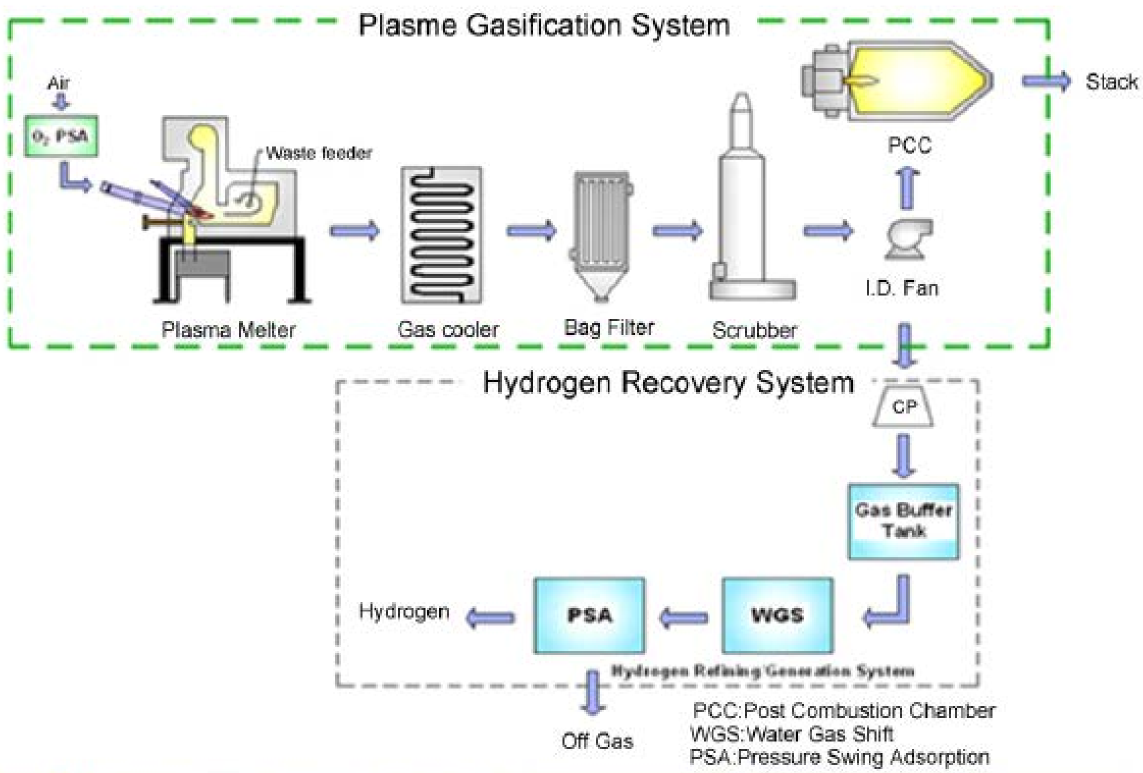


Figure 4. Schematic diagram of the thermal plasma process for the recovery of high purity H2 and picture of the overall demonstration plant.

2.1.3. Anaerobic Digestion

Anaerobic digestion (AD) is one of the most favorable organic waste management options because of higher resource recovery potentials [16]. The AD is a natural biological process mediated by microorganisms and takes place in the absence of oxygen. Anaerobic digestion produces biogas and composts (solids). Biogas consists of methane (~ 64 percent) and carbon dioxide (~ 34 percent) and is produced within 2-3 weeks [17]. Figure 5 shows the anaerobic digestion process flow chart.

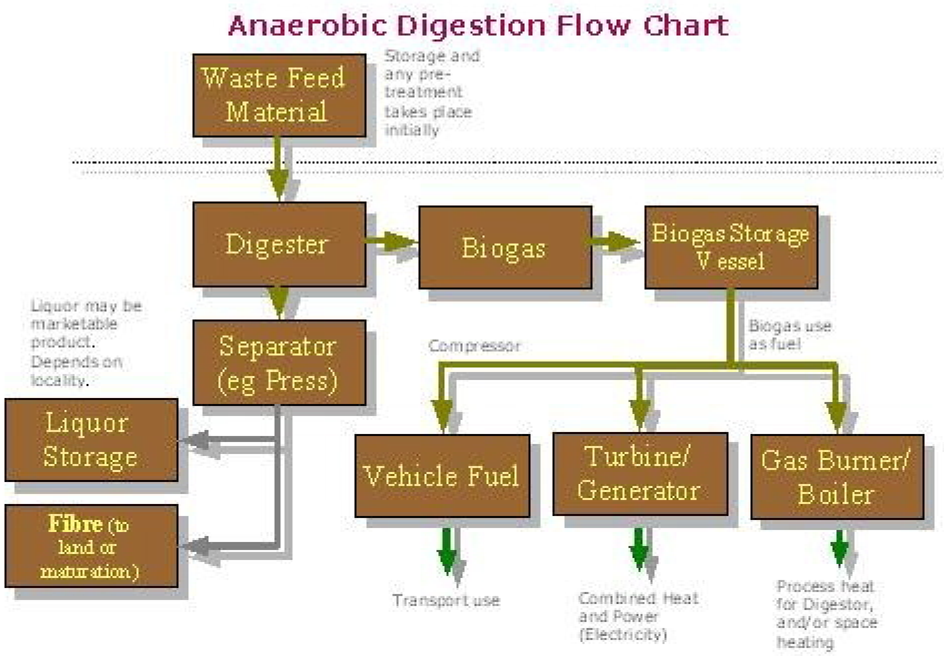


Figure 5. Anaerobic digestion process flow chart

2.2. Goal and Scope

The goal of the study is to develop a life cycle assessment (LCA) and economic assessment model followed by a comparison the three different MSW treatment option (incineration, anaerobic digestion and plasma gasification) for New York, New Jersey and Pennsylvania. SimaPro (7.0 version) software [9] was used for LCA in this study.

2.2.1. Function and Functional Unit

Disposal of the source solid waste is the function of the MSW treatment processes under evaluation. Solid waste is considered as a mixture of compostable or organic, inorganic and other types of waste fractions. We used 59500 Metric tons of solid waste per day as the functional unit for this study. This estimate was calculated based on the total population of NY, NJ and PA multiplied by the municipal solid waste generation rate per Kg/person·day in the U.S. Based on the 2010 U.S. census, the total population of NY, NJ and PA was 29,739,174 people and the municipal solid waste generation rate was 2 Kg/person·day [18].

2.2.2. System Boundaries

Figure 6 shows the system boundary of the waste-to-energy treatment processes. Waste is considered a mixture of compostable or organic, inorganic and other types of waste fractions. It enters the transportation mode (dump truck) and is relocated to a facility. Then, the waste produces different fuel or electricity based on a given process along with different emissions (water & air.) After the process is completed, the waste by-products consisting of ash, solid residue, and digestate (from AD) are transported to a landfill. In this thesis model, the distance to the landfill was assumed to be 50 miles l (section 2.3 Life Cycle Inventory).

We sought access to real data and metrics from an operating anaerobic digestion processing plant. There is a digester at a waste water treatment plant (WWTP) in Elizabeth, NJ. An operations engineer at the WWTP was able to provide some general information about the digester operation. However, literature values for digester inputs and outputs had to be used because of incomplete data from this particular plant. Further, for this modeling study we assumed the solid waste would be mixed directly with the WWTP sludge and then input into the digester where it would produce biogas with 64% methane content [17]. In this example, the biogas product would offset the consumption of natural gas used in natural gas or electric vehicles, or eventually in future hydrogen fuel cell vehicles. Also in this study, the 35-60% of the wastes not digested [19] first are de-watered in a screw press and then transported 55 miles to the Middlesex County Sanitary Landfill to be used as landfill cover. As landfill cover, waste conversion to methane does not occur due to the presence of atmospheric oxygen.

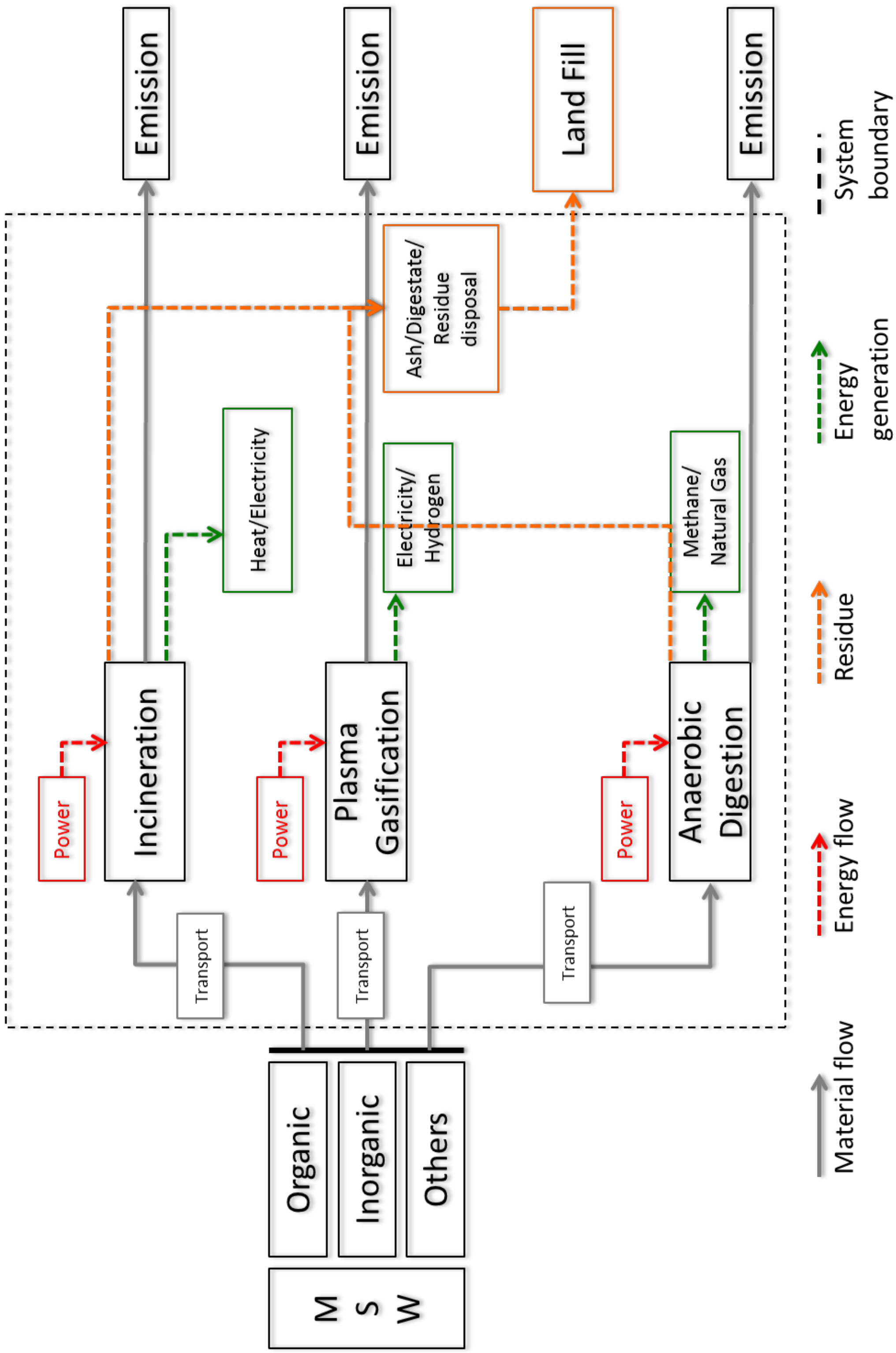


Figure 6. System boundary for different MSW treatment options

2.2.3. Impact Assessment Methodologies and Categories

The impact assessment methods used in this project were Eco-indicator 99(E) [11] and CML 2 baseline (2000) [10]. Environmental impacts from the three different MSW treatment options were analyzed based on eleven different impact categories selected in the Eco-indicator 99(E) application. The impact categories in are carcinogens, respiratory organics, respiratory inorganics, climate change, radiation, ozone layer, ecotoxicity, acidification/eutrophication, land use, minerals, and fossil fuels. Environmental impacts from the three different MSW treatment options were analyzed based on ten selected impact categories in the CML 2 baseline (2000) application. The impact categories are abiotic depletion, acidification, eutrophication, global warming potential, ozone layer depletion, human toxicity, fresh aquatic ecotoxicity, marine aquatic ecotoxicity, terrestrial ecotoxicity, and photochemical oxidation.

2.3. Life Cycle Inventory

The data used in this study was acquired through government reports and literature review. Reports were found primarily from government environmental departments in the U.S. and abroad while the journal articles used were found primarily through database searches for keywords. In our study mainly we used the existing databases in SimaPro Software and Also from UK Department for Environment, Food and Rural Affairs report [12], Zaman [5], Finnveden [6] and Ducharme [15].

2.3.1. Emissions to Air & Water

Table 1 shows the gas and particle emission rates of key products (kg/day) for each process using the input mass unit of 59500 MSW tons per day. Each emission rate was e calculated manually as input to the applications software. All calculations are in Appendix A.1, including references to the data sources for each process.

Table 1. Emissions to the air from different waste to energy processes (kg/day)

Atmospheric emission rates of key products from different waste-to-energy processes (kg/day)			
Substance	*Incineration*	*Plasma Gasification*	*Anaerobic Digestion*
Nitrogen oxides	95165.35	46393.11	11181.92
Particulates	2260.17	713.74	No data
Sulfur dioxide	2498.09	3092.87	178.43
Hydrogen chloride	3449.74	1903.3	1.189
Hydrogen fluoride	59.478	20.22	0.41
VOC	475.82	654.26	No data
Cadmium	0.297	0.41	0.0059
Nickel	2.973	2.37	0.017
Arsenic	0.297	3.56	0.029
Mercury	2.973	4.1	0.035
Dioxins and furans	0.237×10^{-5}	2×10^{-6}	5759410
Polychlorinated biphenyls	0.005	No data	No data
Carbon dioxide	59478348	59478348	No data

Table 2 shows the amount of emissions to processing water for anaerobic digestion. All calculations are in Appendix A.1.

Table 2. Emissions to water for Anaerobic Digestion (kg)

Emissions to water for anaerobic digestion (kg)	
Substance	*Anaerobic Digestion*
Nitrogen	594.78
COD, Chemical Oxygen Demand	5947.83
BOD, Biological Oxygen Demand	148.6

2.3.2. Input-Output (Energy)

Table 3 compares the amount of energy input (consumption) to the energy output (generation) for 59500MSW tons per day for each process. All calculations are in Appendix A.2.

Table 3. Input and output energy comparisons for MSW conversion processes

Input and output energy comparison			
Input/ Output	*Incineration*	*Plasma Gasification*	*Anaerobic Digestion*
Start-up energy	4627.4 MWh	21114.8 MWh	247.1MWh
Energy generation	32356.2 MWh	48058.5 MWh	196278548.4 ft^3 CH_4

2.3.3. Waste Scenario

We assumed the end waste product from each MSW treatment processing facility is disposable material. A truck transports this processed material from each treatment plant to landfill which is 50 miles away. All the calculations are in Appendix A.4.

2.4. Life Cycle Impact Assessment

The normalized values are summarized below for the selected impact categories for the three waste-to-energy-processes based on the CML 2 (Table 4) and Eco indicator 99(E) (Table 5) methods and using a materials processing rate 59500 tons of MSW per day. A positive value indicates a deleterious effect where pollutant material is added; a negative value indicates net pollutant removal. The CML 2 environmental impact results (Table 4), show all three processes have positive (deleterious) for the categories of terrestrial ecotoxicity and global warming potential (GWP). GWP is as the largest environmental emission category by several orders of magnitude in each case. Also, incineration and anaerobic digestion processes have positive (deleterious) impacts on ozone layer depletion due to linked electricity generation. Conversely, switching to plasma gasification and anaerobic digestion show the greatest benefits in the environmental impact categories of marine aquatic ecotoxicity and abiotic depletion. Incineration has significant positive pollutant release in the same environmental categories. Incineration has a significant environmental impact on carcinogens. In Table 5, all three waste-to-energy processes show the largest positive (deleterious) results in the category of climate change. This category ranks as the largest impact category in the EcoIndicator method. Incineration always has positive net pollutant emissions compared to plasma gasification and anaerobic digestion processes. In addition, plasma gasification has only one positive environmental impacts and that is climate change. Also, in Table 5 the EcoIndicator analysis shows plasma gasification to be the process with greatest overall reductions of pollutant mass emissions to the environment. Both plasma gasification and anaerobic digestion have large benefits (negative mass release rates) compared to incineration which has a net positive mass release. Tables 4 and 5 results demonstrate the incineration waste-to-energy process has the highest impacts to the environment and ecology impact categories. Significant benefits are possible by switching to plasma gasification and anaerobic digestion.

Table 4. Comparative normalization results for processes (CML 2 method)

Comparative normalization results for processes (CML 2 method)				
Impact category	*Unit*	*Incineration*	*Plasma Gasification*	*Anaerobic Digestion*
Abiotic depletion	kg Sb eq	9.17E-08	-1.06E-06	-6.92E-07
Acidification	kg SO2 eq	1.86E-07	-2.46E-07	6.47E-09

Eutrophication	kg PO4--- eq	1.04E-07	-4.96E-08	1.56E-08
Global warming (GWP100)	kg CO2 eq	1.40E-06	8.37E-07	1.06E-07
Ozone layer depletion (ODP)	kg CFC-11 eq	4.09E-10	-7.01E-10	9.78E-12
Human toxicity	kg 1,4-DB eq	1.77E-08	-2.28E-08	-1.07E-08
Fresh water aquatic ecotox.	kg 1,4-DB eq	1.91E-08	-6.57E-08	-1.31E-07
Marine aquatic ecotoxicity	kg 1,4-DB eq	2.66E-07	-1.36E-06	-1.26E-06
Terrestrial ecotoxicity	kg 1,4-DB eq	3.41E-07	2.99E-07	1.23E-09
Photochemical oxidation	kg C2H4 eq	4.73E-09	-3.89E-08	-5.04E-09

Table 5. Comparative normalization results for processes (Eco indicator 99(E) method)

Comparative normalization results for processes (Eco indicator 99(E) method)				
Impact category	*Unit*	*Incineration*	*Plasma Gasification*	*Anaerobic Digestion*
Carcinogens	DALY	156.76194	-761.72122	7.6386447
Respiratory organics	DALY	0.22756535	-0.52740965	-0.39725348
Respiratory inorganics	DALY	1210.2977	-799.82485	123.90984
Climate change	DALY	1462.2313	878.39648	112.01268
Radiation	DALY	44.579362	-15.359457	0.38900164
Ozone layer	DALY	0.055585182	-0.095614318	0.001240271
Ecotoxicity	PAF*m2yr	19.02472	-78.464171	0.99902085
Acidification/ Eutrophication	PDF*m2yr	104.40151	-4.3399142	11.96743
Land use	PDF*m2yr	4.6204869	-20.474165	0.27550694
Minerals	MJ surplus	11.773089	-8.9886495	1.644394
Fossil fuels	MJ surplus	372.57513	-3386.0703	-3257.0149

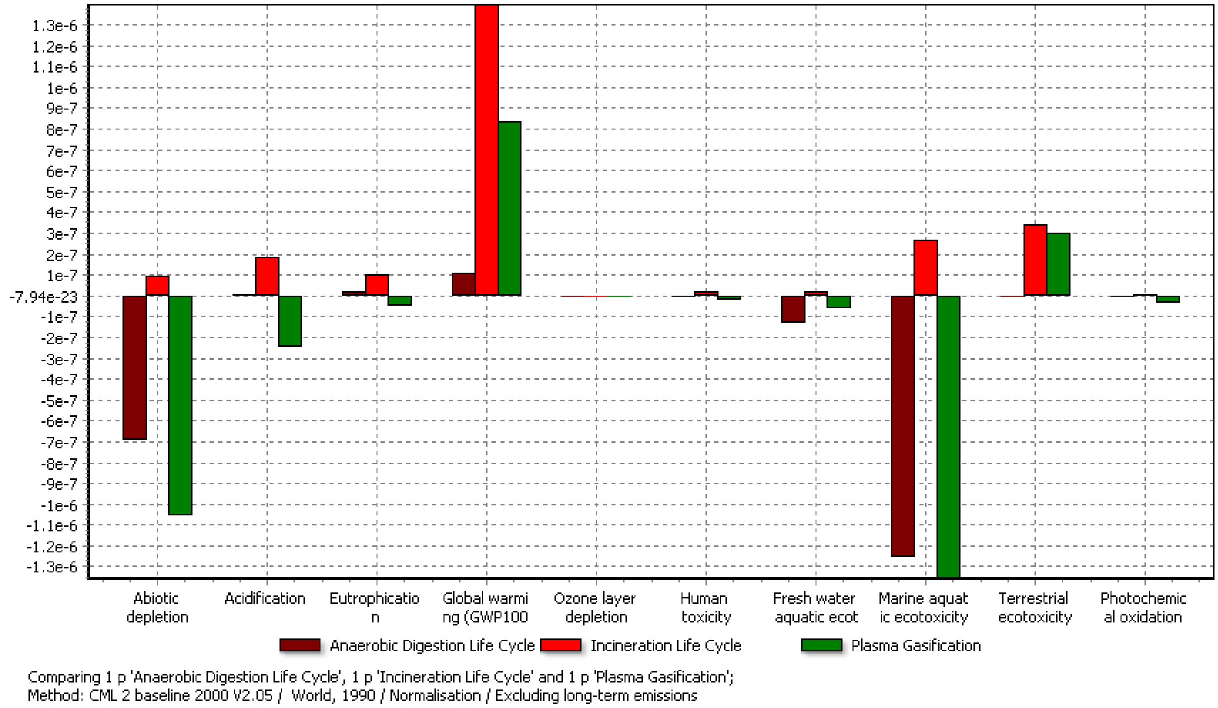


Figure 7. Comparative LCA normalization graph for three MSW treatment options using CML 2

Figures 7 and 8 show the comparative LCA normalization graphs for the three MSW treatments based on CML2 and EcoIndicator 99(E). The more negative the result, the greater the benefit to the environmental and ecological category. Here incineration has a significant environmental impact on global warming, climate change, and respiratory inorganics. In this analysis, natural gas is an offset for anaerobic digestion (brown bar) and electricity for plasma gasification (green bar). By replacing natural gas and electricity generation from fossil fuels with these two MSW waste-to-energy processes, the largest impacts on the environment can be avoided. Therefore, anaerobic digestion and plasma gasification could be good options for waste-to-energy processes especially for the transportation sector. Note all the life cycle networks for each process are in Appendix A.3.

Furthermore, it is clear from this analysis the largest avoided impacts on the environment are from displacing natural gas consumption and electricity consumption. Note that Based on my understanding from results both

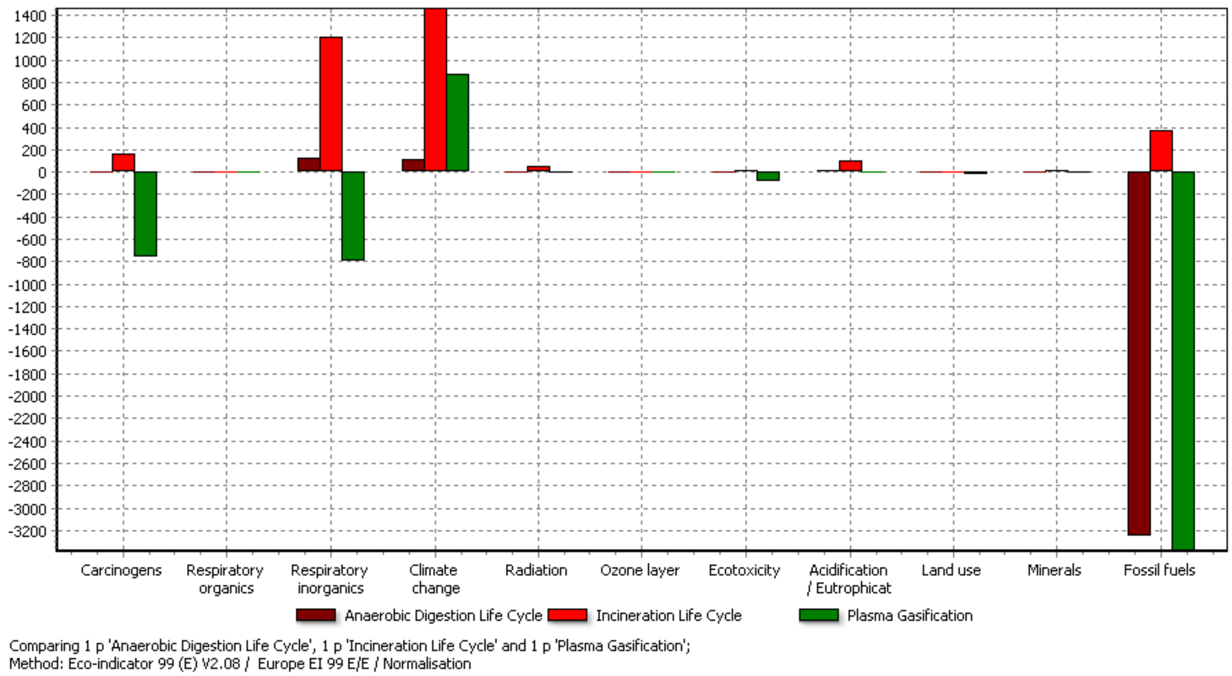


Figure 8. Comparative LCA normalization graph for three MSW treatment options using Eco Indicator 99(E)

2.5. Economic Assessment

In this section, after performing an LCA, we performed an economic assessment. Economic assessment methods are used in a comparative manner. For example, two alternative projects are compared to each other or a project is compared to the status quo. The economical assessments can be used to identify the project that gives the most environmental benefit/improvement for the least cost, and thereby society can utilize its resources in the most effective manner. There are different methods to perform welfare economic calculations. One of the most common methods is cost-benefit analysis. It includes all costs and all benefits associated with a project and calculates the total value of performing this specific project. The project that gives the highest net benefits is the project that is the most advantageous to perform [20].

In our study, except for incineration, there were not enough data for plasma gasification and anaerobic digestion processes. Therefore, most of the data were used from project proposals and literature review especially in other countries [12-19].

In the case of plasma gasification, the economic assessment of this new technology is crucial to its development as it uses electricity, the most expensive source of energy. The capital costs are likely to be high as the technology is not mature enough to lower the prices. In our study we consider capital cost, operating cost, which includes labor and maintenance costs. The revenues (benefit) are the results of sales: electricity, natural gas, metals recovered, and the gate (tipping) fees. All the cost and benefit values are based on in the 2010 U.S. dollar. For the gate fees paid by the neighboring communities, the average cost was assumed: for every ton of garbage processed by the plant, $65 is paid to the plant.

2.5.1. Economic Assessment for Incineration

Table 6 shows the cost and benefits for the incineration process. Cost values were accessed from California Integrated Waste Management Board report [21]. Gate fee and electricity sale price were taken from Ducharme [15]. We assumed the electricity sale is 10 cents per kWh and based on Circeo [22] and energy generation (electricity) is 544 kWh/tonne. Consequently, in this study the sale of electricity from incineration is $54.4 per tonne of MSW. The total costs ($135/tonne) is more than the total benefits ($119/tonne), so incineration is not beneficial.

Table 6. Costs and Benefits for Incineration

Costs categories	($/ton)	**Benefits categories**	($/ton)
Operating costs	$104	Gate fee	$65
Annual Capital Cost	$31	Sales of electricity	$54
Total	*$135*	*Total*	*$119*

2.5.2. Economic Assessment for Plasma Gasification

The economic analysis is based on software created by Sunbeam for Credit Suisse on a proposal to build a Europlasma plant. The application is adapted for the case of the construction of a 400 tons per day plant in New Jersey [15]. Although plasma gasification can produce a great amount of hydrogen (H2), it is a future energy option that could figure significantly. Hydrogen has long been proposed as an ideal long-term solution to energy-related environmental and supply security problems. Therefore, the recovery of H2 from the thermal plasma treatment of waste has been considered as a useful and economically feasible tool [23]. In order to calculate revenues for energy generation, we used the amount of electricity which can be generated from this process. Based on Ducharme [15], energy generation is 808 kWh/tonne with the sales of electricity per ton resulting in $80.80 for in our NJ study. The sale of electricity is 10 cents per kWh. All other costs were estimated from Ducharme [15]. The results in Table 7 show the input cost total ($149.00) is only slightly higher than total benefits ($148.27). This slight cost differential could be change based by increasing the operational efficiency of plasma gasification process.

Table 7. Costs and Benefits for Plasma Gasification

Costs categories	($/ton)	**Benefits categories**	($/ton)
Labor cost	$10	Gate fee	$65
Other operating costs	$53	Sales of electricity	$80.8
Total operating cost	$63	Metal & slag recovery	2.47
Annual Capital Cost	$86		
Total	*$149*	*Total*	*$148.27*

2.5.3. Economic Assessment for Anaerobic Digestion

Table 8 shows the costs and benefits for the anaerobic digestion process. Cost values were obtained from the California Integrated Waste Management Board [21]. Gate fees were from Ducharme [15]. We assumed there is a 1 to 1 ratio of methane gas produced from natural gas with a methane production rate of 3,300 ft3 CH4/wet ton based on estimates from the EPA and the East Bay Municipal Utility District [17]. The natural gas price is $0.00988 per ft3 based on EIA data [24] with sales of natural gas at $32.6 per ton. The economic assessment results in Table 8 show the total benefit is higher than the total costs, indicating anaerobic digestion is a beneficial process overall.

Table 8. Costs and Benefits for Anaerobic Digestion

Costs categories	($/ton)	**Benefits categories**	($/ton)
Operating costs	$3.0	Gate fee	$65.0
Annual Capital Cost	$2.0	Sales of natural gas	$32.6
Total	*$5.0*	*Total*	*$97.6*

2.6. Life Cycle Interpretation and Conclusions

Based on the system boundaries (Figure 6)for which data was gathered and input into SimaPro, the life cycle analyses indicate that diverting NY, NJ and PA wastes to anaerobic digestion and plasma gasification processing options each reduce substantially negative impacts in the indicator categories on human health and eco-system quality. In terms of resource consumption, the production of methane and natural gas from anaerobic digestion and the production of electricity and hydrogen from plasma gasification offset significant impacts from fossil fuel consumption compared to the incineration process and conventional landfill methods. These LCA results are in contrast to current MSW waste management practices which do not consider environmental factors showing anaerobic digestion of the waste is a better option than the incineration and landfill. Also, the economic assessment results of our study indicate the anaerobic digestion process for MSW as more beneficial than incineration and plasma gasification.

In the future, decisions also will be influenced by the regulatory environment for alternative energy within the NJ State government. The NJ Energy Master Plan, released on December 6th 2011 [25], affirms that “energy from waste is an attractive option” and calls for the State to “consider opportunities to support further use of biomass as an energy source and consider innovative mechanisms for the development of new plants that can make use of a variety of biomass types to produce electricity as well as fuels [25]. Therefore, cost-effective growth of biomass to energy technologies are important to energy supply and security which in turn support economic growth within NJ and the region.

Also mentioned in the NJ Energy Master Plan are specific energy technologies involving waste streams. When waste is used directly as an energy resource, 80% or more of the hydrocarbons are converted to energy. These efficiencies can be achieved, not only through incineration, but also by utilizing plasma gasification, pyrolysis, and in-vessel anaerobic digestion. Potential energy products include heat, electric power, biogas, and bio-liquids. These energy conversion technologies can be designed, permitted, and operated with state-of-the-art pollution control systems in conformance with strict emissions limits" [25].

As NJ and other states move ahead in exploring opportunities for waste to energy, it is the hope of the practitioners that environmental life cycle assessments - such as the one conducted in this study - will be considered and utilized to help inform decision making and energy investments..

2.6 Conclusion

In this work, a life cycle assessment (LCA) and economic assessment model was developed to compare three different municipal solid waste (MSW) treatments of incineration, anaerobic digestion, and plasma gasification options. Together these MSW treatments produce energy outputs in the form of electricity and thermal heat, hydrogen and methane gas for the states of New York, New Jersey and Pennsylvania. Based on the system boundaries in which data was gathered and input into SimaPro, this analysis indicates that diverting NY, NJ and PA wastes to anaerobic digestion and plasma gasification prevents negative impacts on human health and eco-system quality. In terms of resource consumption the production of methane and natural gas in digestion and production of electricity and hydrogen in gasification does offset more fossil fuel consumption than does the incineration and landfill methods. Also results shows that anaerobic digestion might be more beneficial in economic assessment method compare to other two. As the states move ahead in exploring opportunities for waste to energy, it is the hope of the practitioners that environmental life cycle assessments - such as the one conducted in this study - will be utilized to help inform decision makers.

Chapter 3- Planning Sustainable Hydrogen Infrastructure under Demand Uncertainty

3.1. Introduction

This chapter addresses the problem of the optimal planning of a sustainable regional infrastructure for hydrogen fuel supply chain network under uncertain demand. The planning includes sizing and location of nodes from production to delivery of hydrogen as a fuel within the supply chain. The problem of planning also includes accurate estimation of demand for hydrogen-fueled vehicles and fuel consumption. The transition from the current energy infrastructure to one where hydrogen plays a major role as an energy carrier has stimulated public and private interest in hydrogen economy [3]. The hydrogen economy comprises the production of molecular hydrogen (H2) using coal, natural gas, nuclear energy, or renewable energy such as biomass, MSW, wind, solar; the delivery and storage of hydrogen in some fashion; and the end use of hydrogen in fuel cells. Building hydrogen infrastructure (production plants, storage facilities and delivery modes) is expensive and needs significant investment with substantial risks [26]. Presently, the attention from industry and academia are on alternative fuel production processes and power train technologies. The infrastructure planning is under investigation only sporadically and on limited basis.

Here, we create a multi-period optimization model taking into account the stochasticity and the effect of uncertainty in the hydrogen production, storage and usage. The objective function includes minimization of the total daily social cost of the supply chain network with uncertain demand. This model formulates the infrastructure problem as a network flow problem with different types of nodes and flow types. The dynamics of the network are partially defined by the demand at some of these nodes. There are two network extents employed as part of this study. The first is a macro view which encompasses components at a large scale. Here, the demand is defined on regional basis and the objective is to decide on the major infrastructure elements. The second is a micro view which focuses in at various regions and considers the demand and supply with finer granularity.

The underlying model for the two network extents is stochastic and uses a two-stage programming approach for optimization. Uncertainty in demand is assumed for each region – this can be estimated using an energy economy model, statistical data, and survey results. There are several factors and key attributes, which influence a consumer's choice to buy a fuel cell vehicle. At the same time, consumer preference on the demand side is the most important factor in predicting changes in the auto market. We develop a spatially aggregated demand model to estimate the potential demand for fuel cell vehicles based on different household attributes such as income and education. Vehicle demand at the aggregate level usually focuses on household income, land use, and household demographic characteristics. The results of this work can be used towards the development of an advanced decision support system that can assist in multi-period planning for hydrogen refueling infrastructure.

Many researchers used different optimization techniques such as linear programming, stochastic programming, dynamic programming and multi-objective programming to design and model the hydrogen supply chain infrastructure [26]. Almansoori and Shah [27] introduced a deterministic mathematical model with an objective function on the basis of a hydrogen supply chain which included facility capital cost, transportation capital cost, facility operating cost and transportation operating cost. Later, Almansoori and Shah [28, 29] expanded their work to take into account the uncertainty arising from long-term variation in hydrogen demand using a scenario-based approach in Great Britain. Their results showed the future hydrogen supply chain network was somewhat similar to the existing petroleum infrastructure in terms of production, distribution and storage. Kim et al. [30] developed a steady-state mixed integer linear programming (MILP) model for hydrogen infrastructure under demand uncertainty in the Republic of Korea. This work was the first stochastic approach for hydrogen infrastructure optimization. They used similar cost elements as Almansoori and Shah [27]. Kim and Moon [31] developed a multi-objective optimization model to minimize the cost of the hydrogen supply chain network and to maximize the network safety. The safety objective was treated in terms of a risk index calculated on the basis of region's population risk. Not many studies addressed risk based optimization of the hydrogen supply chain [26].

Guillen-Gosalbez et al. [32] developed a deterministic and multi-period MILP framework model for a hydrogen supply chain network optimization that considered cost and environmental impacts. The environmental impact was measured by the contribution to climate change through emissions due by hydrogen supply chain network operation. Sabio [33] developed a multi-scenario MILP optimization model to allow for the control of variations in the economic performance of the hydrogen infrastructure in Spain. Konda et al. [34] developed a multi-period optimization framework based on a techno-economic analysis in the Netherlands. Their results showed transitioning toward a large-scale hydrogen based transport system is economically feasible for any given demand scenario.

The earliest studies of aggregate vehicle demand evaluated the role of income, price, vehicle stocks, and financial markets on per capita car ownership in the United States (Dyckman [35]). Mokhtarian and Cao [36] presented a thorough review of these and related works. Virtually all studies employed some measure of aggregate economic activity. Studies which used incomes include Dyckman [35], Tanner [37], Train [38], Manski [39], Dargay and Gately [40], Chung and Lee [41]. The works by Hicks [42] and Melendez and Milbrandt [43] focused on alternative fuel vehicles. Melendez and Milbrandt [43] developed a model which geographically optimized locations for hydrogen refueling stations. With the exception of Chung and Lee [41], each of these authors found a positive relationship between household income and automobile ownership (measured in many different ways). Other important variables included automobile stocks [35, 39], average automobile price [35, 39], and driving time, trips or distance [38, 41]. A variety of variables were found and classified at the aggregate level through these studies. These classes were: income-related (income or discretionary income, income index, gross national product, per-capita income, and household income); cost-related (price, cost index of motoring, transportation consumer price index, and personal transportation expenditure); land use-related (urbanized area and population density or percentage of population in an urbanized area); demographic characteristics (number of workers, household size, percentage of population within a specific age range, and economically active population); and miscellaneous variables (automobile stocks, annual transit trips per capita in the area).

3.2. Problem Description

In this chapter we address the problems of sizing and locating a sustainable hydrogen supply chain network under uncertain demand, and of detecting the important factors that play major roles in designing an optimal network design. The hydrogen supply chain (HSC) consists of hydrogen production plants, storage facilities, and delivery modes. Each node in the network has its own costs, which are categorized by economy, ecology, energy, and risk. The capital cost and operating cost for each node are in the *economy cost* category. The emission cost for each node is in the *ecology cost* category, and energy consumption cost for each node is in the *energy cost* category. Each node has associated GHG emission costs. In the case of hydrogen, which is, produced from a zero emission power source such as solar, produces zero emissions. However, it still has emissions in the production and delivery nodes (e.g. delivered by tanker truck).

In addition to the mentioned problems, other questions are how safe is hydrogen as a fuel and how can a safe and feasible infrastructure be developed. Hydrogen has a long history of safe use in the chemical, manufacturing, and utility industries, which are operated predominantly by highly trained people. However, as a large-scale energy carrier in the hands of the general public, where untrained people will deal with hydrogen, safety issues might develop unique to energy projects. For example, the technical installations used in production, storage and delivery could fail. Therefore, it is reasonable to determine at an early stage the safety technological conditions and the associated operating procedures required for hydrogen infrastructure [44]. In this application a risk cost is assumed for each network node which uses a quantitative risk assessment (QRA) method to calculate and evaluate risk quantitatively. QRA is a systematic methodology for the identification and quantification of a facility's risk contributors. A QRA can provide authorities and stakeholders with a sound basis for creating awareness about existing and potential hazards and risks [44, 45]. Based on the findings from the QRA, potential measures to control and/or reduce the risk can be suggested, and the effect of potential measures evaluated.

The model we develop will be used to establish and investigate a number of strategic decisions required to fulfill the customers' needs. These decisions include: the number, location, type and capacity of hydrogen production plants and storage facilities;

delivery modes and the total production rate of hydrogen in each region; the determination of the total average inventory in each region; and the size and type of delivery flow with uncertain demand over a long time horizon. Taking these decisions into account, the model also minimizes the total social costs of the hydrogen supply chain network. The network described by the model is demand-driven, which means the establishment of production plants, storage facilities and transportation links depend mainly on the demand structure. This is a stochastic, multi-period model, formulated as a mixed integer linear programming solution with two stages. This work also includes spatially aggregated demand modeling to estimate the potential demand for those who are interested in purchasing fuel cell vehicles, and eventually consuming hydrogen as a fuel based on different household attributes.

3.3. Problem Formulation

3.3.1. Mathematical Model

The objective function in this model is the Total Social Cost (TSC) of a multi-period HSC network under uncertain daily demand. TSC consists of 15 separate costs: production capital cost (PCC); storage capital cost (SCC); delivery capital cost (DCC); production operating cost (POC); storage operating cost (SOC); delivery operating cost (DOC); production emission cost (PEC); storage emission cost (SEC);, delivery emission cost (DEC); production energy consumption cost (PECC); storage energy consumption cost (SECC); delivery energy consumption cost (DECC); production risk cost (PRC); storage risk cost (SRC); and delivery risk cost (DRC). In this formulation, the production (all cost categories) and storage capital cost variables are considered in the first stage, while the storage operating, emission, energy consumption and risk cost, and delivery decisions variables are included in the second stage of the model. In this treatment, the first stage calculates the costs incurred in production and storage nodes. The second term quantifies the costs of the delivery decisions and is obtained by applying the expectation variable called Q to an embedded optimization problem. The role of Q is to average over the second stage cost occurred in given demand scenarios.

The two-stage stochastic linear programming problem can be stated as [46-49]:

$$\text{minimize } C^{T}x + E_{w}Q(x, w) \tag{3.1}$$

$$Ax=b$$

$$x \geq 0$$

where,

$$Q(x, \omega) = \min\ d_{\omega}^{T} y$$

$$T_{\omega x} + W_{\omega} y = h_{\omega}$$

$$y \geq 0$$

E_{ω} is the expectation and *w* denotes a scenario with respect to the probability space (Ω, *P*). Vector *x* includes first-stage variables – these have to be decided before the outcome of the stochastic variable ω is observed. The variables within vector *y* are second-stage variables: they can be calculated after the outcome of ω is known.

We will consider discrete distributions *P* only, so we can write:

$$E_{\omega} Q(x, \omega) = \sum_{\omega \in \Omega} p(\omega) Q(x, \omega) \tag{3.2}$$

Using this we can formulate a large Linear Programming that forms the deterministic equivalent problem:

$$\text{Minimize } C^{T} x + \sum_{\omega} p(\omega)\, d_{\omega}^{T} y \tag{3.3}$$

$$Ax=b$$

$$T_{\omega}\, x + W_{\omega}\, y_{\omega} = h_{\omega} \quad \forall\, \omega$$

$$x \geq 0\,, y_{\omega} \geq 0$$

To solve this model, a scenario-based approach was applied with P_j as the probability of each scenario. For the model formulation we borrow some ideas from Almansoori, Shah [27-29] and Kim et al. [30], and Lin [50], especially for the economy categories such as capital cost and operation cost for each node. The remaining equations related to ecology, energy and risk cost categories were derived by us through researching the literature and data, and by understanding the problem. In addition, Kim et al. [30] developed a steady-state mixed integer programming (MILP) model for hydrogen infrastructure under demand uncertainty in Republic of Korea; however, they didn't consider the time dependence. Also, the scenarios were limited to three levels and they considered only the economy cost category. Our model is capable of running many scenarios with different probabilities which can be defined by the user.

The multi-period two-stage stochastic model under demand uncertainty is:

$$\text{Min TSC}=\frac{1}{NT}\left(\frac{1}{\alpha CCF}(\text{PCC+SCC}) + \text{POC+PEC+PECC+PRC}+ \text{Q}\right) \tag{3.4}$$

Q=E

$$\frac{\sum_j P_j\, DCC_j}{\alpha CCF} + \sum_j P_j\, SOC_j + \sum_j P_j\, SRC_j + \sum_j P_j\, DOC_j + \sum_j P_j\, SEC_j + \sum_j P_j\, \text{SECC}_j + \sum_j P_j\, \text{DEC}_j + \sum_j P_j\, \text{DECC}_j + \sum_j P_j\, \text{DRC}_j$$

Subject to:

$$P_{irt}=\sum_d \sum_{r'}(Q_{idrr'tj} - Q_{idr'rjt}) + D_{irtj} \qquad \forall\, i,r,t$$

$$P_{irt}=\sum_P P_{Pirt} \qquad \forall\, i,r,t$$

$$S_{irtj}=\beta\, D_{irtj} \qquad \forall\, i,r,t,j$$

$$X_{idrr'tj} + X_{idr'rtj} \le 1 \qquad \forall\, i,d,r,r',t,j \;\; ; r \ne r'$$

$$Y_{irtj} \ge X_{idrr'tj} \qquad \forall\, i,d,r,r',t,j \;\; ; r \ne r'$$

$$Z_{irtj} \ge X_{idr'rtj} \qquad \forall\, i,d,r,r',t,j \;\; ; r \ne r'$$

$$Y_{irtj}+Z_{irtj} \le 1 \qquad \forall\, i,r,t,j$$

$$Q_{id}^{min}\, X_{idrr'tj} \le Q_{idrr'tj} \le Q_{id}^{max}\, X_{idrr'tj} \qquad \forall\, i,d,t,r,r',t,j \;\; ; r \ne r'$$

$$SOC_j=\sum_i \sum_r \sum_s \sum_t USC_{si} * S_{irtj} \qquad \forall\, j$$

$$DCC_j=NTU_j * TMC_{id} \qquad \forall\, j$$

$$DOC_j=LC_j + MC_j + GC_j \qquad \forall\, j$$

$$SEC_j=\sum_i \sum_r \sum_s \sum_t S_{irtj} * (EMS_{si} + EMSE_{si} * ConvC_{si}) * ETax \qquad \forall\, j$$

$$\text{DEC}_j=\sum_{i,d,r,r',t}(L_{drr'} * Q_{idrr'tj} * DsUse_{id} * ConvC_d) * ETax \qquad \forall\, j$$

$$SECC_j=\sum_i \sum_r \sum_s \sum_t S_{irtj} * EMSE_{si} * EC \qquad \forall\, j$$

$$SRC_j=\sum_i \sum_r \sum_s \sum_t \text{SR}_{si} * NS_{sirtj} * RC_{si} \qquad \forall\, j$$

$$DECC_j=\sum_{i,d,r,r',t}(L_{drr'} * Q_{idrr'tj} * DsUse_{id} * \text{Dscost}) \qquad \forall\, j$$

$$NTU_j= \sum_{i,d,r,r',t} \frac{Q_{idrr'tj}}{TMA_d * Tcap_{id}}\left(\frac{2L_{drr'}}{SP_d} + LUT_d\right) \qquad \forall\, j$$

$$LC_j = \sum_{i,d,r,r',t} DW_d (\frac{Q_{idrr'tj}}{Tcap_{id}}(\frac{2L_{drr'}}{SP_d} + LUT_d)) \quad \forall j$$

$$MC_j = \sum_{i,d,r,r',t} ME_d (\frac{2L_{drr'} * Q_{idrr'tj}}{Tcap_{id}}) \quad \forall j$$

$$GC_j = \sum_{i,d,r,r',t} GE_d (\frac{Q_{idrr'tj}}{TMA_d * Tcap_{id}}(\frac{2L_{drr'}}{SP_d} + LUT_d)) \quad \forall j$$

$$\sum_p PCap_{pi}^{min} * NP_{pirt} \leq \sum_P P_{Pirt} \leq \sum_p PCap_{pi}^{max} * NP_{pirt} \quad \forall i, r, t$$

$$\sum_s SCap_{si}^{min} * NS_{sirtj} \leq S_{irtj} \leq \sum_s SCap_{si}^{max} * NS_{sirtj} \quad \forall i, r, t, j$$

$$DRC_j = \sum_t NTU_{tj} * NF_{tj} * HC \quad \forall j$$

Subject To:

$$PCC = \sum_i \sum_r \sum_p \sum_t PCC_{pi} * NP_{pirt}$$

$$SCC = \sum_i \sum_r \sum_s \sum_t \sum_j SCC_{si} * NS_{sirtj}$$

$$POC = \sum_i \sum_r \sum_p \sum_t UPC_{pi} * P_{pirt}$$

$$PEC = \sum_i \sum_r \sum_p \sum_t P_{pirt} * (EMP_{pi} + EMPE_{pi} * ConvC_{pi}) * ETax$$

$$PECC = \sum_i \sum_r \sum_p \sum_t P_{pirt} * EMPE_{pi} * EC$$

$$PRC = \sum_i \sum_r \sum_p \sum_t PR_{pi} * NP_{pirt} * RC_{pi}$$

<u>Notations</u>

Indices

i	Hydrogen type
r	region
r'	region such that r $= r'$
p	plant type with different production technologies
s	storage facility type with different storage technologies
d	transportation mode
t	time periods

Parameters

CCF	Capital charge factor – payback period of capital investment, year

D_{irtj}	Total demand required by region r itself during time period t in scenario j, kg/day
P_j	Probability of scenario j occurrence
$PCap_{pi}^{min}$	Minimum production capacity of type p for hydrogen type i, kg/day
$PCap_{pi}^{max}$	Maximum production capacity of type p for hydrogen type i, kg/day
Q_{id}^{min}	Minimum flow rate of hydrogen type i by transportation mode d, kg/day
Q_{id}^{max}	Maximum flow rate of hydrogen type i by transportation mode d, kg/day
PCC_{pi}	Capital cost of plant type p producing hydrogen type i, $
$SCap_{si}^{min}$	Minimum storage capacity of storage type s for hydrogen type i, kg
$SCap_{si}^{max}$	Maximum storage capacity of storage type s for hydrogen type i, kg
SCC_{si}	Capital cost of establishing storage type s for storing hydrogen type i, $
TMC_{id}	Cost of establishing transportation mode d of hydrogen type i, $
$L_{drr'}$	Delivery distance between regions, by transportation mode d, km/trip
UPC_{pi}	Unit production cost for hydrogen type i by plant type p, $/km
USC_{si}	Unit storage cost for hydrogen type i at storage type s, $/kg day
DW_d	Driver wage of transportation mode d, $ per hour
FE_d	Fuel economy of transportation mode d, km / litter
FP_d	Fuel price of transportation mode d, $ per litter
GE_d	General Expenses of transportation mode d, $ day
LUT_d	Load/unload time of hydrogen for transportation mode d, hour per trip
ME_d	Maintenance expenses of transportation mode d, $ /km
SP_d	Average speed of transportation mode d, km /hour
$TCap_{id}$	Capacity of transportation mode d transporting hydrogen type i, kg /trip
TMA_d	Availability of transportation mode d, hour per day
$ConvC_{pi}$	Carbon emission rate of production type p for hydrogen type i, kgC/ 1 kg hydrogen
$EMPE_{pi}$	Flow rate of electricity in plant type p for hydrogen type i, kWh/kg hydrogen
$ConvC_{si}$	Carbon emission rate of storage type s for hydrogen type i, KgC/1 kg hydrogen
$ETax$	Carbon tax rate, $/Kg C
EMS_{si}	Emission rate for storage type s for hydrogen type i, kg/ 1 kg hydrogen
$EMSE_{si}$	Flow rate of electricity in storage type s for hydrogen type i (kWh/kg Hydrogen)
$DsUse_{it}$	Diesel consumption for hydrogen type i with transport mode d gallon/ (mile.kg hydrogen)
$ConvC_d$	Carbon emission rate for diesel, kgC/gallon
EC	Electricity cost $/kWh
$Dscost$	Diesel cost $/gallon

NT	Number of time periods
PR_{pi}	Relative risk of plant p for hydrogen type i, per year
RC_{pi}	Cost associated to the risk for plant p for hydrogen type i, $ per person
SR_{si}	Relative risk of storage s for hydrogen type i, per year
RC_{si}	Cost associated to the risk for storage s for hydrogen type i , $ per person
NF_{dj}	Number of causalities in fatal crashes which hydrogen delivery mode was involved number of causalities in fatal crashes which hydrogen delivery mode was involved (hydrogen release)
HC	Human Cost, $ per person

Continuous Variables

TSC	Total Social Cost, $/day
PCC	Production Capital Cost, $
POC	Production operation cost, $/day
PCEC	Production carbon emission cost, $/day
PECC	Production energy consumption cost, $/day
PRC	Production risk cost, $/day
SCC	Storage Capital Cost, $
SOC	Storage operation cost, $/day
SEC	Storage emission cost, $/day
SECC	Storage energy consumption cost, $/day
SRC	Storage risk cost, $/day
DCC	Delivery Capital Cost, $
DOC	Delivery operation cost, $/day
DEC	Delivery emission cost, $/day
DECC	Delivery energy consumption cost, $/day
DSRC	Delivery risk cost, $/day
P_{pirt}	Production rate of hydrogen type i by plant type p in region r during time period t, kg/day
P_{irt}	Total Production rate of hydrogen type i in region r during time period t, kg/day
$Q_{idrr'tj}$	Flow rate of hydrogen type i by transportation mode d entering region r during time period t from region r to r' in scenario j, kg/day
$Q_{idr'rtj}$	Flow rate of hydrogen type i by transportation mode d entering region r during time period t from regions r' to r in scenario j, kg/day
S_{sir}	Average inventory of hydrogen type I by storage facility s in region r, kg
S_{ir}	Total average inventory of hydrogen type i in region r, kg
GC	General cost, $/day

LC	Labor cost, $/day
MC	Maintenance cost, $/day

Integer variables

NP_{pirt}	Number of plants of type p hydrogen type i in region r during time period t
NS_{sirtj}	Number of storage facilities of type s for hydrogen type i in region r during time period t in scenario j
NTU_{tj}	Number of transport units during time period t for each scenario j

Binary Variables

$X_{idrr'tj}$	1 if hydrogen type i is to be transported from regions r to r' by transport at mode d during time period t in scenario j, 0 otherwise
$X_{itr'rtj}$	1 if hydrogen type i is to be transported from regions r' to r by transportation mode d during time period t in scenario j, 0 otherwise
Y_{irtj}	1 if hydrogen type i is to be exported from region r during time period t in scenario j, 0 otherwise
Z_{irtj}	1 if hydrogen type i is to be imported into region r during time period t in scenario j, 0 otherwise

Greek Letters

α	Network operating period, day/year
β	Storage holding period _ average number of worth of stock, day

3.3.2. Constraints

3.3.2.1. Production node constraints

The mass balance must be satisfied in each node embedded in the supply chain. Assuming a multi-period operation during each scenario *j*, the sum of the total flow rate of hydrogen type *i* (such as liquid hydrogen) which transported by mode *d* entering region *r* during time period *t* ($Q_{idr'rjt}$) plus the total production rate of the same region during time period *t* (P_{irt}), must equal the total outflow rate leaving that region ($Q_{idrr'tj}$) plus the total demand required by region *r* itself during time period *t* in scenario *j* (D_{irtj}) .

$$P_{irt} = \sum_d \sum_{r'} (Q_{idrr'tj} - Q_{idr'rjt}) + D_{irtj} \qquad \forall\, i, r, t \tag{3.5}$$

The total production rate of a hydrogen type *i* in region *r* during time period *t* is equal to the production rate of all plants of type *p* established in that same region:

$$P_{irt} = \sum_P P_{Pirt} \qquad \forall\, i, r, t \tag{3.6}$$

The production rate of hydrogen type *i* produced by any plant of type *p* in region *r* during time period t (P_{Pirt}) cannot exceed its capacity. Thus, there is always a maximum production capacity for any hydrogen type ($PCap_{pi}^{max}$). Moreover, there is often a minimum production rate ($PCap_{pi}^{min}$) that must be maintained while the plant is operating:

$$\sum_p PCap_{pi}^{min} * NP_{pirt} \leq \sum_P P_{Pirt} \leq \sum_{\mathrm{p}} PCap_{pi}^{max} * NP_{pirt} \qquad \forall\, i, r, t \tag{3.7}$$

Note that NP_{pir} (number of plants type p for hydrogen type i in region *r* during time period) and P_{irt} and P_{Pirt} are first-stage variables, so this value will not change by applying the scenarios. The production capital cost (PCC) is equal to sum of multiplication of capital cost of plant type *p* producing hydrogen type *i* ($\mathrm{PCC_{pi}}$) by the number of plants (NP_{pirt}) .

$$\mathrm{PCC} = \sum_i \sum_r \sum_p \sum_t \mathrm{PCC_{pi}} * NP_{pirt} \qquad \forall\, i, r, t \tag{3.8}$$

The production operation cost is equal to production rate of a hydrogen type *i* produced by any plant of type *p* in region *r* during time period *t* (P_{Pirt}) multiplied to the unit production cost for hydrogen type *i* by plant type *p*:

$$\mathrm{POC} = \sum_i \sum_r \sum_p \sum_t \mathrm{UPC_{pi}} * P_{pirt} \tag{3.9}$$

The production carbon emission cost is equal to equation below:

$$\mathrm{PEC} = \sum_i \sum_r \sum_p \sum_t P_{pirt} * ConvC_{pi} * ETax \tag{3.10}$$

Note that $ConvC_{pi}$ is the carbon emission rate of production type *p* for hydrogen type *i* per 1 kg of hydrogen (kgC/kg hydrogen) and, in order to convert this equation to cost, we need to have a factor such as carbon tax (ETax). Note the tax rate can change based on region.

The Equation below calculates the production energy consumption cost. Note all costs are per day, and $EMPE_{pi}$ is the flow rate of electricity in plant type p for hydrogen type i (kWh/kg hydrogen) and EC is electricity cost per kWh.

$$\text{PECC}=\sum_i \sum_r \sum_p \sum_t P_{\ pirt} * EMPE_{pi} * EC \tag{3.11}$$

The production risk cost can be calculated from equation below:

$$\text{PRC}=\sum_i \sum_r \sum_p \sum_t PR_{\ pi} * NP_{\ pirt} * RC_{pi} \tag{3.12}$$

Where $PR_{\ pi}$ is the relative risk of plant *p* for hydrogen type *i* and RC_{pi} is the cost associated to the risk for plant *p* for hydrogen type *i*.

3.3.2.2. Storage facilities constraint

An important issue in the operation of the above network is the ability of the storage facilities to hold the hydrogen for a certain period of time in order to accommodate any fluctuations in demand and supply. Therefore, storage facilities can be built either locally in a specific region next to the production facility—if established—or outside the region boundary away from the production source [27].

During steady-state operation, the total inventory rates of a hydrogen type *i* in region *r* during time period *t* in scenario *j* (S_{irtj}) is equal to a function of the corresponding demand D_{irtj} multiplied by the storage period (β) days of cover:

$$S_{irtj}=\beta\, D_{irtj} \qquad \forall\, i,r,t,j \tag{3.13}$$

The capacity of each storage facility type *s* storing hydrogen type *i* ($SCap_{si}$) cannot exceed its capacity. This consideration will guarantee that the total inventory of each product in each region will be bound within certain limits:

$$\sum_s SCap_{si}^{min} * NS_{sirtj} \le S_{irtj} \le \sum_s SCap_{si}^{max} * NS_{sirtj} \qquad \forall\, i,r,t,j \tag{3.14}$$

This constraint also implies the total inventory of hydrogen type *i* stored in a grid g is constrained by the number of storage facilities NS_{sirtj}. Note, NS_{sirtj} is a first-stage variable so it will not change over different scenarios. The storage capital cost (SCC) is equal to the sum of multiplication of the capital cost of establishing storage type *s* for storing hydrogen type (SCC_{si}) by the number of storage facilities:

$$\mathrm{SCC}=\sum_i \sum_r \sum_s \sum_t \sum_j \mathrm{SCC}_{\mathrm{si}} * NS_{sirtj} \tag{3.15}$$

The storage operation cost is equal to the inventory rates of hydrogen type *i* in region *r* during time period *t* in scenario *j* (S_{irtj}) multiplied by the unit storage cost for fuel type *i* at storage type *s* (USC_{si}):

$$SOC_j = \sum_i \sum_r \sum_s \sum_t USC_{si} * S_{irtj} \qquad \forall j \tag{3.16}$$

The storage carbon emission cost for scenario j is equal to equation below:

$$SEC_j = \sum_i \sum_r \sum_s \sum_t S_{irtj} * ConvC_{si} * ETax \qquad \forall j \tag{3.17}$$

Note, the term $ConvC_{si}$ is the carbon emission rate of storage type *s* for hydrogen type *i* per 1 kg hydrogen (kgC/kg hydrogen). In order to convert this equation to cost we need to have a factor such as a carbon tax (ETax). The tax rate can change based on the region. The equation below calculates the storage energy consumption cost for scenario *j*. All costs are in units of per day, and $EMSE_{si}$ is the flow rates of electricity in storage type *s* for hydrogen type *i* (kWh/kg hydrogen). EC is electricity cost per kWh.

$$SECC_j = \sum_i \sum_r \sum_s \sum_t S_{irtj} * EMSE_{si} * EC \qquad \forall j \tag{3.18}$$

The storage risk cost is calculated from the following equation:

$$SRC_j = \sum_i \sum_r \sum_s \sum_t \mathrm{SR}_{\mathrm{si}} * NS_{sirtj} * RC_{si} \qquad \forall j \tag{3.19}$$

Where $SR_{\ pi}$ is the relative risk of storage facility type *s* for hydrogen type *i* and RC_{si} is the cost associated with the risk for storage type s for hydrogen type i.

3.3.2.3. Delivery constraints

There must be a continuous flow of hydrogen between different regions in order to satisfy the required demand. The flow of a hydrogen type i from region r to a different region r' in each scenario will exist only if the transportation mode is established. Thus, there always are a minimum and a maximum flow rate of hydrogen (Q_{id}^{min} and Q_{id}^{max}) needed to justify the establishment of a transportation mode between two regions in the network for each scenario:

$$Q_{id}^{min}\, X_{idrr'tj} \leq Q_{idrr'tj} \leq Q_{id}^{max}\, X_{idrr'tj} \qquad \forall\, i,d,t,r,r',t,j\ \ ; r \neq r' \tag{3.20}$$

A region only can import a hydrogen type from other regions or export a hydrogen type to other regions:

$$X_{idrr'tj} + X_{idr'rtj} \leq 1 \qquad \forall\, i,d,r,r',t,j\ \ ; r \neq r' \tag{3.21}$$

A particular region only can import hydrogen from neighboring regions or *export* hydrogen, but not both. This constraint follows from the reason that if a region can only satisfy its needs by importing from other regions, it could not export to other regions:

$$Y_{irtj} \geq X_{idrr'tj} \qquad \forall\, i,d,r,r',t,j\ \ ; r \neq r' \tag{3.22}$$

$$Z_{irtj} \geq X_{idr'rtj} \qquad \forall\, i,d,r,r',t,j\ \ ; r \neq r' \tag{3.23}$$

$$Y_{irtj} + Z_{irtj} \leq 1 \qquad \forall\, i,r,t,j \tag{3.24}$$

The capital cost of different types of delivery modes takes into account the number of the delivery units, *i.e.*, tanker trucks or tube trailers, required to satisfy the demand and the cost of each unit. The number of transport units during time period *t* for each scenario (NTU_{tj}) depends fundamentally on the average distance travelled between different regions ($L_{\ drr'}$). Long delivery distances mean more trucks or tube trailers are required to deliver a given quantity of hydrogen, which can result in a higher delivery capital cost, operating cost, emission cost, or energy cost. The capacity of a transport container ($TCap_{id}$) also is an important factor, especially for long distances, since it determines the number of trips that must be made between the production plant and the storage facility. It is clear that large transport containers will reduce the cost of transportation as fewer tanker trucks or tube trailers are required. In addition, the flow rate of hydrogen between regions ($Q_{idrr'tj}$) and the delivery mode availability (TMA_d), average speed (SP_d), and loading/unloading time (LUT_d) are other main factors that affect the capital cost of transporting hydrogen. On the other hand, the cost of the transport unit (TMC_{id}) includes the cost of the transport container, the cost of the undercarriage and the cost of the cab. The number of tanker trucks and/or tube trailers required to satisfy a certain flow between different regions are given by the following relationship:

$$NTU_{tj} = \sum_{i,d,r,r'} \frac{Q_{idrr'tj}}{TMA_d * Tcap_{id}} (\frac{2L_{drr'}}{SP_d} + LUT_d) \qquad \forall\ t, j \tag{3.25}$$

It can be noted from equation above that $L_{drr'}$ is multiplied by two for a roundtrip.

Therefore, the delivery capital cost for each scenario is given by the following equation:

$$DCC_j = \sum_{i,d,t} NTU_{tj} * TMC_{id} \qquad \forall\ j \tag{3.26}$$

The daily labor cost associated with transporting the hydrogen between different regions is given as a function of the total delivery time and driver wage for each scenario:

$$LC_j = \sum_{i,d,r,r',t} DW_d (\frac{Q_{idrr'tj}}{Tcap_{id}} (\frac{2L_{drr'}}{SP_d} + LUT_d)) \qquad \forall\ j \tag{3.27}$$

Again, the first and second terms in the above equation represent the driver wage and the total delivery time, respectively. The maintenance cost includes general maintenance of the transportation systems. It is a function of the total daily distance driven and the cost per unit distance travelled for each scenario:

$$MC_j = \sum_{i,d,r,r',t} ME_d\left(\frac{2L_{drr'} * Q_{idrr'tj}}{Tcap_{id}}\right) \qquad \forall\, j \qquad (3.28)$$

The last operating cost is the general cost. It consists of transportation insurance, license and registration, and outstanding finances. It depends on the number of transport units and the corresponding expenses for each scenario:

$$GC_j = \sum_{i,d,r,r',t} GE_d\left(\frac{Q_{idrr'tj}}{TMA_d * Tcap_{id}}\left(\frac{2L_{drr'}}{SP_d} + LUT_d\right)\right) \qquad \forall\, j \qquad (3.29)$$

Finally, the total transportation operating cost for each scenario is equal to the sum of labor, maintenance and general costs:

$$DOC_j = LC_j + MC_j + GC_j \qquad \forall\, j \qquad (3.30)$$

The delivery carbon emission cost for scenario j is equal to equation below:

$$DEC_j = \sum_{i,d,r,r',t}(L_{drr'} * Q_{idrr'tj} * DsUse_{id} * ConvC_d) * ETax \qquad \forall\, j \qquad (3.31)$$

Note the $DsUse_{id}$ is the diesel consumption rate for hydrogen type *i* with transport mode *d* per mile.kg hydrogen. $ConvC_d$ is the carbon emission rate for diesel fuel consumed during transport, and its units are kgC/gallon. In order to convert this equation to cost, we need to a factor such as carbon tax (ETax) [50]. The equation below calculates the delivery energy consumption cost for scenario *j*. Note all *costs* are *per day* and *Dscost* is the cost of diesel fuel.

$$DECC_j = \sum_{i,d,r,r',t}(L_{drr'} * Q_{idrr'tj} * DsUse_{id} * \text{Dscost}) \qquad \forall\, j \qquad (3.32)$$

The delivery risk cost can be calculated from equation below:

$$DRC_j = \sum_t NTU_{tj} * NF_{dj} * HC \qquad \forall\, j \qquad (3.33)$$

Where NF_{dj} is the number of causalities in fatal crashes for a hydrogen delivery mode (hydrogen release) and *HC* is the human cost. The required data for human costs can be obtained from questionnaires taken by accident victims and their friends and relatives. In the absence of information from surveys, insurance payments to victims or their families can be used as social willingness-to-pay. Section 3.3 and Appendix A describe these elements in more detail.

3.3.3. Determining the Relative Risk of Hydrogen Infrastructure Activities

Each node in the network is associated with a risk cost which can be calculated according to quantitative risk assessment (QRA) method. QRA is a systematic methodology for the identification and quantification of risk contributors. A QRA can provide authorities and stakeholders with a sound basis for creating awareness about existing and potential hazards and risks [44, 45]. Based on the findings from the QRA, potential measures to control and/or reduce the risk can be suggested, and the effect of the measures evaluated. The QRA methodology [45] applied is schematically illustrated in figure below:

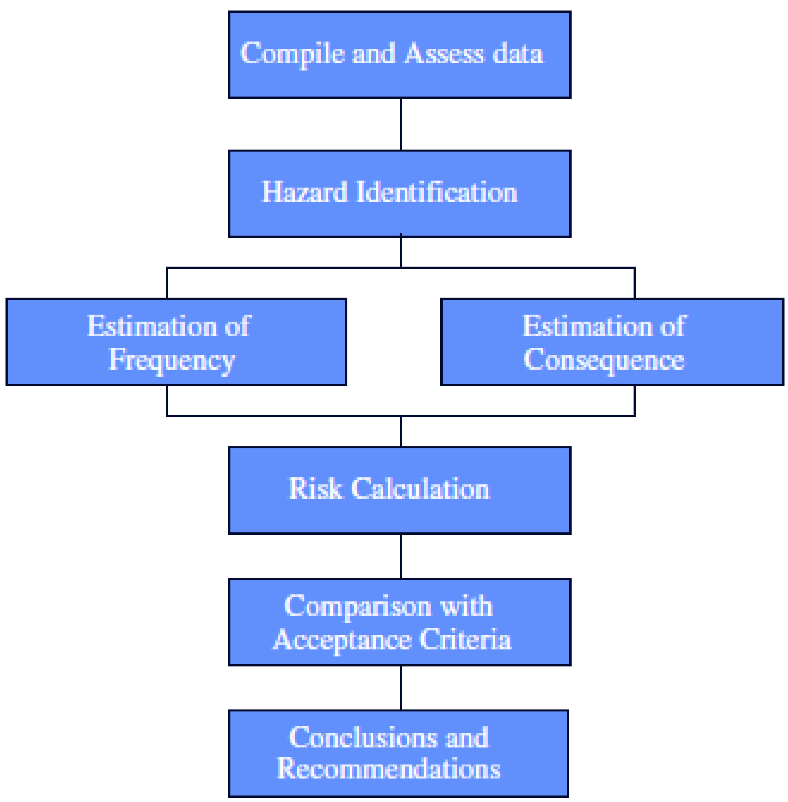


Figure 9. QRA process

In this study, Failure Modes Effect Analysis (FMEA) method was selected to identify potential hazards related to the hydrogen infrastructure. FMEA is a systematic and structured method for identifying product and process problems, assessing impacts and identifying potential solutions that can reduce them. FMEA computes all failure modes together with their causes and potential effects [44]. Fault tree analysis (FTA) [44] is an analytical tool that uses deductive reasoning to determine the occurrence of an undesired event (called “Top” Event). The FTA, along with component failure data and human reliability data, allows us to compute the frequency of occurrence (probability) of an accidental event. It yields both qualitative as well as quantitative information. In order to quantify the negative impacts of these accidents, we conduct consequence analysis. We calculate the number of fatalities in a given accident along with number of injuries and property damage or loss. Risk is then calculated by multiplying frequency and consequences.

As mentioned earlier, there are costs associated to risks in our model. With the lack of reliability data for components in hydrogen infrastructure, especially in the production and storage nodes, we compiled accident probability data from several safety papers [44, 45].

3.3.4. Spatially Aggregated Demand Model

In order to design a sustainable energy infrastructure for hydrogen, the demand for hydrogen must be estimated accurately. The main objective of the spatially aggregated demand model is to estimate the population (demand), which is interested in purchasing fuel cell vehicles. In order to estimate this population, the factors and key attributes which influence consumer choice are identified. Our approach uses some basic results developed by Melendez and Milbrandt [43], which geographically optimizes locations for hydrogen refueling stations. In our proposed model, consumers are households and not individuals because every household may have more than one vehicle. The main steps in this model are:

Step 1: Identify the key attributes affecting consumer acceptance of fuel cell vehicles

Key attributes affecting fuel cell vehicle penetration into the consumer market are listed below. This is not an exhaustive list, and there are additional variables that can influence consumer decisions.

1. **Household Income**: Based on literature review, initial customers for fuel cell vehicles will be those with higher income levels.
2. **Households with two or more vehicles:** Initial customers for fuel cell vehicles will be those households that have two or more vehicles because of limited hydrogen range and refueling opportunities.
3. **Education:** Based on literature review, initial customers for hydrogen vehicles will be those with higher education levels.
4. **Commute Distance:** More time spent in a vehicle commuting may make consumers more interested in newer and more efficient vehicles especially fuel cell vehicles.

The data to support the analysis for these attributes can be collected from U.S. Census Bureau [52].

Step 2: Classify and score and normalize attributes

In this step the above household attributes (1-4) were classified based on different groups and scored by each group. For instance *household income* was classified into different number of groups (based on U.S dollar income) and each scored based on their importance level on the purchase of fuel cell vehicles. The education category can be classified based on the number of people with a bachelor's degree or higher; the same applies to the other two attributes. Also, scores were normalized so the group scores for each attribute were equal to 100%.

Step 3: Weight each attribute based on its impact level

In this step each attribute can be weighted based on the level of impact on consumers (based on assumption):

- Household Income (W1)
- Households with two or more vehicles (W2)
- Education (W3)
- Commute Distance (W4)

Step 4: Calculate hydrogen demand based on weights and scores

In this step the hydrogen demand can be calculated based on the weights and scores, which were computed in the previous steps.

$$HD = MPR \times HC \times PGR \times \sum \Big(Attribute\ Weights \times \sum (Scoring\ Weights \times Number\ of\ People\ in\ each\ group) \Big) \tag{3.34}$$

The above equation shows the *Hydrogen Demand* (*HD*) for a given year based on the *MPR*. *MPR* is the market penetration. *HC* is the vehicle hydrogen consumption rate, which can be assumed to be 0.6 kg H_2/day·vehicle. This estimate is based on the assumption that the average vehicle travels 15,000 miles/year and has a fuel economy of 65 miles/kg (roughly equivalent to a gasoline fuel economy of 65 miles per gallon). *PGR* is the population growth rate. Note the energy in 2.2 pounds (1 kilogram) of hydrogen gas is about the same as the energy present in 1 gallon of gasoline.

3.4. Case Study - Hydrogen Infrastructure for New Jersey

Hydrogen and fuel cell projects are becoming increasingly popular throughout the Northeastern U.S. Natural gas is one of the main sources of hydrogen and it is widely available throughout the region, is relatively inexpensive, and is primarily a domestic energy supply. These technologies are viable solutions that can meet the demand for renewable energy in New Jersey. In addition, the deployment of hydrogen and fuel cell technology would reduce the dependence on oil, improve environmental performance, and increase the number of jobs within the state. As mentioned earlier the main objective of the proposed model is to minimize the total social cost (daily) for a hydrogen supply chain network over a long time horizon. Total social cost is the summation of economy, ecology, energy and risk costs for the total supply chain network. This case study model application takes the following input data: 1) production plant cost data for each technology in the four categories of economy, ecology, energy and risk, and the plant capacities: 2) storage cost and technology data, such as storage capacity and their type (liquid or gaseous); and 3) delivery and transportation mode (tanker truck or tube trailer) data, such as lead time and the transport capacity. The model output includes the number and locations of hydrogen production plants and storage facilities and the number of delivery modes.

For this case study two production plant types were chosen: *steam methane reforming* (SMR) plant and an *electrolysis* plant. The reasoning for these two production processes is that natural gas, electricity and water, which are the primary sources for these production plant types, are widely available in New Jersey. Most of the cost data were obtained from [27, 30, and 51]. The capital costs and the unit production costs of hydrogen production technologies and their capacities are shown below:

Table 9. Capital and unit production costs of hydrogen production technologies and their capacities

	Plant Type			
	Steam Methane Reforming		*Electrolysis*	
	Gaseous(GH2)	Liquid(LH2)	Gaseous(GH2)	Liquid(LH2)
Production Capacity (thousand kg/day)	480	480	50	50
Capital Cost (million $)	379	519	54	112
Unit Production Cost ($/kg)	0.94	1.53	3.25	4.18

Two storage types are chosen: *liquid hydrogen* (LH2) storage facility and compressed *gaseous hydrogen* (GH2) storage facility. Capital costs and unit storage cots of GH2 storage and LH2 storage and their capacities are shown in the table below. The storage facility holding period β is assumed to be 5 days.

Table 10. Capital costs and unit storage cots of GH2 storage and LH2 storage and their capacities

	GH2 storage facility	*LH2 storage facility*
Storage capacity (thousand kg/day)	80	540
Storage capital cost (million $)	155	122
Unit storage cost ($/kg day)	0.075	0.005

Two transportation modes were considered to transport hydrogen: *tube trailer* for compressed hydrogen and *tanker truck* for liquid hydrogen. Parameters used to estimate the costs of tube trailer and tanker truck containers are shown in Table 11. The capital charge factor (payback period of capital investment, year) for production plants and storage facilities are assumed to be 10 years and for delivery modes is 5 years. The network operating period is 365 days per year. The *Carbon Tax* rate is assumed to be $50 per ton C. The *Electricity Consumption* rate for *SMR* is 0.57 kWh/kg hydrogen and for *Electrolysis* is 53.48 kWh/kg hydrogen. The Carbon Emission rate for SMR is assumed to be 0.06 kgC/ gallon and 4.71 kgC/ gallon for Electrolysis [51, 53]. The Diesel Cost is assumed to be $4.027 per gallon.

Table 11. Parameters used to estimate the costs of hydrogen transport by tube trailer and tanker truck

	Transportation Mode	
Parameter	*Tube trailer*	*Tanker truck*
Capacity (kg/trip)	200	4000
Container cost($)	150,000	650,000
Undercarriage cost($)	60,000	60,000
Cab cost($)	90,000	90,000
Total cost($)	300000	800000
Fuel Economy (mile/gallon)	5.88	5.88
Average speed (mile/hour)	31.00	31.00
Mode availability (h/day)	24.00	24.00
Load/unload time (h/trip)	1.00	3.00
Driver wage ($/h)	28.75	28.75
Fuel price ($/gallon)	4.02	4.02
Maintenance expenses ($/mile)	0.16	0.16
General expenses ($/day)	8.22	8.22

In order to calculate the risk cost for each node, we used the results of the work [44, 45] to obtain the associated risk for each node which the authors evaluated using the quantitative risk assessment (QRA) method. As mentioned in section 3.3.3, QRA is a systematic methodology for the identification and quantification of risk contributors. Table 12 shows the risk associated for each node. The cost associated to the risk for production, storage and delivery assumed to be $ 3,536,568 per person.

Table 12. Risk occurrences associated for each node

	GH2	LH2
Production	2.3×10^{-4} /year	6.5×10^{-4} /year
Storage	4.1×10^{-4} /year	5.5×10^{-4} /year
Delivery	1.15×10^{-7} /year	3.7×10^{-4} /year

In order to estimate hydrogen demand in the future, we developed a spatially aggregated demand model (described in section 3.3.4.). The Demand estimation was created from the U.S. Census Bureau 2010 data [52]. Regions were based on New Jersey counties. The vehicle hydrogen consumption rate was 0.6 kg per day. The population growth rate for each county was calculated based on the growth rate from year 2000 to 2010 using the U.S. Census 2010 data [52]. In order to estimate the hydrogen demand, the factors and key attributes, which influence consumer choice, were identified as: *household income*, *households with two or more vehicles*, *education*, and *commute distance*. Household income was classified into five different groups (based on U.S dollar Income) and each was scored according to purchase level of fuel cell vehicles (Table 13). The households with two or more vehicles category was classified to three different groups based on the number of households with two or more vehicles (Table 14). The education category was classified based on the number of people with a bachelor's degree or higher (Table 15). The commute distance category was classified into three different groups based on the number of households with travel to work durations more than 20 minutes every day (Table 16). Also note that scores were normalized so the groups for each attribute equal 100%.

Table 13. Classification for household income ***Income Level*** *($U.S.)*	***Scoring of Classification***
0 - 24,999	1
25,000 - 49,999	2
50,000 - 74,999	3
75,000 - 99,999	4
over 100,000	6

Table 14. Classification for households with two or more vehicles

Values and Classification *(Number of people)*	***Scoring of Classification***
0 – 49,999	3
50,000 - 99,999	4
over 100,000	6

Table 15. Classification for education

Values and Classification *(Number of people)*	***Scoring of Classification***
0 – 29,999	3
30,000 - 59,999	4
60,000 - 89,999	5
over 90,000	6

Table 16. Classification for commute distance

Values and Classification *(Number of people)*	***Scoring of Classification***
0 – 49,999	3
50,000 - 99,999	4
over 100,000	6

Each attribute can be weighted based on its level of impact on consumer behavior. We weighted these assumed attributes as follows:

- Household Income (30%)
- Households with two or more vehicles (30%)
- Education (20%)
- Commute Distance (20%).

We applied a scenario based approach to solve the proposed multi-period two-stage stochastic model. Ten scenarios with different market penetration rates were selected for four time periods (2013-2022, 2023-2032, 2033-2042, 2043-2052). Figure 10 shows the results for these demand scenarios.

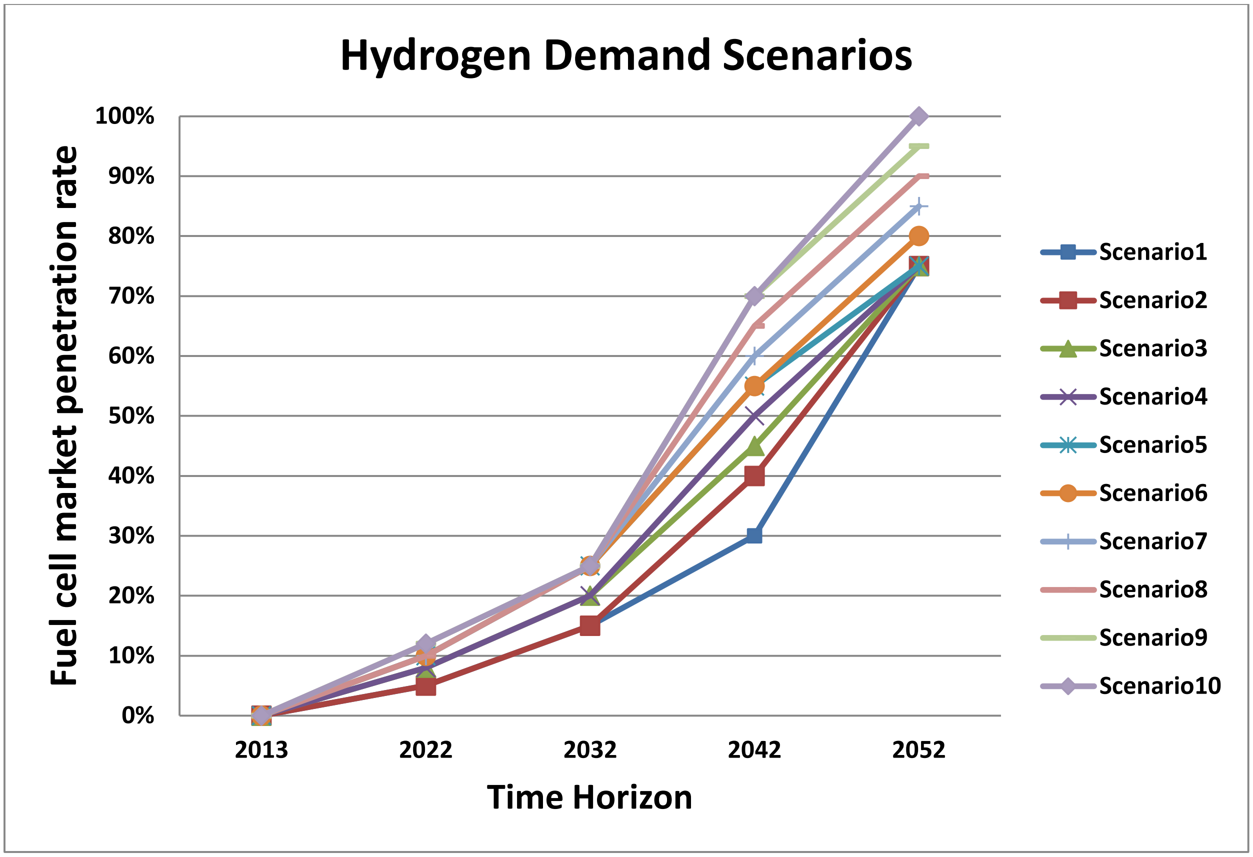


Figure 10. Hydrogen demand scenarios

Table 17 shows the results of the spatially aggregated demand model for the four time periods and the ten hydrogen demand scenarios based on market penetration of hydrogen fuel cell as we discussed above.

Table 17. Results of hydrogen demand with 10 scenarios and four time periods in the state of New Jersey

Time period	t1	t1	t1	t1	t2	t2	t2	t3	t3	t3	t3	t3	t3	t3	t3	t4	t4	t4	t4	t4	t4
Scenario J	**J1-J2**	**J3-J4**	**J5_J8**	**J9-J10**	**J1-J2**	**J3-J4**	**J5-J10**	**J1**	**J2**	**J3**	**J4**	**J5-J6**	**J7**	**J8**	**J9-J10**	**J1-J5**	**J6**	**J7**	**J8**	**J9**	**J10**
market penetration	**5%**	**8%**	**10%**	**12%**	**15%**	**20%**	**25%**	**30%**	**40%**	**45%**	**50%**	**55%**	**60%**	**65%**	**70%**	**75%**	**80%**	**85%**	**90%**	**95%**	**100%**
Atlantic	743	1,188	1,485	1,782	2,322	3,097	3,871	4,843	6,457	7,264	8,071	8,879	9,686	10,493	11,300	12,623	13,464	14,306	15,147	15,989	16,830
Bergen	3,720	5,952	7,440	8,929	11,294	15,058	18,823	22,857	30,476	34,286	38,095	41,905	45,714	49,524	53,333	57,824	61,679	65,534	69,389	73,244	77,099
Burlington	1,798	2,877	3,597	4,316	5,554	7,406	9,257	11,437	15,249	17,155	19,061	20,968	22,874	24,780	26,686	29,437	31,400	33,362	35,325	37,287	39,250
Camden	1,672	2,676	3,345	4,013	5,039	6,719	8,399	10,124	13,499	15,186	16,873	18,561	20,248	21,935	23,623	25,424	27,119	28,813	30,508	32,203	33,898
Cape May	237	379	474	569	693	924	1,155	1,352	1,802	2,028	2,253	2,478	2,704	2,929	3,154	3,296	3,515	3,735	3,955	4,175	4,394
Cumberland	329	526	657	789	1,021	1,361	1,701	2,113	2,817	3,169	3,521	3,873	4,225	4,577	4,929	5,466	5,830	6,194	6,559	6,923	7,287
Essex	2,486	3,978	4,973	5,967	7,414	9,885	12,357	14,739	19,652	22,108	24,565	27,021	29,478	31,934	34,391	36,625	39,067	41,509	43,950	46,392	48,834
Gloucester	1,063	1,700	2,125	2,550	3,391	4,522	5,652	7,217	9,622	10,825	12,028	13,230	14,433	15,636	16,839	19,195	20,475	21,755	23,034	24,314	25,594
Hudson	2,350	3,759	4,699	5,639	7,195	9,594	11,992	14,690	19,587	22,035	24,483	26,932	29,380	31,828	34,277	37,488	39,987	42,487	44,986	47,485	49,984
Hunterdon	503	805	1,006	1,207	1,548	2,063	2,579	3,175	4,233	4,762	5,291	5,820	6,349	6,878	7,407	8,140	8,683	9,226	9,768	10,311	10,854
Mercer	1,256	2,010	2,512	3,015	3,852	5,136	6,421	7,876	10,501	11,814	13,127	14,439	15,752	17,065	18,377	20,128	20,128	22,812	24,154	25,496	26,838
Middlesex	3,220	5,152	6,441	7,729	10,040	13,386	16,733	20,867	27,823	31,301	34,779	38,257	41,734	45,212	48,690	54,215	57,829	61,443	65,058	68,672	72,286
Monmouth	2,459	3,934	4,918	5,902	7,469	9,958	12,448	15,123	20,164	22,684	25,205	27,725	30,246	32,766	35,287	38,277	40,829	43,380	45,932	48,484	51,036
Morris	2,111	3,378	4,222	5,067	6,480	8,641	10,801	13,262	17,683	19,893	22,103	24,313	26,524	28,734	30,944	33,925	36,187	38,448	40,710	42,972	45,233
Ocean	1,997	3,195	3,994	4,793	6,363	8,484	10,604	13,515	18,020	20,273	22,525	24,778	27,030	29,283	31,535	35,885	38,278	40,670	43,062	45,455	47,847
Passaic	1,409	2,254	2,817	3,381	4,278	5,704	7,131	8,663	11,551	12,994	14,438	15,882	17,326	18,770	20,214	21,926	23,388	24,850	26,312	27,773	29,235
Salem	166	265	331	397	504	671	839	1,021	1,362	1,532	1,702	1,872	2,042	2,212	2,383	2,588	2,761	2,933	3,106	3,279	3,451
Somerset	1,401	2,242	2,802	3,363	4,382	5,843	7,304	9,138	12,184	13,707	15,230	16,753	18,276	19,799	21,322	23,818	25,406	26,994	28,582	30,170	31,757
Sussex	544	871	1,089	1,307	1,662	2,216	2,770	3,381	4,508	5,072	5,635	6,199	6,762	7,326	7,889	8,599	9,173	9,746	10,319	10,893	11,466
Union	1,852	2,963	3,704	4,445	5,631	7,508	9,385	11,413	15,217	17,120	19,022	20,924	22,826	24,728	26,630	28,915	30,843	32,771	34,698	36,626	38,554
Warren	361	577	721	866	1,115	1,486	1,858	2,296	3,062	3,444	3,827	4,210	4,592	4,975	5,358	5,913	6,307	6,701	7,096	7,490	7,884
Total Demand	**31,676**	**50,682**	**63,353**	**76,023**	**97,247**	**129,663**	**162,079**	**199,101**	**265,468**	**298,651**	**331,834**	**365,018**	**398,201**	**431,385**	**464,568**	**509,709**	**542,347**	**577,670**	**611,651**	**645,631**	**679,612**

This study assumes in the first time period the market penetration rate is categorized into four sets (J1-J2, J3-J4, J5-J8, and J9-J10). The second time period for all scenarios was categorized into three sets (J1-J2, J3-J4 and J5-J10). The third time period for all scenarios was categorized into eight sets (J1, J2, J3, J4, J5-J6, J7, J8, J9-10) and for the fourth period was categorized into six sets (J1-J5, J6, J7, J8, J9, J10). The reason we defined different scenarios was to ensure the model could handle the hydrogen demand with different market penetration rates. In this example, the lowest market penetration rate we considered in our scenarios was 5 percent based on aggregated demand model for households that would eventually purchase hydrogen fuel cell vehicles, and the highest market penetration was 100 percent of households. In order to run multi-period two-stage stochastic programming, we used GAMS software with MILP. The probability of each scenario occurring assumed to be 10 percent in this case study, with a total sum of all scenarios equal to 100 percent.

Our results show for first time period year 2013-2022, only three Steam Methane Reforming (SMR) plants needed to be added, and one additional plants were required for second time period year 2023-2032, in addition to the previous time period infrastructure. For the third time period, 2033-2042, ten SMR plants and five electrolysis plants needed to be added to the production infrastructure. For last time period, 2043-2052, two SMR plants and two electrolysis plants needed to be added to previous time period. This analysis indicates the optimal total number of production plants required from 2013 to 2052, should be 18 SMR and 7 Electrolysis plants to be added in specific numbers in the different time periods. For storage facilities, the hydrogen demand model results indicated 21 liquid facilities and 53 compressed facilities would be necessary by time 2052.

The result from our optimization model for scenario ten during time period 2013-2022 is shown in Figure 11. In this model we assume the SRM plants alone can meet the total hydrogen demand by producing 50 percent from LH2 type and the other 50 percent from compressed gaseous hydrogen (GH2). In this scenario there are three SMR plants in the network and no Electrolysis plants. The reasons are a SMR plant has higher capacity, and lower unit production and emission costs due to lower carbon emission rates. A SMR plant also has lower energy cost compared to an Electrolysis plant due to a lower electricity consumption rate. Figures 12-14 show the optimal hydrogen infrastructures in New Jersey for scenario 10 in 2023-2032, 2033-2042 and 2043-2052.

The red color facilities indicate the new facilities which are needed to be added to the hydrogen production infrastructure for that time period. In terms of the number of production and storage plants for the different scenarios within a specific time period, the results are the same as scenario 10. The reason for this outcome is because (as mentioned earlier) we consider all production node variables and storage capital cost variables in the first stage stochastic programming model. However, for each scenario in a specific time period the number of variables relating to storage, operating, emission, energy and risk costs, and all delivery costs, can be different because they are in the second stage of the stochastic programming model where demand uncertainty can affect them. As shown in Figures 11-14, different types of production and storage facilities needed to be added over time in each NJ State county (region) and as demand increases. As the time periods change, each county will need its own production facility so that the decreased hydrogen delivery costs will be eliminate or reduce significantly the cost of hydrogen imported from other regions. .

When taken over all time periods, the average total cost of hydrogen production in this model is 3.07×10^6 dollars (U.S.) per day. The average cost categories within the network and the cost per kg hydrogen for the entire planning horizon are summarized in Table 18. All dollar ($U.S.) values are based on the year 2013. As seen in this table, the hydrogen cost per kg decreases over the entire planning horizon because as demand increases hydrogen production plants and storage facilities and delivery modes are using their full capacity and the cost per unit decreases.

Table 18. Summary of hydrogen infrastructure network costs over entire planning horizon

Cost categories		**Time period , *t***			
		t_1	t_2	t_3	t_4
Economy					
Capital cost ($)					
	Production facilities	9.03×10^{8}	2.46×10^{9}	7.79×10^{9}	8.77×10^{9}
	Storage facilities	5.28×10^{9}	6×10^{9}	7.83×10^{9}	9.69×10^{9}
	Delivery modes	5.72×10^{7}	9.48×10^{7}	6.93×10^{7}	8.91×10^{7}
Operating cost ($/d)					
	Production facilities	1.96×10^{5}	4.01×10^{5}	1.21×10^{6}	1.84×10^{6}
	Storage facilities	2.39×10^{4}	5.71×10^{4}	1.43×10^{5}	2.23×10^{5}
	Delivery modes	5.26×10^{4}	8.08×10^{4}	5.66×10^{4}	7.07×10^{4}
Ecology					
Emission cost ($/d)					
	Production facilities	2.63×10^{4}	5.63×10^{4}	1.62×10^{5}	2.045×10^{5}
	Storage facilities	29.85	71.32	179.19	279.11
	Delivery modes	71.88	154.89	234.82	308.37
Energy					
Energy consumption cost ($/d)					
	Production facilities	4.54×10^{3}	9.26×10^{3}	9.7×10^{4}	2.045×10^{5}
	Storage facilities	1.31×10^{5}	3.12×10^{5}	7.85×10^{5}	1.22×10^{6}
	Delivery modes	3.18×10^{3}	6.84×10^{3}	1.04×10^{4}	1.36×10^{4}
Risk					
Risk cost ($/d)					
	Production facilities	14.82	33.70	115.93	132.98
	Storage facilities	19.5	19.9	24.6	29.4
	Delivery modes	390	647	473	680
Total network cost ($/d)		$\mathbf{1.86\times10^{6}}$	$\mathbf{2.24\times10^{6}}$	$\mathbf{3.51\times10^{6}}$	$\mathbf{4.66\times10^{6}}$
Hydrogen cost per kg ($)		**16.31**	**7.86**	**4.89**	**4.16**
Network average cost ($/d)		$\mathbf{3.07\times10^{6}}$			

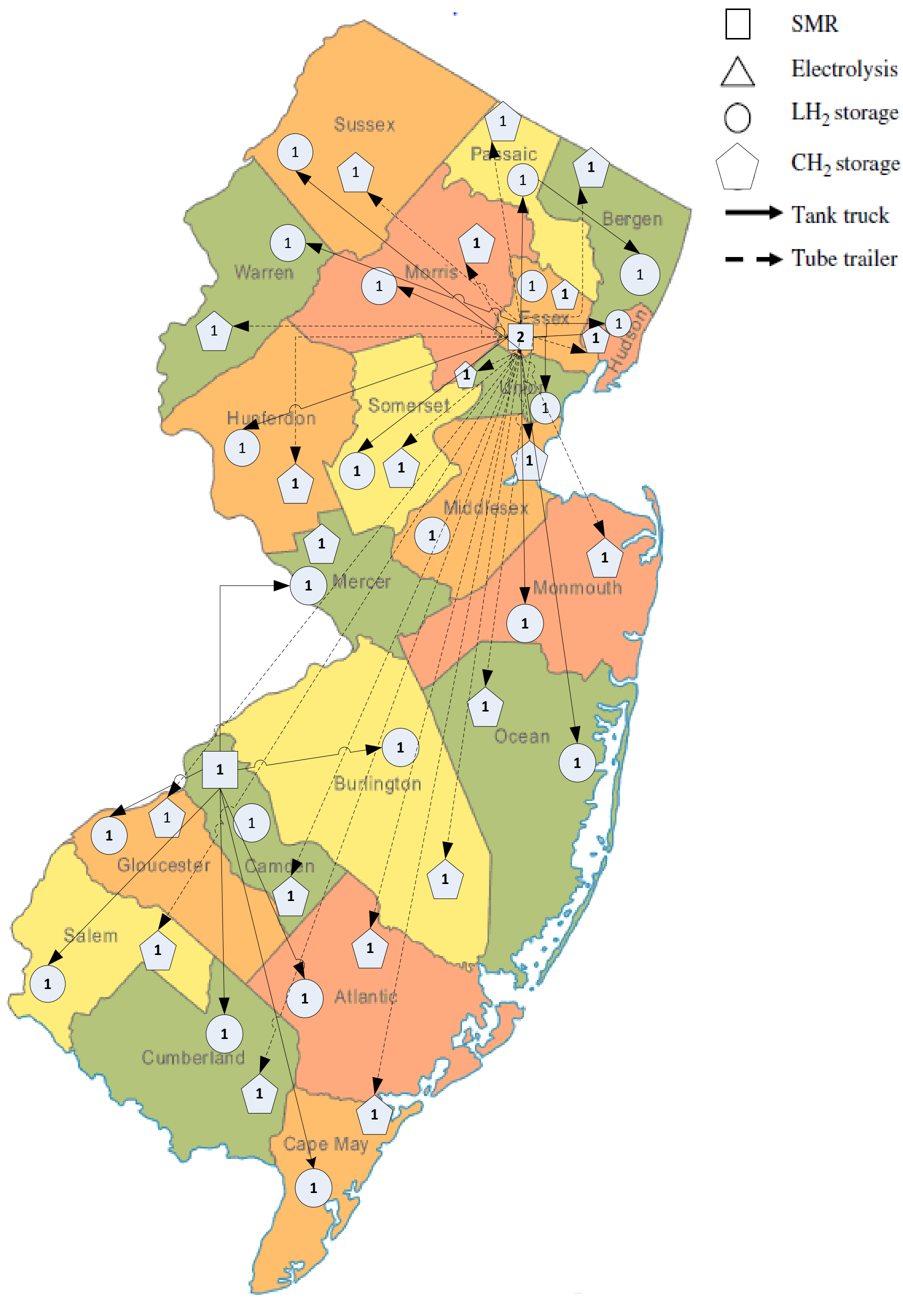


Figure 11. Optimal hydrogen infrastructure in New Jersey for scenario 10 in 2013-2022. All hydrogen demand met by SMR plants and existing storage infrastructure.

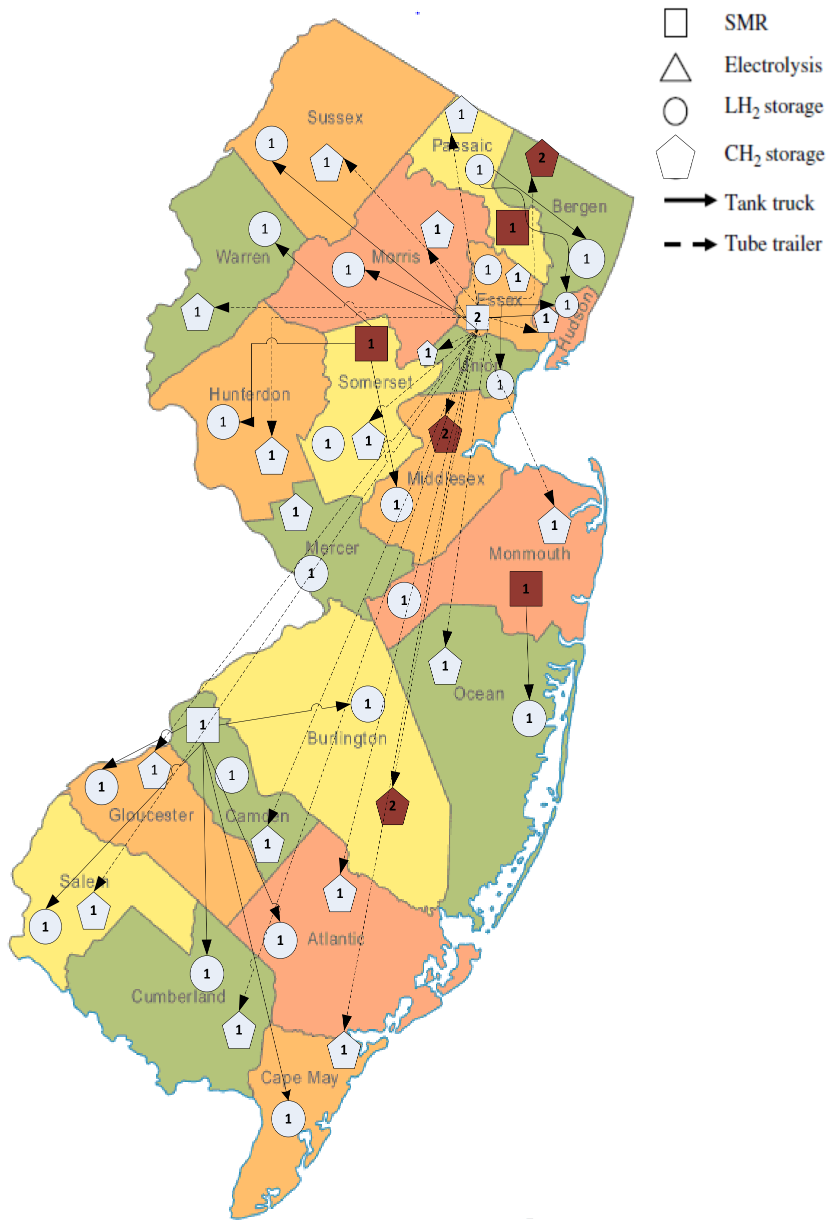


Figure 12. Optimal hydrogen infrastructure in New Jersey for scenario 10 in 2023-2032. New SMR plants and storage facilities needed for increased consumer demand.

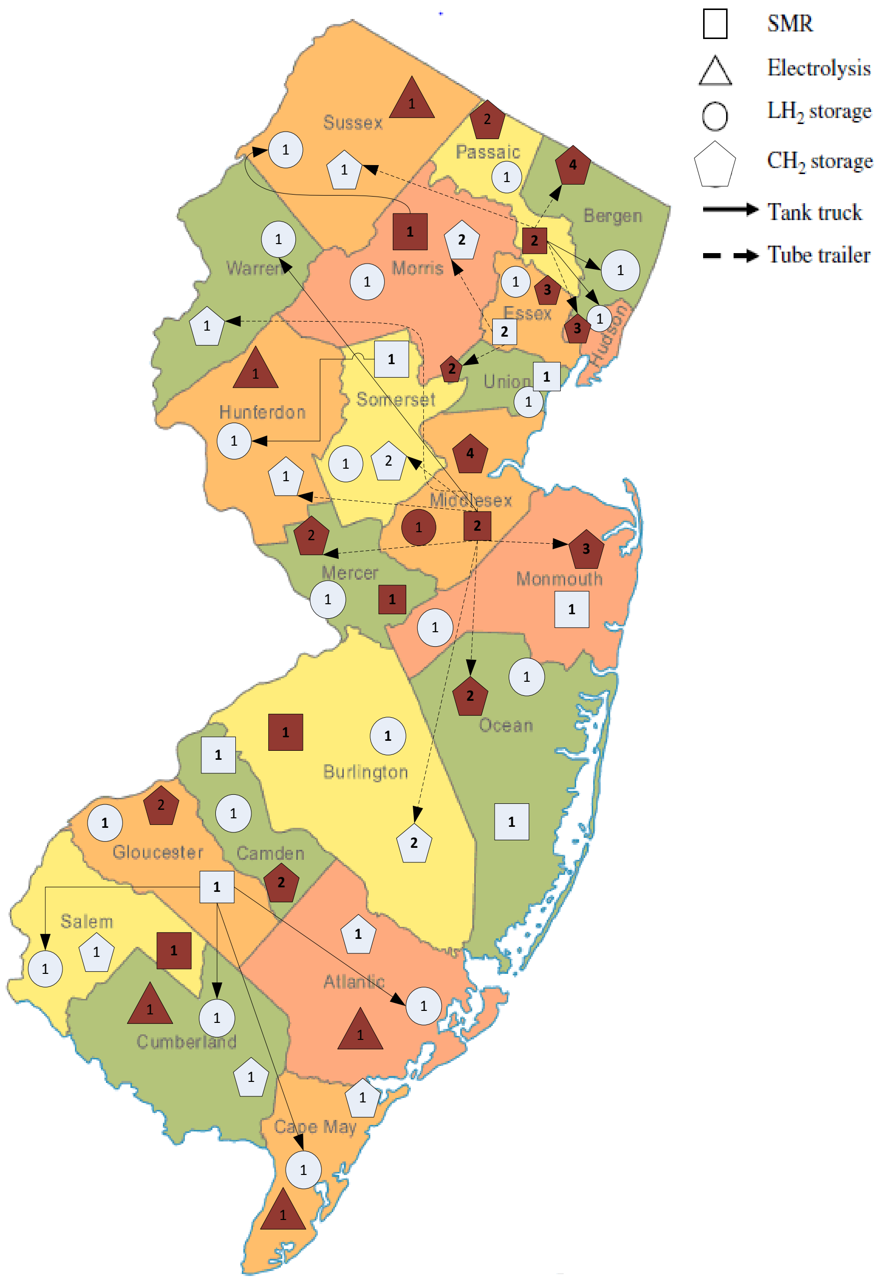


Figure 13. Optimal hydrogen infrastructure in New Jersey for scenario 10 in 2033-2042. Additional SMR and new Electrolysis production plants required to meet regional demands for the state. Additional storage facilities needed across New Jersey.

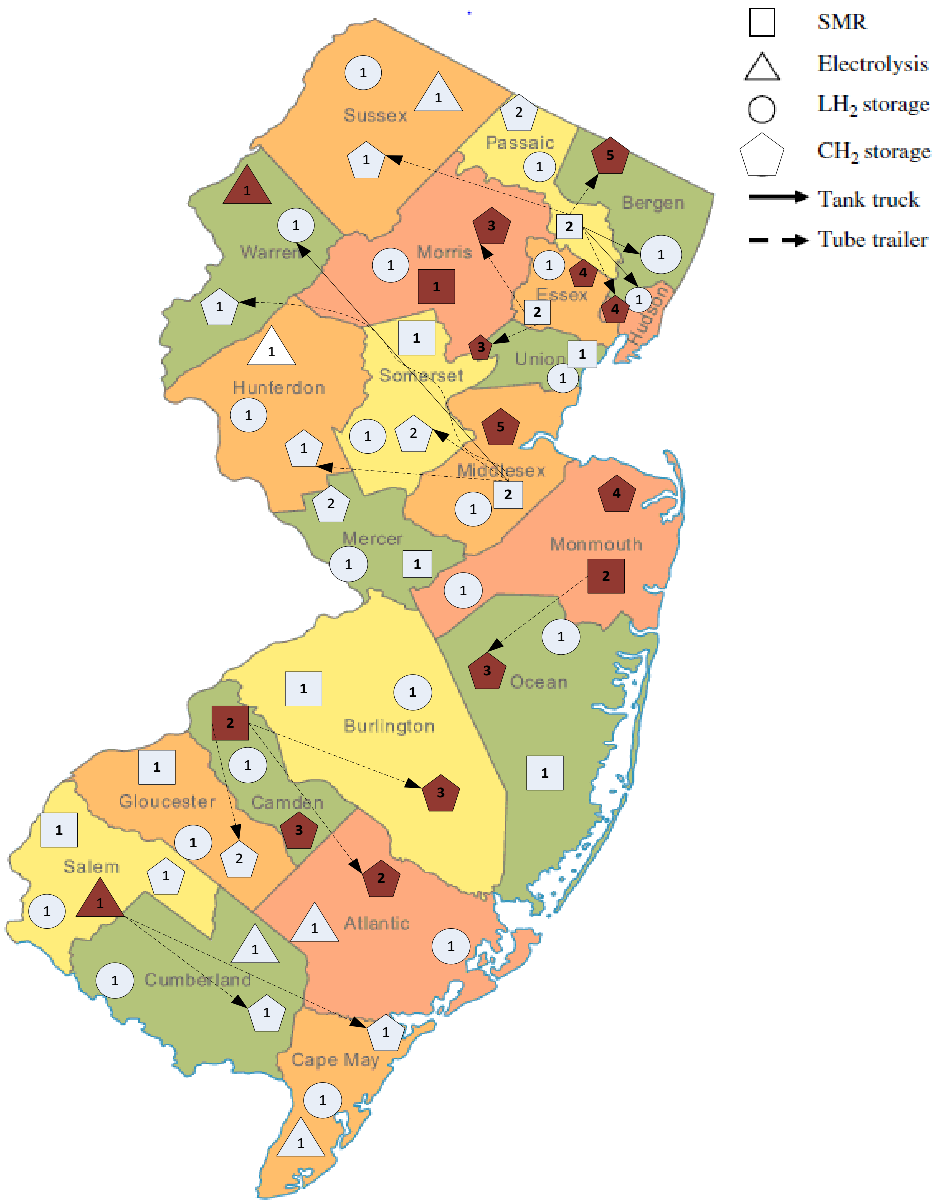


Figure 14. Optimal hydrogen infrastructure in New Jersey for scenario 10 in 2043-2052. Additional SMR and Electrolysis production plants required to meet regional demands for the state. Additional storage facilities needed across New Jersey.

3.5 Conclusion

In this chapter we proposed a multi-period optimization model taking into account the stochasticity and the effect of uncertainty in the hydrogen production, storage and usage in macro view (e.g. county level). The objective function includes minimization of total daily social cost of the hydrogen supply chain network with uncertain demand. There are several factors and key attributes, which influence consumer choice to buy a fuel cell vehicle. At the same time, consumer preference on the demand side is the most important factor in predicting changes in the auto market. A spatially aggregated demand model was developed to estimate the potential demand for fuel cell vehicles based on different household attributes such as income, education etc. These models were applied to evaluate the future hydrogen supply chain for State of New Jersey.

Chapter 4- Multi-Criteria Spatial Decision Analysis for Location Suitability (Micro Level)

4.1 Introduction

Finding suitable and optimal locations for hydrogen fueling stations are significant issues in planning energy infrastructure, especially in high-density regions such as New Jersey. In this study, a Geographic Information System (GIS)-based Multi-Criteria Decision Making (MCDM) tool was developed to find suitable locations for hydrogen fueling stations by considering factors such as land availability, air quality, energy source availability, for example. The MCDM results were used to choose the optimal locations for the location allocation model (Chapter 5). In this analysis, customer demand coverage is maximized that the model will choose the locations in which all or a high % of estimated customer demand is within a specified impedance cutoff. This scenario was carried out using a Analytic Hierarchy Process (AHP), a multi-criteria decision analysis approach. We integrate AHP with the suitable locations identified by GIS analysis. The purpose of integrating the GIS-based location suitability analysis with the multi-criteria AHP approach is to create an enhanced method for solving complex problems related to land-use planning.

AHP is recognized as an effective multi-criteria decision support system [54]. There are many research applications which have used this approach such as finding suitable locations for public parks [69] and ecotourism [56,70,71,72,75], and choosing acceptable MSW landfill sites [73]. No papers have been published at the current time relating to alternative fueling stations, especially in hydrogen. However, there might be some effort in private sector and energy agencies, but these are not accessible to the public. Siting hydrogen fueling stations is a very important topic in near future for investment and planning purposes. In this thesis section, we attempted to develop a framework which involves analytics. It would be a new analysis tool aimed at assisting decision makers and planners in making better decisions regarding alternative energy, particularly hydrogen infrastructure. It is intended this new analysis tool can be used in different regions as long as the necessary data is available.

4.2 Methodology

In this application, GIS-based location suitability analysis and the AHP [55] method based on multi-criteria decision making (MCDM), were used. First, we applied GIS-based location suitability modeling for site suitability [56]. The GIS modeling and analysis is a logically ordered procedure that works by breaking down a problem into smaller and smaller elements [57]. Then, we applied AHP, which is a systematic method to guide decision- making based on priorities to solve the problems [58].

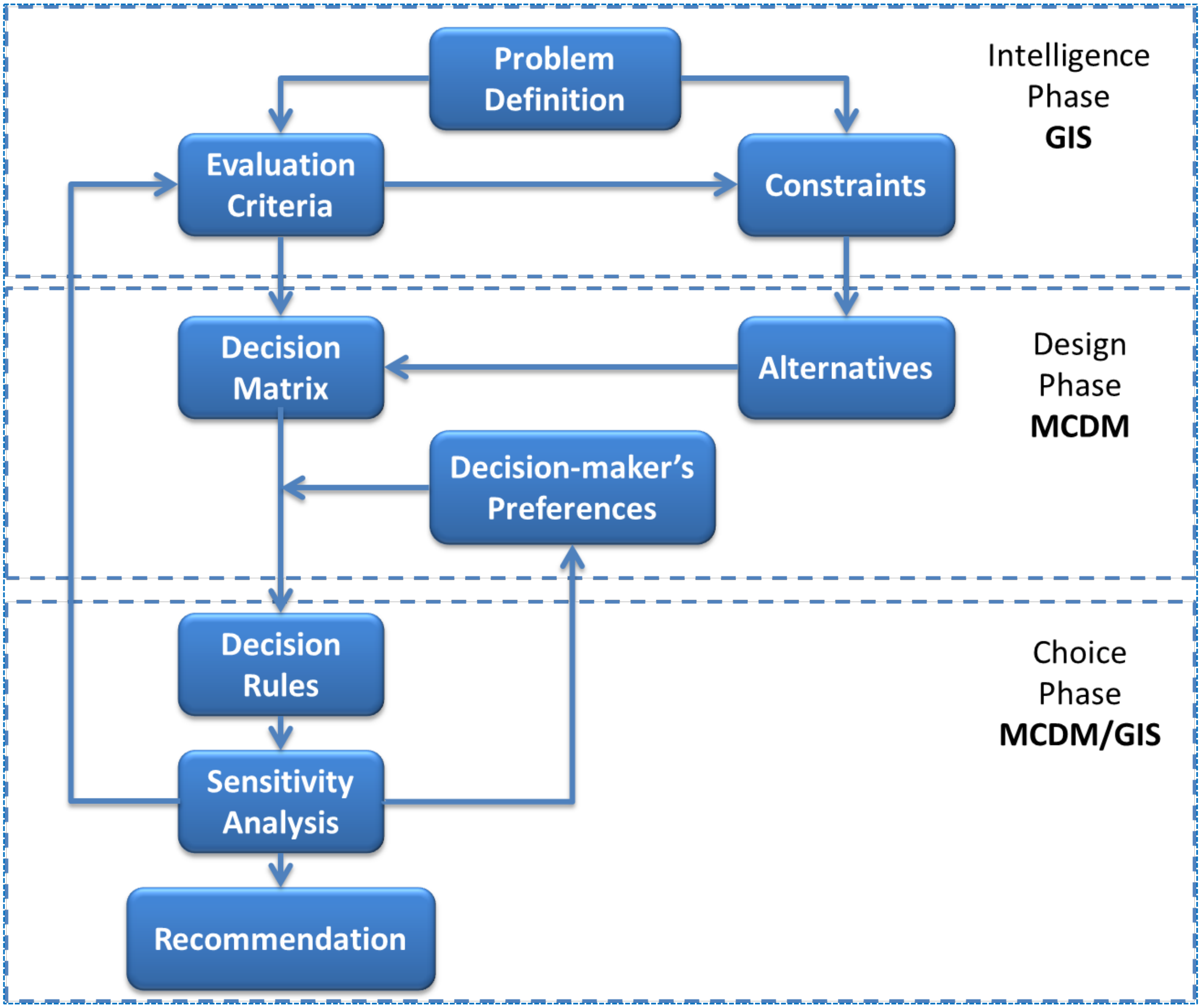


Figure 15. Framework for spatial multi-criteria decision analysis [59]

The main purpose of GIS analytics is to provide support for making spatial decisions [59]. There are different frameworks for informing the decision process. In this study, we used one of the most widely accepted generalizations of the decision making process introduced by Simon [60], and then extended by Malczewski [59]. The later framework was combined with MCDM concepts and is outlined in Figure 15. Simon suggested any decision making process can be structured into three major phases: *intelligence*, which defines a problem or an opportunity for change, *design* which identifies possible alternatives, and *choice* which recommends and ranks alternatives.

Figure 16 shows the schematic diagram we used for modeling the problem of how to identify and choose suitable locations for hydrogen fueling stations in New Jersey. It is important to perform a preliminary study on a region of interest to determine critical attributes which should be considered in the evaluation. One of the important steps in this model is relevant data collection. In order to run this model both spatial and non-spatial data are needed. Recently advances in state and federal data and information practices has made it easier to collect key spatial data through government websites. However, still there may be some limitations in some states.

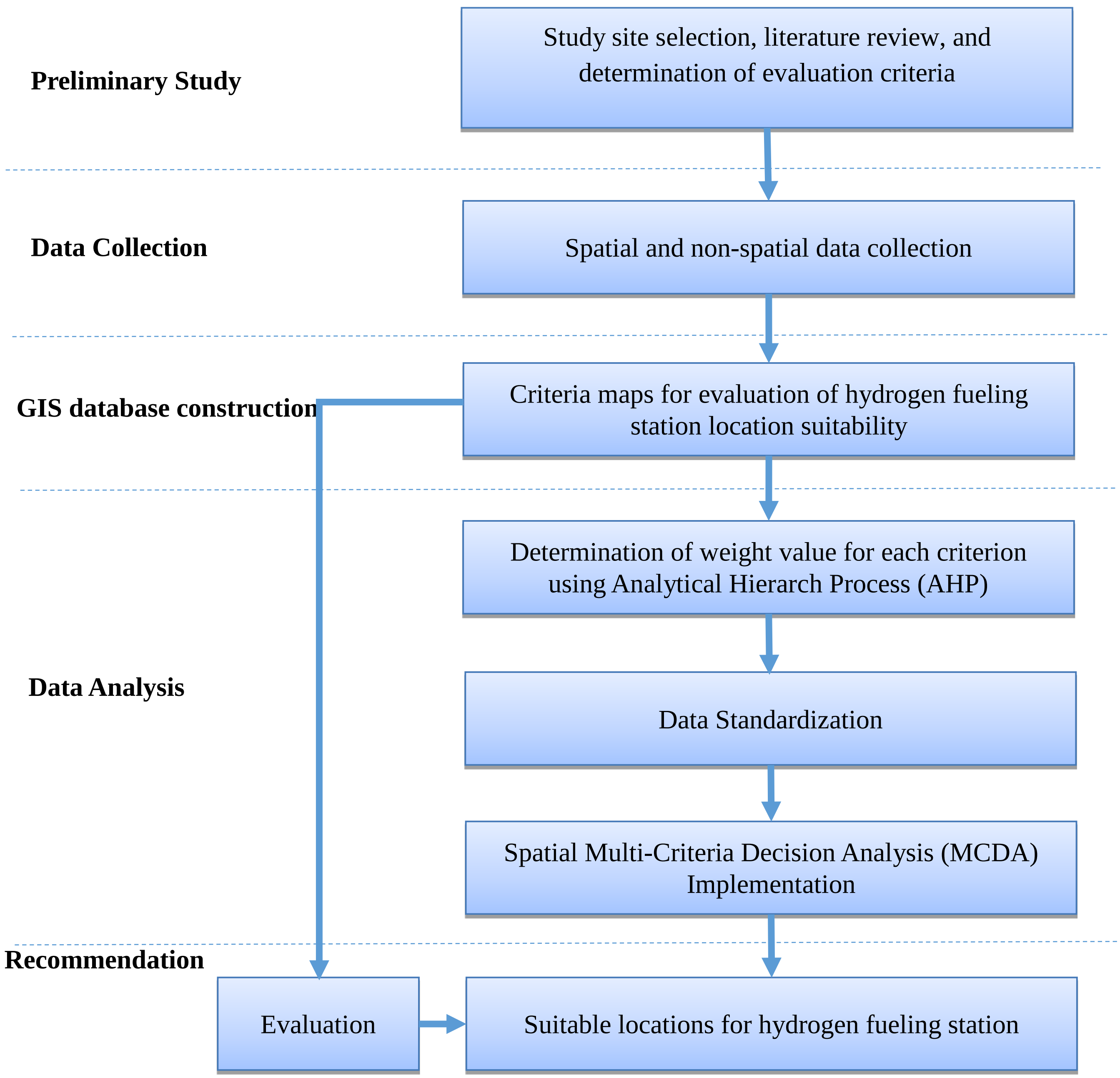


Figure 16 A schematic diagram for modeling suitable locations of hydrogen fueling station

Five criteria were defined in this study, along with their sub-criteria: *Land Availability*, *Transportation Risk*, *Primary Energy Source Availability*, *Air Quality*, and *Entertainment Facilities* (Table 19). The criteria and sub-criteria were chosen according to experience, experts' opinions, and information from various sources. Knowledge acquisition was accomplished through discussions with experts in fields related to this study, surveys of authenticated literature, and analysis of historical data. The GIS database for this study was developed by using criteria and sub-criteria in different data layers (rasterized information).

Table 19. Criteria and sub-criteria for evaluation of hydrogen fueling station location suitability

Criteria/Factor	**Sub-criteria**
Land Availability	Vacant Land
	Existing gas station
Transportation Risk	Major Roads hydrogen transportation risk
	Local Roads hydrogen transportation risk
Primary Energy Source Availability	Exiting natural gas pipeline
	Waste water treatment facilities
	Power line Network
	Landfill Locations
Air Quality	Volatile organic compounds (VOCs)
	Ozone
	NOx
	Particulate Matter-PM2.5
Entertainment Facilities	Shopping Malls
	Golf Courses
	Parks

The AHP method is one of the most extended Multi-Criteria Decision Making (MCDM) techniques. This method provides a structural basis for quantifying the comparison of decision factors and criteria in a pairwise manner [61]. Usually experts are asked to rank the value of a criterion map for a pairwise matrix on a Saaty's scale [62]. The method evaluates the relative significance of all parameters by assigning weight for each of them in the hierarchical order, and in the last level of the hierarchy, the suitability weight is given for each class of the used factors. The priority of each factor involved in the AHP analysis is determined based on the suggestions of experts most of the time [63].

A nine-point scale is used for these evaluations as shown in Table 20. For example, when comparing criteria land availability to criteria transportation risk, a score of 1 indicates that they are equally relevant to the evaluation of suitability and a score of 9 indicates that transportation risk is of little significance relative to land availability. All scores can be assembled in a pair-wise comparison matrix with 1's on the diagonal and reciprocal scores in the lower left triangle (e.g., if land availability to transportation risk is 5, then transportation risk to land availability is 1/5).

Table 20. Pairwise Comparison Matrix

Intensity of Importance	**Definition**
1	Equal importance
2	Equal to moderate importance
3	Moderate importance
4	Moderate to strong importance
5	Strong importance
6	Strong to very strong importance
7	Very strong importance
8	Very to extremely strong importance
9	Extreme importance

A standardized eigenvector is extracted from each comparison matrix in order to assign weights to criteria and sub-criteria. These weights give a suitable value for each location in GIS. For each level in the hierarchy, it is necessary to know whether the pairwise comparison has been consistent. We use a Consistency Ratio (CR) for this assessment. The CR is a measure of how much variation is allowed, and must be less than 10 percent. It can be calculated with the formula below:

$$CR = \frac{CI}{RI} \tag{4.1}$$

The CI term, referred to as the consistency index, provides a measure departure from consistency and RI is the random index, the consistency index of a randomly generated pairwise comparison matrix. RI depends on the number elements being compared.

For AHP weights calculation, Expert Choice 11.5 software [64, 65] or Microsoft Excel can be used to build the GIS database. We used ESRI ArcGIS 10.2 Advanced Desktop software (Redlands, CA) [66]. This was done to automate and model suitability analysis using the ArcGIS Model Builder application.

We calculated a suitability score for each lowest level of the hierarchy (which in our case is level 2) Eastman et al. [67] developed a formula, which applies for each location. That is,

$$S = \left(\sum_{i=1}^{n} w_i \; x_i\right) \prod c_j \tag{4.2}$$

S: Suitability index
w_i: weight of criterion i
x_i: Score of criterion i
c_j: Boolean value of limited criterion

The higher value for the *Suitability index,* the more suitable was the site for the hydrogen fueling station. Boolean values were used for constraints. The value of 0 was assigned to a location not suitable for a hydrogen fuel station. In our model, flood zones were the only exclusion constraints, but more contrarians can be added to this model. This process was automated by using ArcGIS Model Builder for ArcGIS 10.2 (ESRI, 2013) [66].

The location suitability analysis was performed using rasterized geospatial location data. The raster data model is a better technique because the structure of raster data is grid cell based, which can easily delineate suitable sites. Raster data facilitates the user in carrying out a weighted overlay on numerous layers. Combining raster layers are quite complex because it requires an understanding of the characteristics of the data sources to combine, the rules for combining spatial data, strategies for ranking data and how to implement spatial multi-criteria decision analysis. Each raster cell represents a portion of the earth, such as a square meter or square mile, and usually has an attribute value associated with it, such as soil type. Typical raster datasets are very detailed and store a large amount of information, because information about each and every cell must be recorded.

ArcGIS Model Builder is an application which allows users to create, edit, and manage models. Models are workflows that string together sequences of geo-processing tools, feeding the output of one tool into another tool as input. Model Builder can also be thought of as a visual programming language for building workflows (Figure 17).

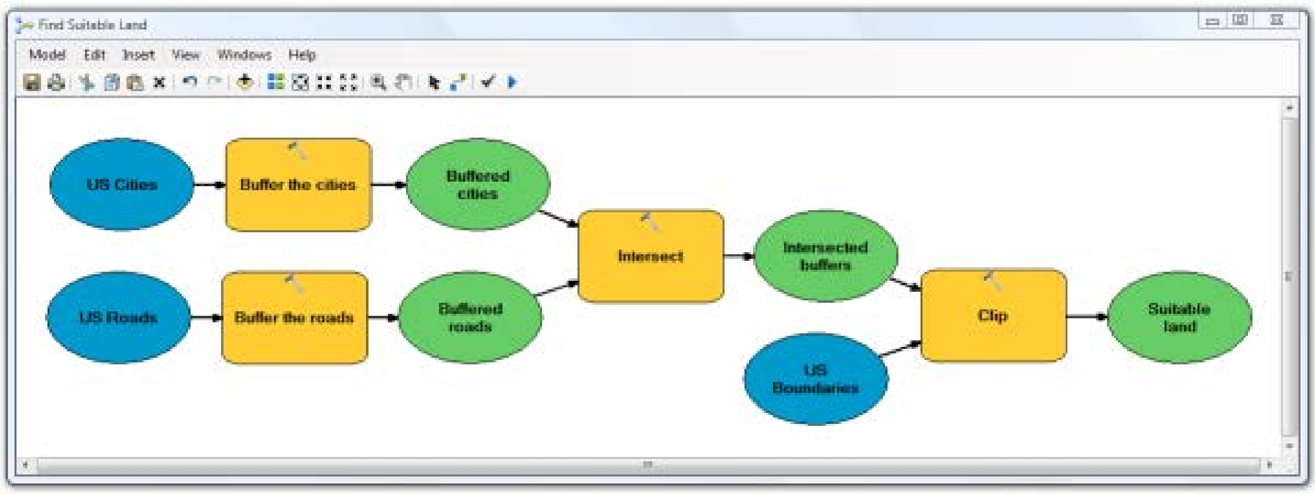


Figure 17. Snapshot of ArcGIS Model Builder

We will now use the ArcGIS Model Builder to find suitable locations for the hydrogen fueling stations using five data layers (rasters) that correspond to the siting criteria mentioned earlier: *Land Availability*, *Transportation Risk*, *Primary Energy Source Availability*, *Air Quality*, and *Entertainment Facilities*. More criteria can be added as long as the data are available for them. These criteria and their sub-criteria weights and score might vary in different locations. The first one is land availability criteria, which has two sub-criteria: *vacant land* and *existing gas station*. Vacant land sub-criteria might be not easy to apply in practice since some land might be public or private, but it can be an important sub-criteria in regions with high-density population. The location of existing gas stations is a very important sub-criteria, especially if gas stations are located in high traffic volume locations, which can meet the high amount of demand for hydrogen. This helps decision makers to consider upgrading the gas station by merging a hydrogen station with an existing gas station, which can reduce operational cost. The second criterion is transportation risk, which is related to transporting hydrogen. Its related risk will be described in more detail in next section. The third criterion is *Primary Energy Source Availability*, which has four sub-criteria: *exiting natural gas pipeline*, *wastewater treatment facilities*, *power line network*, and l*andfill locations*. These four sub-criteria are crucial for on-site hydrogen production as part of a fueling station since each can save significant cost and risk of hydrogen transportation because the primary energy sources are near the hydrogen fueling station. The fourth criterion is air quality which has four sub-criteria: *volatile organic compounds* (VOCs), *ozone*, *NOx*, and *particulate matter-PM2.5*. The air quality criterion is crucial in reducing emissions of criteria pollutants controlled by the federal Clean Air Act. Model locations with high airborne concentrations of these chemical sub-criteria are better suited for hydrogen-fueling stations because of the reductions of these air pollutant species with hydrogen transportation fuels. The last criterion is *Entertainment Facilities* which has three sub-criteria: *shopping malls*, *golf courses*, and *parks*. These locations usually have high traffic volumes, and would be convenient for those customers with limited time and multitask as they refuel their vehicles while they are in these entertainment facilities.

4.2.1 Risks Associated With Hydrogen Transportation

4.2.1.1 Introduction

Long distances between hydrogen production facilities and hydrogen end-use require design of an advanced delivery system, which is efficient and reliable. In general, compact forms of hydrogen storage are more economical to transport while diffuse forms are more costly. Liquid hydrogen (LH_2) is delivered by truck or rail over distances of up to several hundred miles. Compressed gas hydrogen pipelines (up to several hundred miles in length) are used commercially today to bring hydrogen to large industrial users like refineries.

Hydrogen can be transported by different options like rail and barge, but road transport always will play an important role, especially for liquid transport. Hydrogen can be transported on the road by truck as a cryogenic liquid in double-walled and super-insulated, vacuum-lined tanks. Since LH_2 does not have to be transported under pressure, transporting LH_2 is much more efficient than transporting a high-pressure gas, particularly when larger quantities are needed. Unfortunately, maintenance costs are much higher for liquid transportation.

Several models exist to design and optimize hydrogen transport routes, number of filling stations, and truck delivery times, for example Ogden's model at UC Davis [74]. Unfortunately, the authors did not include risk analysis in their models. What these transport models work with mostly are hydrogen safety regulations. These regulations focus solely on physical characteristics of hydrogen as a fuel and they tend to neglect potential risks due to infrastructure design [44].

In this study we developed a framework to calculate the risk of hydrogen transport via roadways. Such a framework is necessary to identify which routes have higher road transport risk than others. There can be many different causes for a truck crash and cargo release, but these can be divided into two major categories, *i.e.*, *crash-initiated releases* and *non-crash initiated releases*. The crash-initiated releases with a truck represent a great potential for substantial damage and large releases of hydrogen. These include a collision between two vehicles, collisions with fixed objects, and overturn. Collisions between two vehicles and with fixed objects present the potential for substantial damage and also can represent relatively energetic impact accidents (explosions) with the potential for significant damage and/or cargo release. Overturned vehicles are most likely during trucking operations where, for some truck designs and cargoes, the vehicle's center of gravity is high, especially on tight curves such as ramps.

It has been recognized that among the factors that contribute to truck crashes, human error ranks the highest [44]. The most common causes of truck crashes are due to excessive speed, following too close to the preceding vehicle, non-observance of rest-time leading to driver over fatigue, and failure to observe traffic warnings.

Meanwhile, the non-crash initiated releases are characterized by equipment failures associated with accidents such as leaks of pipes and fittings or failures of relief valves and ruptured connections. These mechanisms result in relatively small quantities of cargo being released. We evaluated only the crash- initiated releases for risk calculation in in this study of hydrogen transportation.

The overall hydrogen transportation risk is found through the following steps: (1) calculate the probability of hydrogen release from segments of a road; (2) design a consequence model for different accident scenarios; (3) calculate the road segment risk by multiplying the potential consequences and crash probabilities; and (4) determine the overall risk for the road by creating the cumulative summation across all roadway segments.

4.2.1.2 Estimation of the probability for hydrogen release from road transport

As CCPS (Center for Chemical Process Safety) 2005 [44, 68] mentions, crash-initiated releases tend to dominate the risk of hazardous material transportation. Therefore, the losses of containment frequencies for these systems can be estimated directly from the crash rate data. *Crash rate*, which is defined as a number of crashes per *Million Vehicles Mile Traveled* (MVMT) in a given period, is estimated using the *Average Annual Daily Traffic* (AADT), and the length of a roadway segment. Since this project focuses on truck crashes, the *Average Annual Daily Truck Traffic* (AADTT) should be used. AADTT consists of all commercial vehicles traveling in a defined roadway segment. However, since the AADTT was not available for the majority of roadways in our area of study, the crash rate was calculated based on AADT. Usually AADT can be found from Straight Line Diagrams (SLD) databases owned by the Department of Transportation at each state. The source of the above crash data was obtained from NJDOT's (New Jersey Department of Transportation) website [75].

Crash rate for a roadway segment is calculated using the following formula:

$$\text{Crash rate for roadway segment } i = CR_i = \frac{\text{Number of crashes(N)}}{\text{Exposure per million vehicle per Mile(MVMT)}} \tag{4.3}$$

Where,

$$\text{MVMT} = \frac{\text{AADT}\times\text{Lenght of segment(L)}\times\text{Numberof years}\times 365}{1{,}000{,}000} \tag{4.4}$$

MVMT is the risk rate per hundred million vehicles per mile.

The probability of hydrogen release from road transport is the likelihood or chance that a vehicle carrying hydrogen will be involved in a crash:

$$P_i = CR_i \times P_i(H|C) \times L_i \tag{4.5}$$

where,

P_i : Probability of hydrogen release from road transport from road segment i

CR_i: All Vehicle Crash rate (1/vehicle-mile)

$P_i\ (H|C)$: Conditional probability for hazmat release given a crash occurs in road segment i

L_i : Length of the roadway segment (mile)

In order to calculate this probability, first we need to calculate crash rates for all vehicles for each road segment. Then, we need to obtain conditional probability for hazmat release given a crash occurs for each segment. We can obtain this probability by dividing the number of crashes with hazmat included for each roadway segment, by all vehicle crashes in that specific roadway segment. The reason we use roadway segments is to anticipate if it may be necessary to determine the local risk adjacent to more critical locations or for a road with more sensitive surroundings. For instance, some specific segments of a road might have a higher crash rate than others for the same road.

4.2.1.3 Consequence model

The consequence of each accident scenario is computed, usually in terms of heat flux, explosion overpressure, and toxic exposure using consequence modeling tools. Based on such estimates and the population densities for land use adjoining each route, the number of people affected by the postulated incidents can be determined in terms of injuries or fatalities. Since we considered crash-initiated releases in our study, we created an event tree (Figure 18). Such schema are used in fueling station risk analysis to define the accident scenarios after a crash has occurred either from a collision between two vehicles, collisions with fixed objects, or overturn) [44].

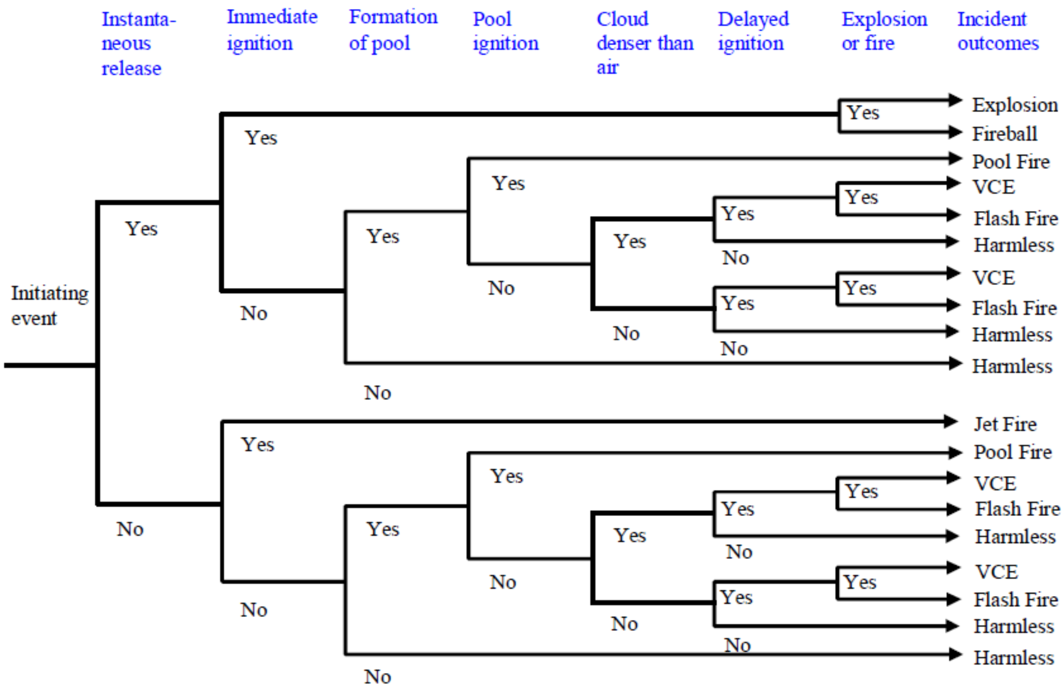


Figure 18. Event tree diagram of LH2 hydrogen release [44]

These are the data needed for defining our consequence model:

1. Probability of each accident scenario (can be obtained from event tree analysis) [44];
2. Potential Impact area for each accident scenario (based on historical data as well as expert opinion) [44]; and
3. Population Density (obtained from U.S. Census data 2010[52]).

For each accident there are a number of possible accident scenarios, S_j, each of which may be considered to be fatal to individuals present within radius, r_j. The expected number of people, N, which may be affected at the location of the accident, depends on population density,

$$N = \pi r^2{}_j D \qquad (4.6)$$

So, if we want to consider the consequence of a crash-initiated release by a hydrogen tanker truck, the expected number of people killed for scenario j is given by:

$$N_{fj} = P_{Sj}\,\pi\,r^2{}_j\,D \tag{4.7}$$

N_{fj}: Number of people being killed in scenario j

P_{Sj} : Probability of each accident scenarios

r_j : Radius of Impact Area for accident scenario j (Mile)

D : Population Density (Number of people / Square mile)

The term, $P_{Sj}\,\pi\,r^2{}_j$, is independent of the route, but the value for *D* depends on the chosen route. We defined a term called *Hydrogen Severity Index* by summing up all the $P_{Sj}\,\pi\,r^2{}_j$ terms for all possible scenarios.

4.2.1.4 Risk computations

As mentioned previously, in order to calculate the risk we need to multiply crash probabilities with the potential consequences for each roadway segment.

These steps involved in calculating the population risk are:

1. Calculate the probability of hydrogen release from road transport for each roadway segment (section 4.2.1.2);
2. Calculate the *Hydrogen Severity Index* by summing up $\sum_j P_{Sj}\,\pi\,r^2{}_j$ values for all postulated scenarios;
3. Obtain the *Population density* data based on the roadway segment location;
4. Multiply the last three steps results together for each roadway segment. The result gives the expected number of people severely impacted:

$$N_{fi} = P_i\,.\,D_i\,.\sum_j P_{Sj}\,\pi\,r^2{}_j\ ; \tag{4.8}$$

5. Compute the overall population risk expected for all road segments by the summing the results in step; and
6. Compare the population risks for different route alternatives.

4.3 Case Study for Central New Jersey

We chose Middlesex County in State of New Jersey for the study area. Based on the spatially aggregated demand model results from Chapter 3, Middlesex County has the highest potential hydrogen demand compared to other counties in the state. Data used in this study were assembled from a variety of resources. Knowledge acquisition was accomplished through discussions with experts of related fields of study, surveying of authenticated literature, and analysis of historical data.

Four criteria were defined with their sub-criteria: *Land Availability*, *Transportation Risk*, *Primary Energy Source Availability*, and *Entertainment Facilities*. We assumed air quality was not significantly different in each location of Middlesex County so it was not considered in our analysis. The criteria and sub-criteria were chosen according to experience, experts' opinions, and information from various sources. Also, GIS database development of this study was developed by using criteria and sub-criteria in different data layers (Figures 18-19). All data sources are available for public use (Table 21). A nine-point scale was used for these evaluations as shown in Table 20. The related factors and criteria are shown in Table 22. The data corresponding to these factors and criteria spatial data were created as GIS layers and then used in the analyses in this format.

Table 21. Data types and sources

Level 1Criteria	Level 2 Criteria	Types	Sources
1. Land Availability	1.1 Vacant land	Spatial	New Jersey Geographic network https://njgin.state.nj.us
	1.2 Existing fueling station	Spatial	OpenStreetMap https://www.openstreetmap.org/
2.Transportation Risk	2.1 Major road hydrogen transport risk	Spatial Non-Spatial	NJDOT (NJ Department of Transportation) Developed manually section 4.2.1
	2.2 Local road hydrogen transport risk	Spatial Non-Spatial	NJDOT (NJ Department of Transportation) Developed manually section 4.2.1
3.Primary Energy Sources	3.1 Power line network	Spatial	OpenStreetMap https://www.openstreetmap.org/
	3.2 Landfill	Spatial	Geocoded manually with ARCGIS10.2
4.Entertainment	4.1 Shopping malls	Spatial	OpenStreetMap https://www.openstreetmap.org/
	4.2 Golf courses	Spatial	OpenStreetMap https://www.openstreetmap.org/

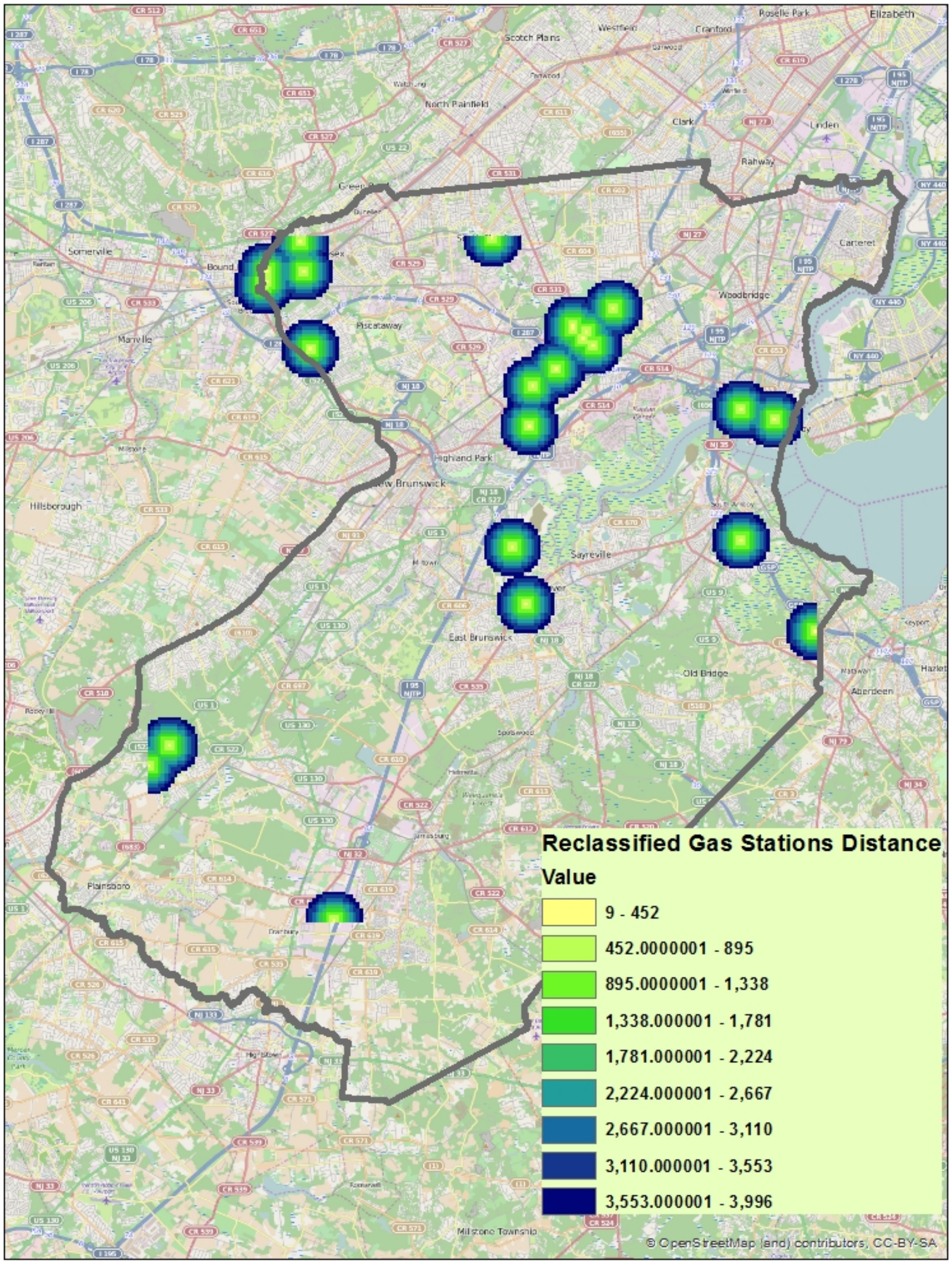


Figure 19. Reclassified Gas Station Distance (feet) raster analysis

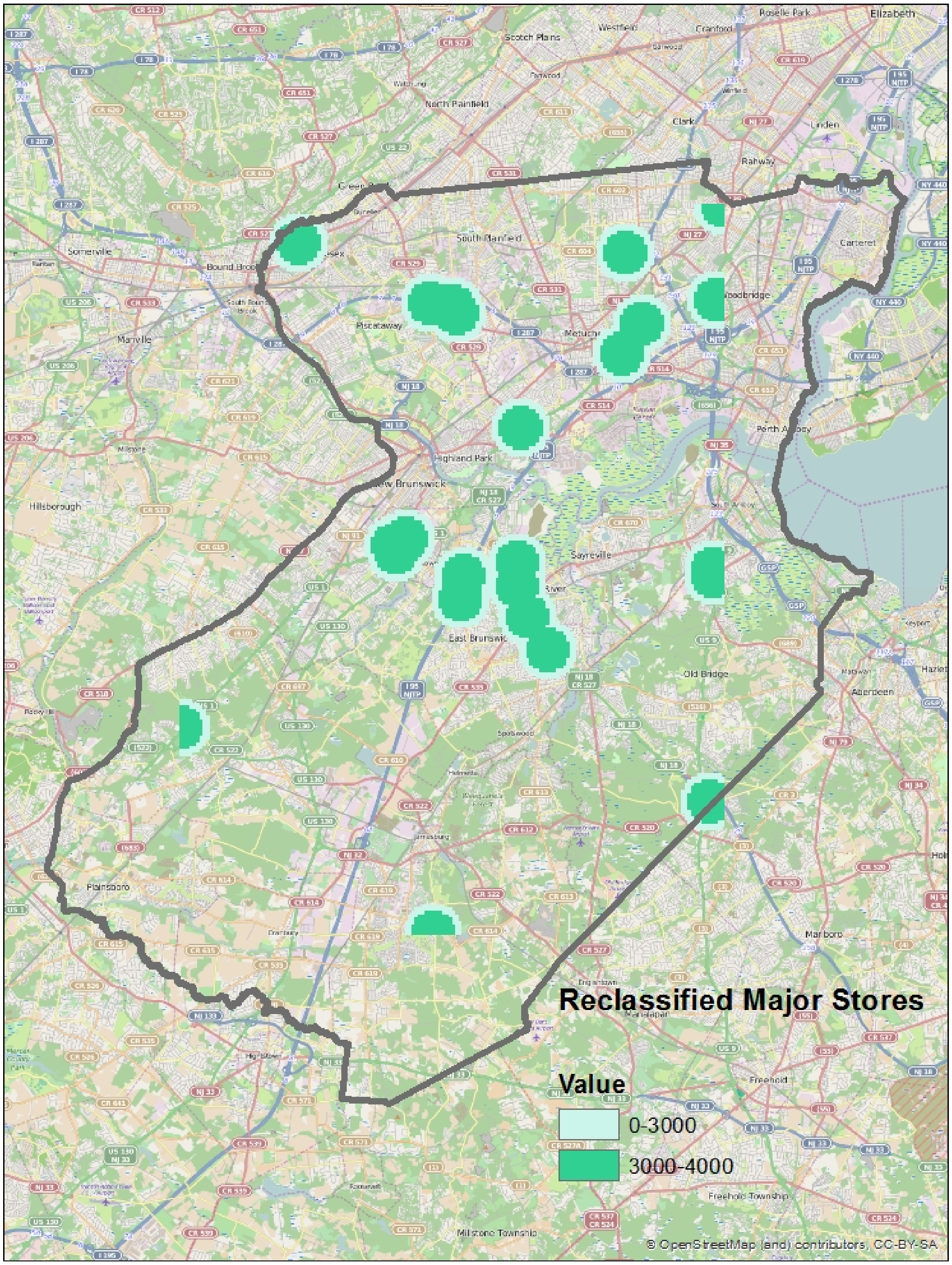


Figure 20. Reclassified Major Stores Distance (feet) raster analysis

Table 22. Standardized score corresponding to criteria attribute values

Level 1 Criteria	Level 2 Criteria	Criteria Attribute Values	Score (Xi)
1. Land Availability	1.1 Vacant Land	0-300 feet	9
		300-1000 feet	1
	1.2 Existing Fueling station	0-250 feet	9
		250-400 feet	6
2. Transportation Risk	2.1 Major Road hydrogen transport risk	<0.01 (Risk of transport)	9
		>0.01	5
	2.2 Local Road hydrogen transport risk	<0.01 (Risk of transport)	9
		>0.01	5
3. Primary Energy Sources	3.1 Power line Network	0-300 feet	9
		300-1000 feet	7
	3.2 Landfill	0-500 feet	9
		500-2000 feet	5
4. Entertainment	4.1 Shopping Malls	0-3000 feet	9
		3000-4000 feet	7
	4.2 Golf Courses	0-3000 feet	9
		3000-4000 feet	6

A standardized eigenvector is extracted from each comparison matrix to assign weights to each criteria and sub-criteria. These weights give a *suitable value* for each location in GIS. For each level in the hierarchy, it is necessary to know whether the pair-wise comparison has been consistent, therefore, a *Consistency Ratio* (CR) can be used. We used Microsoft Excel to calculate the AHP weights and ESRI ArcGIS 10.2 software to build the GIS database. ArcGIS Model Builder was used to automate suitability analysis in the model. Tables 23-26 show results for the calculated criteria weights. The consistency ratio is below 0.1 for all the weight calculations, which shows it’s acceptable for using it in suitability modeling. Table 27 shows the total overall weight calculation combining all criteria weights.

Table 23. Computation of the criteria weights for hydrogen fueling station suitability

Suitability Criteria	Land Availability	Transportation Risk	Primary Energy Sources	Entertainment	Weight
Land Availability	1	1/2	2	4	0.31
Transportation Risk	2	1	1/3	3	0.28
Primary Energy Sources	1/2	3	1	2	0.32
Entertainment	1/4	1/3	1/2	1	0.09

Table 24. Computation of the criteria weights forland availability

Suitability Criteria	Vacant Land	Existing Gas Station	Weight
Vacant Land	1	1/5	0.17
Existing Gas Station	5	1	0.83

Table 25. Computation of the criteria weights for transportation risk

Suitability Criteria	Major Road Hydrogen Transport Risk	Local Road Hydrogen Transport Risk	Weight
Major Road Hydrogen Transport Risk	1	6	0.86
Local Road Hydrogen Transport Risk	1/6	1	0.14

Table 26. Computation of the criteria weights for primary energy sources

Suitability Criteria	Power line Network	Landfill	Weight
Power line Network	1	1/3	0.25
Landfill	3	1	0.75

Table 27. Overall weights of criteria for hydrogen fueling station suitability

Level 1		Level 2		Overall Weight
Criteria	**W1**	**Criteria**	**W2**	**W1*W2**
Land Availability	0.31	Vacant Land	0.17	0.0527
		Existing Fueling Station	0.83	0.2573
Transportation Risk	0.28	Major road hydrogen transport risk	0.86	0.2408
		Local road hydrogen transport risk	0.14	0.0392
Primary Energy Sources	0.32	Power line network	0.25	0.08
		Landfill	0.75	0.24
Entertainment	0.09	Shopping malls	0.5	0.045
		Golf courses	0.5	0.045

We assigned attribute values for each criteria and then calculated *suitability* based on such values. For example, all zones within 3000 feet from a shopping mall were assigned a suitability score of 9 (Table 22). All other criteria had the same suitability scoring method except for *Transportation Risk*. This criterion was calculated for each road as described in section 4.2.1. Roads with risk less than 0.01 score were assigned a value of 9; those with risk more than 0.01 were assigned a suitability score of 5. We illustrate the process of calculating the transportation risk for one specific road in Middlesex County, NJ. This process was performed for most roads in Middlesex County by using our scoring procedure.

In this example, we assume the LH2 truck is the only transportation mode for hydrogen fuel delivery. The LH2 truck *(e.g.,* Linde Corporation, what is the town, NJ) has a capacity of 53 m^3 or about 4000 kg of LH2 (-253°C, 0.13 MPa). It is used regularly to deliver LH2 from a storage depot to the site of an end-use technology (*e.g.,* hydrogen filling station). The objective is to calculate the risk (in terms of number of fatalities for an accident scenario) for a specified roadway route. Roads were chosen based on their crash rates (historical data from 2007-2009, add source of data [76]). All road segments have different risk levels based on where they are located (different population density) and on their tabulated crash rates. Furthermore, it is better to analyze *Transportation Road Risk* using road segments rather than the total length of road for the proposed route. Since the AADTT was not available for the majority of roadways in our study area, the crash rate was calculated based on an overall AADT. AADT data for Middlesex County was obtained from NJDOT (NJ Department of Transportation) Straight Line Diagrams (SLD) [75]. As mentioned earlier, there are two types of hydrogen release conditions: *Instantaneous* and *Continuous*. Each has *accident outcomes* along with their probabilities (P_{Sj}). These probabilities were calculated in using and event tree analysis and are shown in Table 28 [44]. We used both historical data and expert opinions to determine the potential impact area. Table 29 shows the data for the *radius of impact area* for accident scenario, j (r_j), in terms of miles [44].

Table 28. Accident outcome probabilities for LH2 truck [44]

Release Scenarios	**Accident Outcomes**	**Conditional Probabilities**	**Mean**
Instantaneous release	Early explosion	0.036	2,3E-06
	Fireball	0.144	9,2E-06
	Pool fire	0.0064	4,1E-07
	Late explosion	0	1,8E-09
	Flash Fire	0.0001	7,4E-09
Continuous release	Jet fire	0.4	2,6E-05
	Pool fire	0.0064	4,1E-06
	Late explosion	0.0014	9,2E-08
	Flash fire	0.0058	3,7E-07
No effect		0.3423	2,2E-05
Overall frequency		1.0000	**6.4E-04**

Table 29. Radius of impact for an accident outcome

Hydrogen Release Type	**Accident Outcomes**	**Conditional Probabilities**	**Radius of Impact (mi.)**
Instantaneous release	Early explosion	0.036	0.447
	Fireball	0.144	0.072
	Pool fire	0.0064	0.04
	Late explosion	0	0.137
	Flash Fire	0.0001	1.783
Continuous release	Jet fire	0.4	0.045
	Pool fire	0.0064	0.04
	Late explosion	0.0014	0.0256
	Flash fire	0.0058	0.1145

The *Hydrogen Severity Index* for all possible scenarios would be 0.028778 and it is a constant.

$$\sum_j P_{Sj}\, \pi\, r^2{}_j = 0.028778 \qquad (4.9)$$

Table 30 shows the *population risk* or *hydrogen transportation risk* calculated for Route 27 from Milepost 4.11 to 27.29 (the road extent present in Middlesex County, NJ).

Because insufficient Hazmat data involving crashes exists for this road, we assumed equal values for all roadway segments. Year 2007 – 2009 values were used in this study.

$P_i\ (H|C)$ = Conditional probability for hazmat release given a crash occurs in road segment i

$$= \frac{\text{Hazardous Material Crashes in Middlesex county (2007−2009)}}{\text{All vehicle crashes in Middlesex County (2007−2009)}} = \frac{146}{92265} = 0.00158 \qquad (4.10)$$

Note the crash rate unit is (1/10^6 Veh-Mile).

Table 30. Summary of input parameters and the risk results calculated for LH2 transportation segments of Route 27 in Middlesex County, NJ

Road Segment (Milepost)	City	AADT	Crash Rate	Length	P (H|C)	Probability of release	Population Density	Hydrogen Severity Index	Population Risk
4.11 - 6.9	South Brunswick	10484	1.06	2.79	0.00158	2.9574E-06	1008.7	0.028778	8.5848E-05
6.9 - 10.2	South Brunswick	22553	3.17	3.3	0.00158	0.000010461	1008.7	0.028778	0.00030367
10.2 - 16.55	North Brunswick & New Brunswick	38487	1.31	6.35	0.00158	8.3185E-06	6203.45 (Average)	0.028778	0.00148504
16.55 - 20.82	Highland Park & Edison	17520	9.7	4.27	0.00158	0.000041419	5428.55 (Average)	0.028778	0.00647059
20.82 - 21.62	Edison	14386	10.55	0.8	0.00158	0.00000844	3243	0.028778	0.00078768
21.62 - 22.66	Metuchen	23074	8.26	1.04	0.00158	8.5904E-06	4684.8	0.028778	0.00115815
22.66 - 24.69	Edison & Metuchen	21934	11.92	2.09	0.00158	2.49128E-05	3963.9 (Average)	0.028778	0.00284188
24.69 - 27.29	Woodbridge	19780	2.91	2.6	0.00158	0.000007566	4224.5	0.028778	0.00091982
								Overall Risk	**0.01405268**

After calculating weights and assigning score values for each criteria, the suitability for a hydrogen fueling stations (site) were calculated by using equation (4.2) and then implemented in ArcGIS Model Builder (Figure 21). The data raster calculator can find a suitable hydrogen fueling station by integrating all the criteria layers with their associated weights and scores. It then provides a list of suitable locations with their level of suitability. The higher value for the *suitability index*, the more suitable is that site for a hydrogen fueling station. We used Boolean values for constraints. A location value of 0 indicated that site was not suitable for hydrogen fuel station. In our model flood zones, were the only constraints, but more contrarians can be added to this model.

All map coordinates were based on the *NAD 1983 State Plane New Jersey FIPS 2900 Feet* geographic system. Figure 22 shows the model results for the suitable locations of hydrogen refueling stations in NJ. This suitability map provides a decision-making tool for planners and communities. In next chapter we will discuss how we choose the optimal location among suitable locations to maximize the demand coverage.

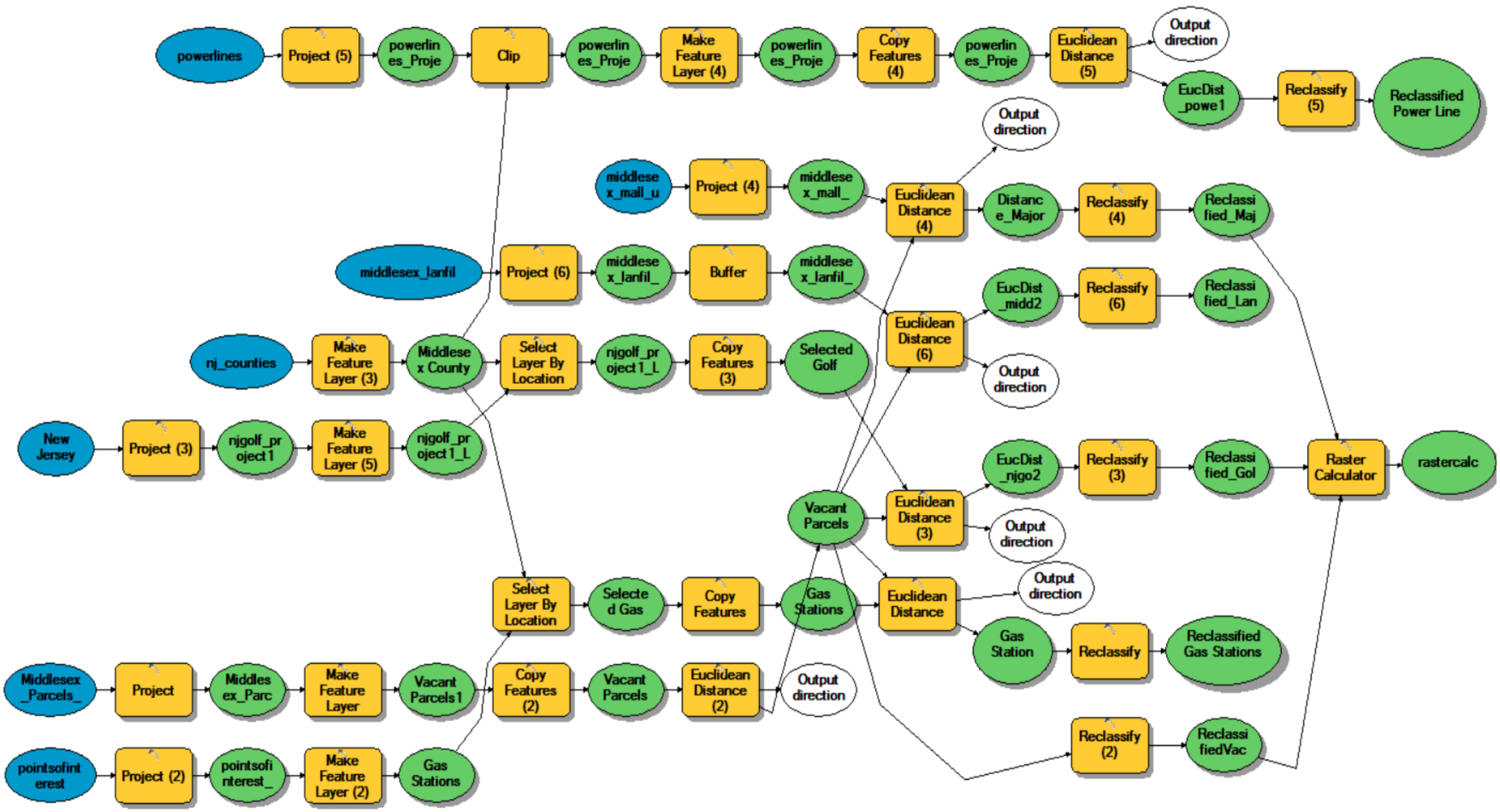


Figure 21. Overall view of suitability model for selecting the location of a hydrogen fueling station using ARCGIS Model Builder

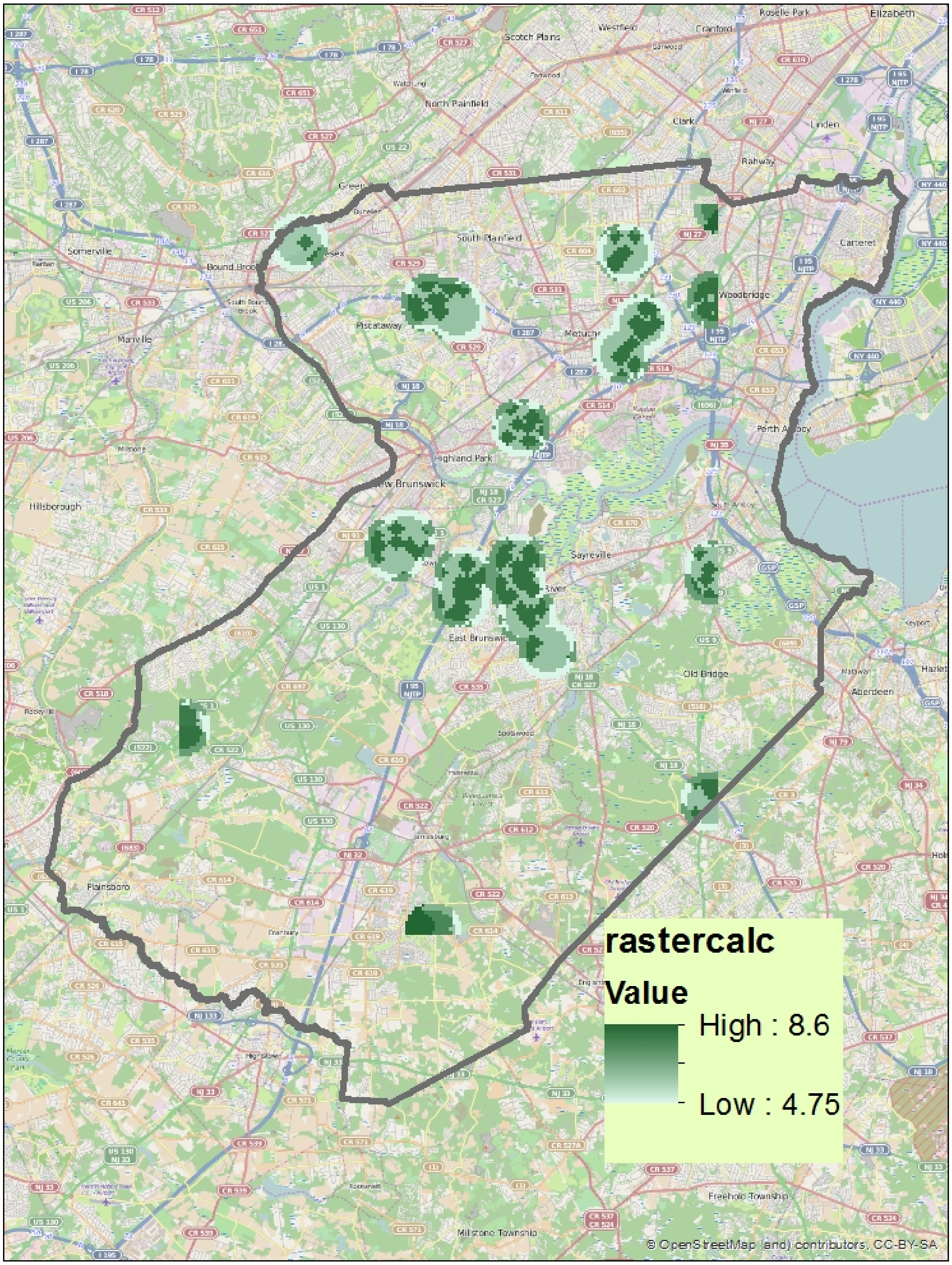


Figure 22. Suitable location model results for hydrogen fueling station in Middlesex County, NJ

4.4 Conclusion

In this study, a Geographic Information System (GIS)-based Multi-Criteria Decision Making (MCDM) tool was developed to find suitable locations for hydrogen fueling stations by considering factors such as land availability, air quality, energy source availability, for example. In this analysis, customer demand coverage is maximized that the model will choose the locations in which all or a high % of estimated customer demand is within a specified impedance cutoff. This scenario was carried out using Analytic Hierarchy Process (AHP), a multi-criteria decision analysis approach. We integrated AHP with the suitable locations identified by GIS analysis.
Also, we proposed a methodology to calculate hydrogen road transport risk so it can identify which routes have higher hydrogen transport risk than others. In this model we only considered the crash-initiated release for risk calculation in hydrogen delivery. In order to calculate overall hydrogen transportation risk we calculated the probability of hydrogen release and then, designed the consequence model for different accident scenarios.

Chapter 5- Development of Hydrogen Infrastructure Optimization Model with Uncertain Demand in Micro View (Street Level) - Location Allocation

5.1 Introduction

The lack of hydrogen fueling stations is a major barrier to the introduction of fuel cell vehicles. Given the high cost of constructing hydrogen fueling stations, an initial strategy might be to build at first the fewest number of fueling stations since the demand at this stage is uncertain. Although several studies have addressed the general question of how many stations are needed, the literature has been largely silent on how to relate the location of stations to a sufficient number of hydrogen stations. In this chapter, we propose a GIS-based location allocation model with uncertain demand. The model is designed a street level which maximizes demand coverage at this scale.

Recently, there have been attempts to combine GIS with optimized location allocation techniques [56]. In most of these studies, integration was achieved sequentially or in a linear fashion; that is, optimized allocation was performed independently using various types of optimization models, then the results of the optimization was exported to a GIS application for mapping and display [77-82]. Our approach imposes the integration simultaneously rather than sequentially, and location allocation optimization is done internally within the GIS application. The proposed model is based on the capacitated *Maximal Covering Location Problem* (MCLP) [83-86]. The best-known facility-location models [86]—such as the median, covering, center, and fixed-charge models—all treat the demand for facilities as if it were located at specified points.

The contribution of this chapter is utilizing the results from chapter 4 and finds the optimal locations for hydrogen fueling station among suitable locations at the micro level. There is much research dealing with choosing optimal locations for hydrogen fueling stations [87-91]. However, none of these accounts consider and provide approaches for modeling site suitability which is essential for implementing real projects.

Since the demand of hydrogen fuel is stochastic, Geometric Brownian Motion (GBM) was used to model the uncertainty of the demand for hydrogen and to measure the risk of future hydrogen fuel shortages. By definition, a Brownian Motion is a Markov process, which implies that only current information is useful in forecasting the future path of the process. This modeling approach provides an analytical framework for siting early hydrogen fueling stations. Initial results suggest a few strategically sited stations could be sufficient to satisfy a large number of prospective consumers. Subsequent years are used for expanding the number and locations of the hydrogen fuel stations as demand grows.

5.2 Problem Description

The problem addressed in this chapter is to choose the optimal location for hydrogen fueling stations. In Chapter 4 a Geographic Information System (GIS)-based Multi-Criteria Decision Making (MCDM) tool was developed to find the suitable locations for hydrogen fueling station by considering factor such as land availability, air quality, energy source availability, etc. The results will be used to choose the optimal locations among suitable locations for location allocation model by maximizing the customer demand coverage so it will chooses the locations such that all or the greatest amount of estimated customer demand is within a specified impedance cutoff. Also the model should capture the hydrogen demand uncertainty and a risk of having hydrogen fuel shortage in future should be measured.

5.3 Problem formulation

The proposed model is based on the capacitated *Maximal Covering Location Problem* (MCLP). Our formulation is based on the strong form of the capacitated p-median problem and is shown below. The objective function (through the use of the binary constant, c_{ij}) maximizes the demand assigned to a hydrogen fueling station within the coverage distance, *S*. Constraint limits the total number of hydrogen fueling station to no more than *p* (*constraint type 5.2*), while *constraint type (5.3)* insures all hydrogen demand points are assigned to a hydrogen fueling station. According to *type (5.4) constraints*, a demand point means a hydrogen fueling station must be constructed at the point. Finally, the fueling station capacity limits are imposed by *constraint set (5.5)*, with the integrality restriction imposed by *sets (5.6)* and *(5.7).*

$$\text{Maximize} \sum_{i\in I}\sum_{J\in L} c_{ij}a_i x_{ij} \tag{5.1}$$

Subject to,

$$\sum_{j \in J} y_j \leq p \tag{5.2}$$

$$\sum_{j \in J} x_{ij} = 1 \quad \forall\, i \in I \tag{5.3}$$

$$x_{ij} \leq y_j \quad \forall\, i \in I\,, j \in J \tag{5.4}$$

$$\sum_{i \in I} c_{ij} a_i\, x_{ij} \leq K_J \quad \forall\, j \in J \tag{5.5}$$

$$y_j = [0,1] \quad \forall j \in J \tag{5.6}$$

$$x_{ij} = [0,1] \quad \forall i \in I\ , j \in J \tag{5.7}$$

Where,

I = the index set of all demand points,

J = the index set of all potential locations for hydrogen fueling station,

a_i = the amount of demand at point i,

K_J = the capacity of hydrogen fueling station,

P = the number of hydrogen fueling stations to be sited,

S = the maximum service distance or time,

d_{ij} = the travel distance or time from j to i,

$$c_{ij} \begin{cases} 1, & if\ d_{ij} \leq S, \\ 0, & otherwise, \end{cases}$$

$$x_{ij} \begin{cases} 1, & \text{if the demand at point i is served by fueling station at } j, \\ 0, & \text{otherwise,} \end{cases}$$

$$y_j \begin{cases} 1, & \text{if a hydrogen fueling station is sited at } j, \\ 0, & \text{otherwise,} \end{cases}$$

One important issue in mathematically formulizing the capacitated MCLP is the measurement of *demand*. A region of analysis is divided typically into small spatial units, or polygons. Each unit can be assigned an attribute category such as city, fire response zone, or census tract. We used the spatially aggregated demand model discussed in section 3.3.4. In the current application we use census tracts as the units, which calculates the demand at the micro level. The second issue is *where* the facilities can be located potentially. In this study, we applied the (GIS)-based Multi-Criteria Decision Making (MCDM) tool detailed in chapter 4; so, only a finite set of potential facility locations was be considered.

Unfortunately, the p-median problem has some limitations in practice. That is, given N candidate facilities and M demand points with a weight, we must choose a subset of the facilities, P, such that the sum of the weighted distances from each M to the closest P is minimized or maximized. This is a combinatorial problem of the type, *N Choose P*, for which the solution space grows extremely large. Optimal solutions cannot be obtained by examining all the possible combinations. For example, even a small problem like 100 choose 10 contains over 17 trillion combinations. In this situation, heuristic approaches can be used to solve location-allocation problems. A heuristic is a technique designed for solving a problem more quickly when classic methods are too slow, or for finding an approximate solution when classic methods fail to find any exact solution.

There are many studies which provide solutions for the p-median problem with different heuristics methods [92]. Heuristics are solution approaches based on some type of search strategy. There is no guarantee the strategy will find the optimal solution, but good heuristic designs are likely to perform well in terms of speed and quality [92] for the solutions identified. A well-known heuristic approach was developed for the p-median problem by Teitz and Bart [93], commonly referred to as an interchange heuristic. This is a neighborhood search approach that begins with a randomly generated configuration of p sites, and an associated allocation of each demand area to its closest fueling station. The starting solution might not be a good solution for our maximization problem, but it starts with a feasible solution where all constraints are satisfied. The heuristic strategy can be thought of as an attempt to find improvements to the starting solution using a process called *swapping* or *interchange* [92].

When an improvement is found, it is adopted and the search continues, but it is focused on finding improvements to the newly adopted solution. When the search fails to find any improvements, the heuristic process stops and the best solution can be found in the results. The interchange heuristic is effective because it is able to focus on the selection of p sites, as the optimal allocation is easy to derive given p facilities.

This problem can be solved in LINGO or LINDO (Software package for linear programming, integer programming, nonlinear programming, stochastic programming and global optimization). However, we opted to use GIS to find suitable locations and to solve the problem with ARCGIS Network Analyst location allocation solver. The location-allocation solver has options to solve a variety of location problems, such as to minimize weighted impedance, maximize coverage, or achieve a target market share. In order to have accurate results, a detailed road network data set should be created or retrieved from valid sources. ArcGIS can only solve this problem deterministically. However, as discussed above hydrogen fuel demand is stochastic and we used Geometric Brownian Motion (GBM) to model demand uncertainty and to measure the risk of having future hydrogen fuel shortages. By definition, Brownian Motion is a Markov process, which implies only current information is useful in forecasting the future path of the process. The GBM process to model hydrogen demand satisfies the following stochastic differential equation:

$$da_t = \mu\, a_t + \sigma a_t\, dW_t \tag{5.8}$$

Where,

a_t is hydrogen fuel demand (kg),

μ is hydrogen fuel demand each period (yearly) drift,

σ is the hydrogen fuel demand each period (yearly) volatility

W_t is standard Brownian Motion,

$dW_t = \sqrt{dt}$, and

e is standard normally distributed.

Since no historical data available exists on hydrogen demand for transportation in NJ, we made our best “guesstimates” on the drift and volatility of the hydrogen demand GBM process and assumed an increasing trend according to a GBM. Monte Carlo sampling technique was applied to generate samples of the stochastic variables. This model generates multiple demand scenarios, and for each scenario ARCGIS Network Analyst location allocation solver computed a deterministic output. There are two important outputs in our model that can be used to define risk measures: *hydrogen fuel shortage* for each scenario and *percentage of hydrogen fuel market coverage*. Combining all scenario outputs can help us to fit them into a distribution.

5.4 Case Study

We selected Middlesex County, NJ, as the study area based on the results of the spatially aggregated demand model in previous chapter. Middlesex County has the highest potential hydrogen demand compared to other NJ counties. In order to estimate deterministic values for hydrogen demand in the future, we developed a spatially aggregated demand model (described in section 3.3.4.). Demand estimation was made from the U.S. Census Bureau 2013 data [52]. Regions were based on the 2013 census tracts. The vehicle hydrogen consumption rate was 0.6 kg per day. Population growth rate for each county was calculated based on the growth rate from year 2000 to 2010 from the U.S. Census 2013 data. In order to estimate the hydrogen demand, the factors and key attributes, which influence consumer choice. These were the same as for those identified in section 3: *household income, households with two or more vehicles*, *education*, and *commute distance*. Household income was classified into five different groups (based on U.S dollar annual income) and each scored according to *purchase level of fuel cell vehicles* (Table 13 from chapter 3). The *households* with two or more vehicles category were classified to three different groups (Table 14 from chapter 3). The *education* category was classified based on the number of people with a bachelor's degree or higher (Table 15 from chapter 3). The *commute distance* category was classified to three different groups based on number of households with travel time more than 20 minutes every day (Table 16 from chapter 3). Also, the scores were normalized so that the groups for each attribute were equal to 100%.

Each attribute was weighted based on its level of impact on consumer behavior. The attributes were weighted as follows:

- Household Income (30%)
- Households with two or more vehicles (30%)
- Education (20%)
- Commute Distance (20%)

If we assume the starting market penetration is 5 percent in next 10 years based on a spatially aggregated model, Middlesex County would need 2660 kg hydrogen per day to meet the demand. We assume each fueling station capacity is around 350 kg hydrogen fuel per day, so the ideal number of fueling stations is 8. However, since there is a high percentage of uncertainty in the hydrogen market, we will start with 5 required hydrogen fueling stations and our capacitated (MCLP) model gives an optimal location output (Figure 23). Also, we ran the model with 6 required hydrogen fueling stations (Figure 24). The impedance cutoff is 25 minutes meaning that the hydrogen fueling station locations accessibility shouldn't exceed 25 minutes and the demand coverage must be maximized. In this case study, ARCGIS Network Analyst was used and a network dataset was developed for Middlesex County in order to run the allocation models. The next step was to generate samples of the stochastic hydrogen demand. We assumed hydrogen demand initially was around 2660 kg per day. There were 6 scenarios with different drift and volatility and required number of hydrogen fueling station. For each scenario, 100 samples were generated by Monte Carlo sampling, requiring 600 runs of the allocation model (Table31).

Table 31. Different scenarios with respective drift, volatility and required number of hydrogen fueling stations

Scenario	**Drift**	**Volatility**	**Required # of hydrogen fueling stations**
Scenario 1	0.05	0.2	5
Scenario 2	0.05	0.2	6
Scenario 3	0.08	0.2	5
Scenario 4	0.08	0.2	6
Scenario 5	0.12	0.2	5
Scenario 6	0.12	0.2	6

After running the capacitated (MCLP) model for each scenario with 100 samples of hydrogen demand, we compared the outputs of each scenario with the other scenario outputs. Two important outputs emerged from our model which can be used to measure the risk: the *hydrogen* *fuel shortage* for each scenario and the *percentage of hydrogen fuel market coverag*e. Figure 25 shows the comparison of shortage values for different scenarios in different years using box plots. For Scenario 1, the mean of the shortage demand over time did not change significantly, however, the variance increased (size of the boxes becomes bigger) with time. Scenario 2 had the same specification of hydrogen demand drift and volatility except we added one more hydrogen fueling station. For Scenario 2, the mean decreased (the line inside the boxes) compared to Scenario 1. Scenarios 3 through 6 had trends similar to Scenarios 1 and 2, but the mean for *shortage* increased over time for each scenario. This result indicates the mean and variance increased over the time duration, and by adding a hydrogen fueling station, the means decreased but not the variances. Figure 26 is a similar to plot, except we grouped the results by year. Again, the means of the distributions for each scenario are better predictors of the demand shortage, and the variances become larger over time, resulting in greater uncertainty in meeting demand.

As mentioned earlier Figures 23 and 2 illustrate the optimal locations for 5 and 6 hydrogen fueling stations, respectively, for the MCLP model runs in GIS format. By adding one hydrogen fueling station to a total of 6, greater coverage of the hydrogen fueling demand is achieved. This outcome shows the importance of number and location for optimally achieving demand coverage for hydrogen.

Figures 27 through 29 show the distributions of the shortages. By adding one hydrogen fueling station to Scenarios 1, 3 and 5, their means decrease which is shown in Scenarios 2, 4 and 6. No changes in variances or standard deviations are seen in any case. Also, we plotted the cumulative distribution functions in Figures 30 through 32. Here, we can see that in Scenario 5 (Figure 30), the probability of having a shortage of 1000 kg hydrogen per day is 0.3 or 30 percent. In addition, we plotted the results based on the percentage of hydrogen fuel coverage. This factor had a similar but inverse trend (Figures 33-40). For instance, by adding one hydrogen fueling station to Scenario 1, the percentage of hydrogen fuel coverage increased and there were no changes in the variances between each scenario.

In this study we only used six scenarios with different drift and volatility and for each scenario, 100 samples were generated by Monte Carlo sampling, requiring 600 runs of the allocation model. This approach can be applied in real project with more scenarios which can help decision makers to capture the uncertainties regarding hydrogen fueling station investment.

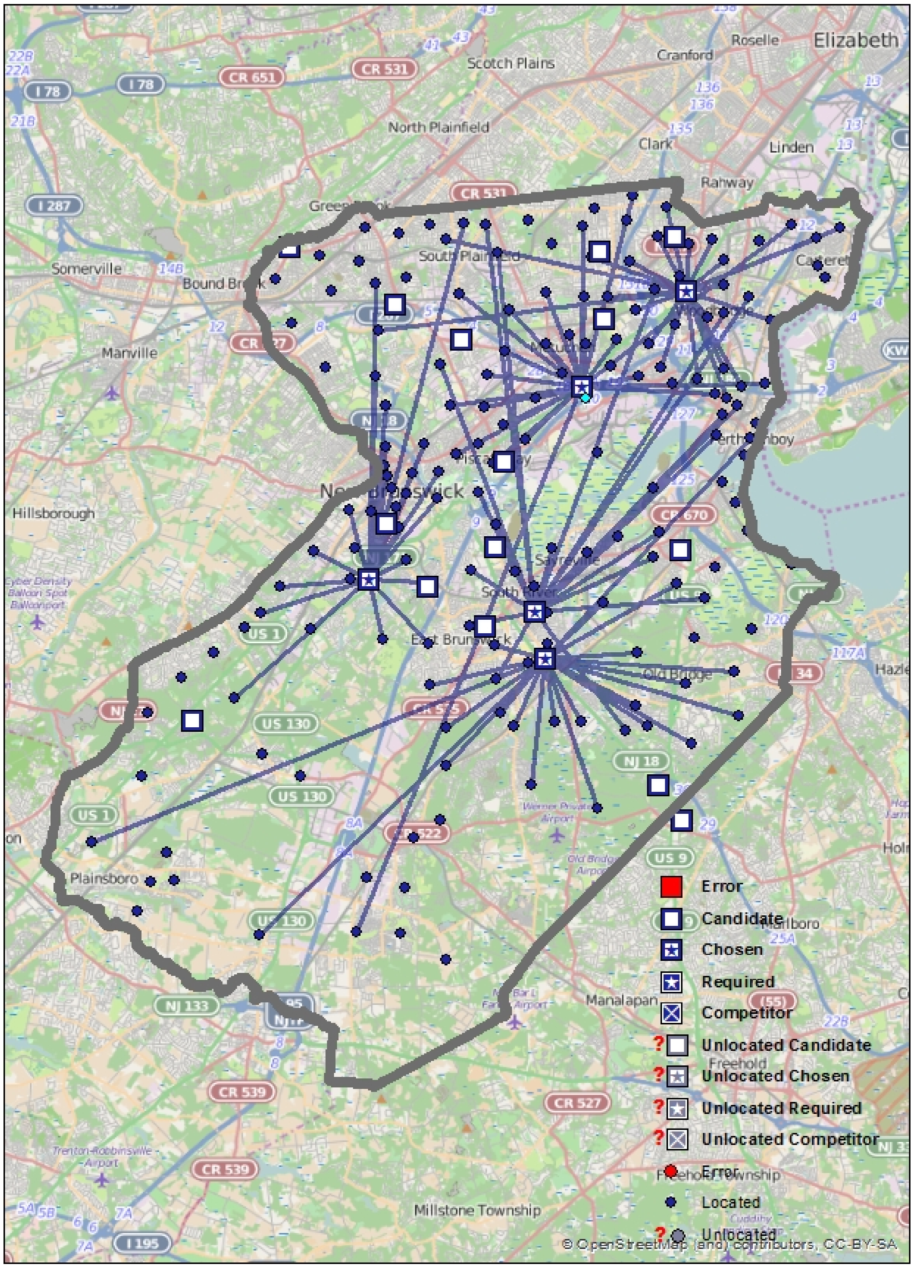


Figure 23. Optimal locations for hydrogen fueling station with 5 required fueling stations for Middlesex County, NJ

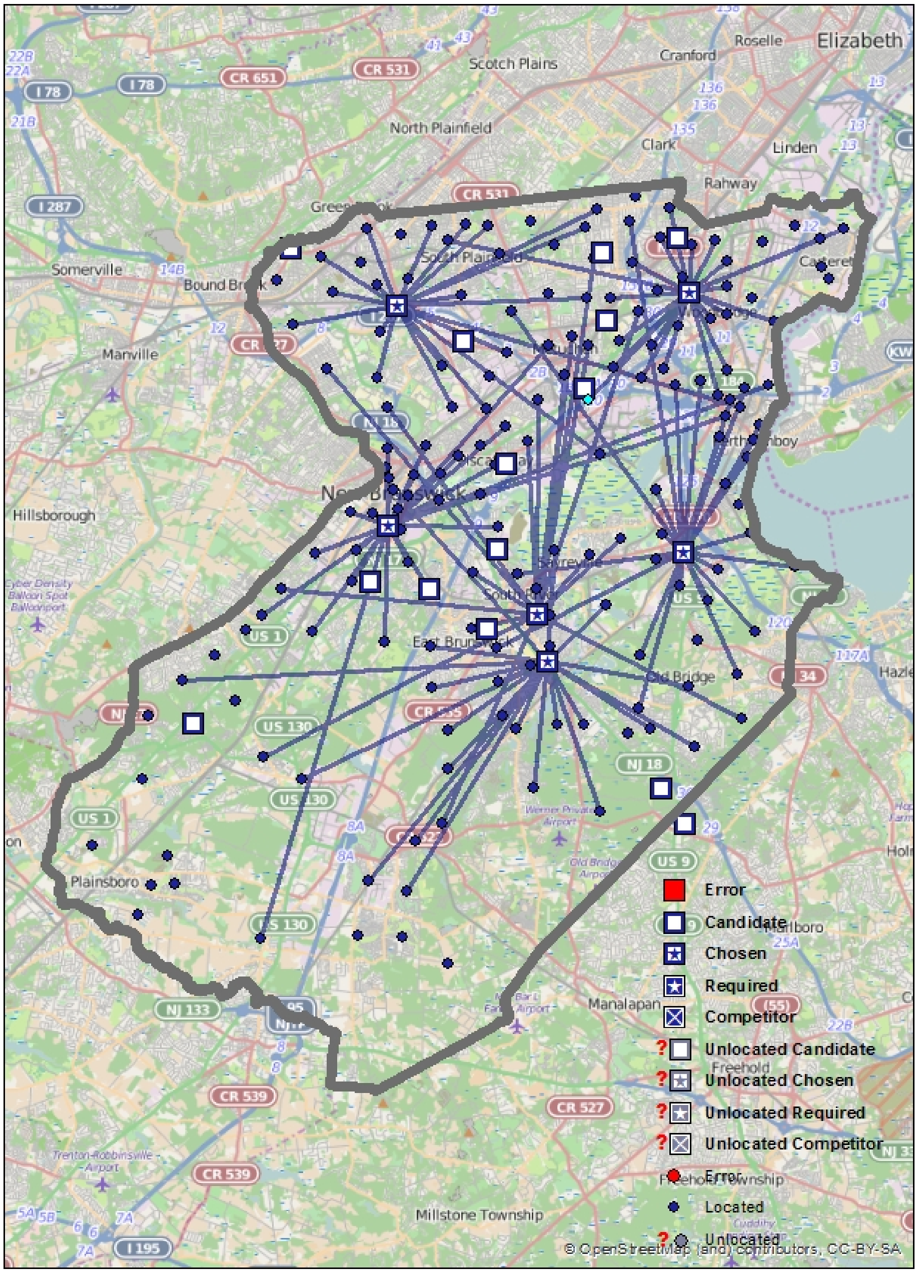


Figure 24. Optimal locations for hydrogen fueling station with 6 required fueling stations for Middlesex County, NJ

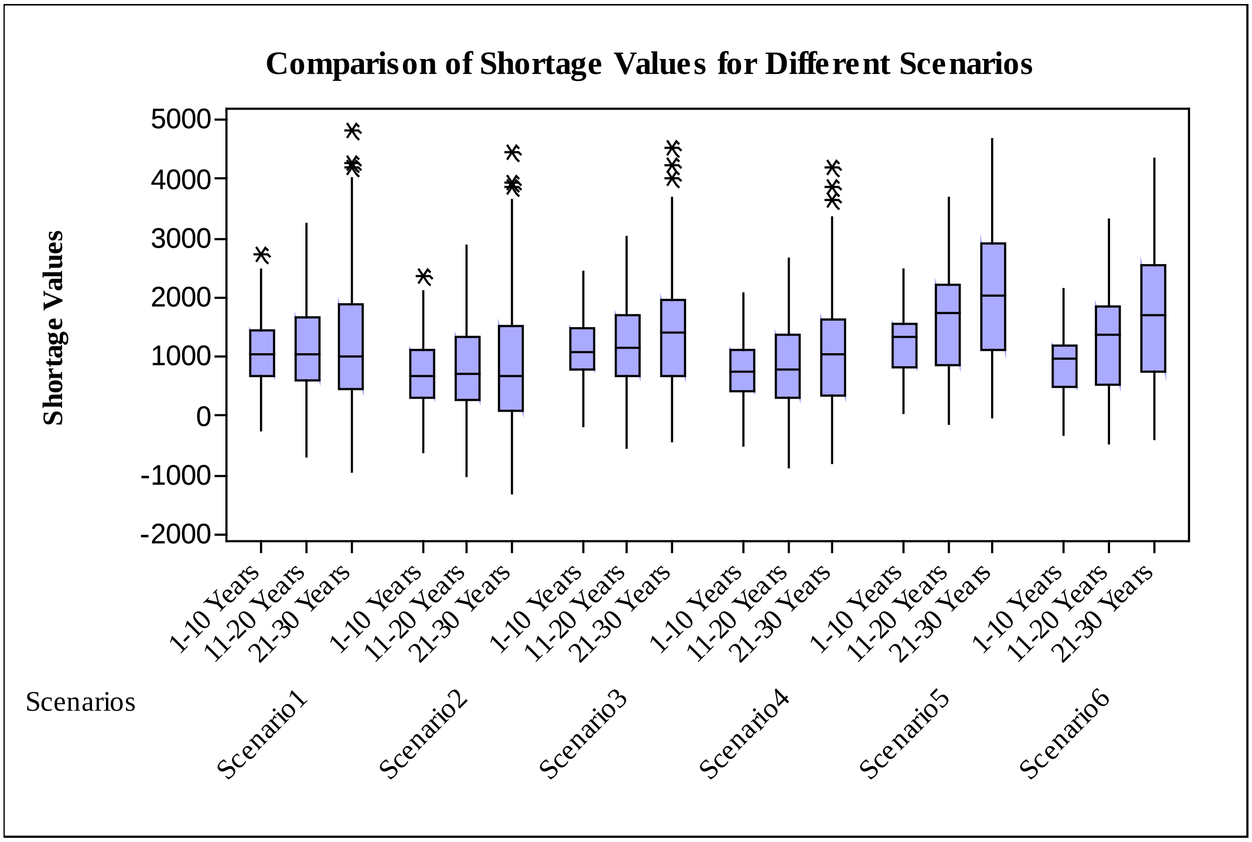


Figure 25. Comparison of hydrogen shortage values for different scenarios

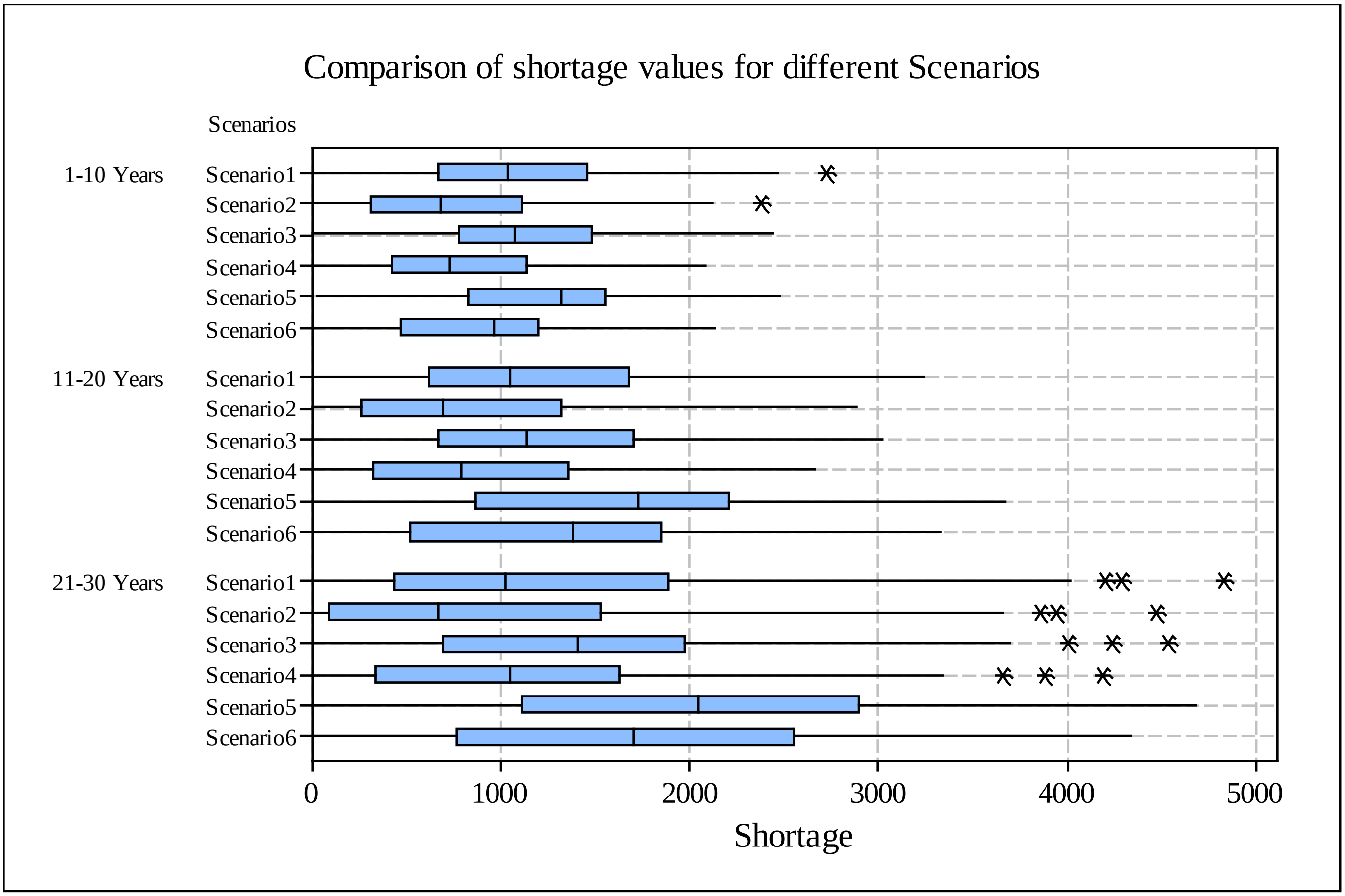


Figure 26. Comparison of hydrogen shortage values for different scenarios by year

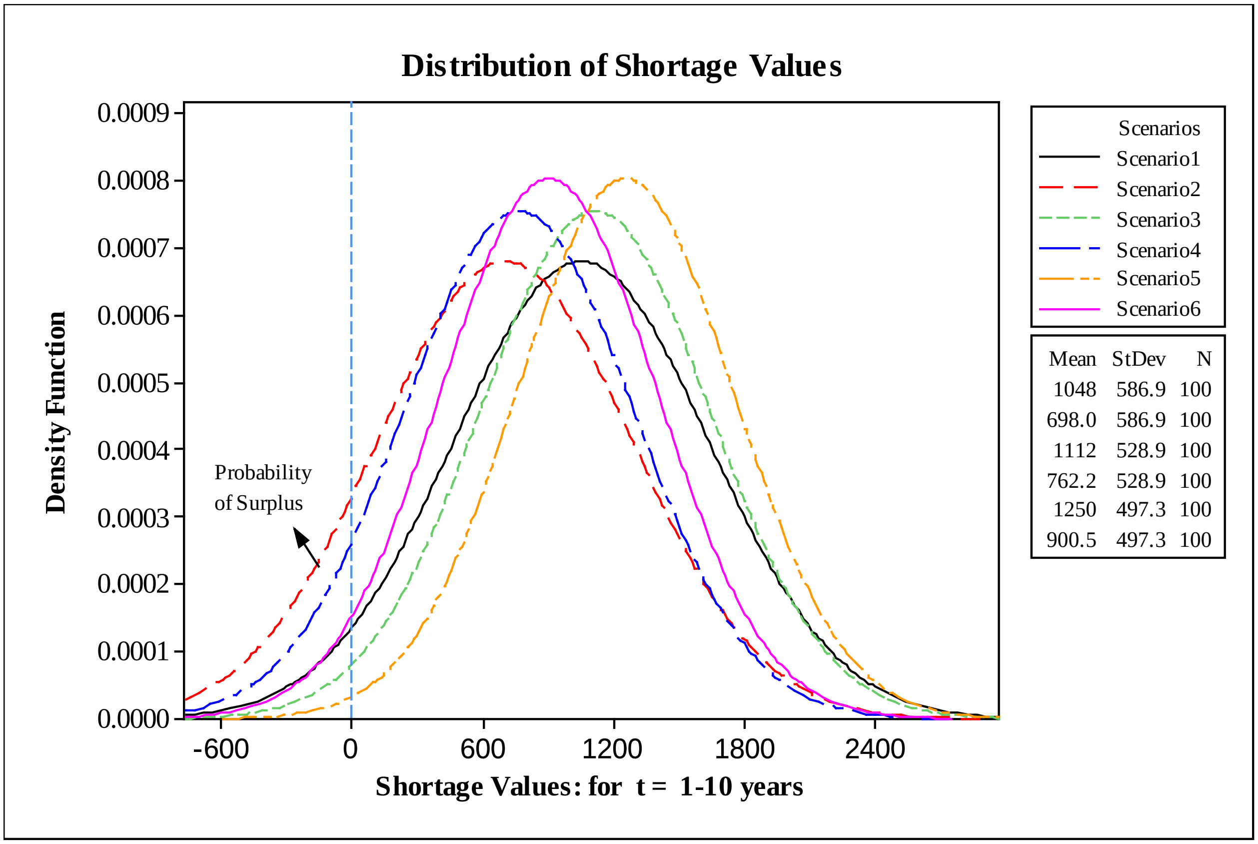


Figure 27. Comparison of the distribution of shortage values for the 1-10 years period

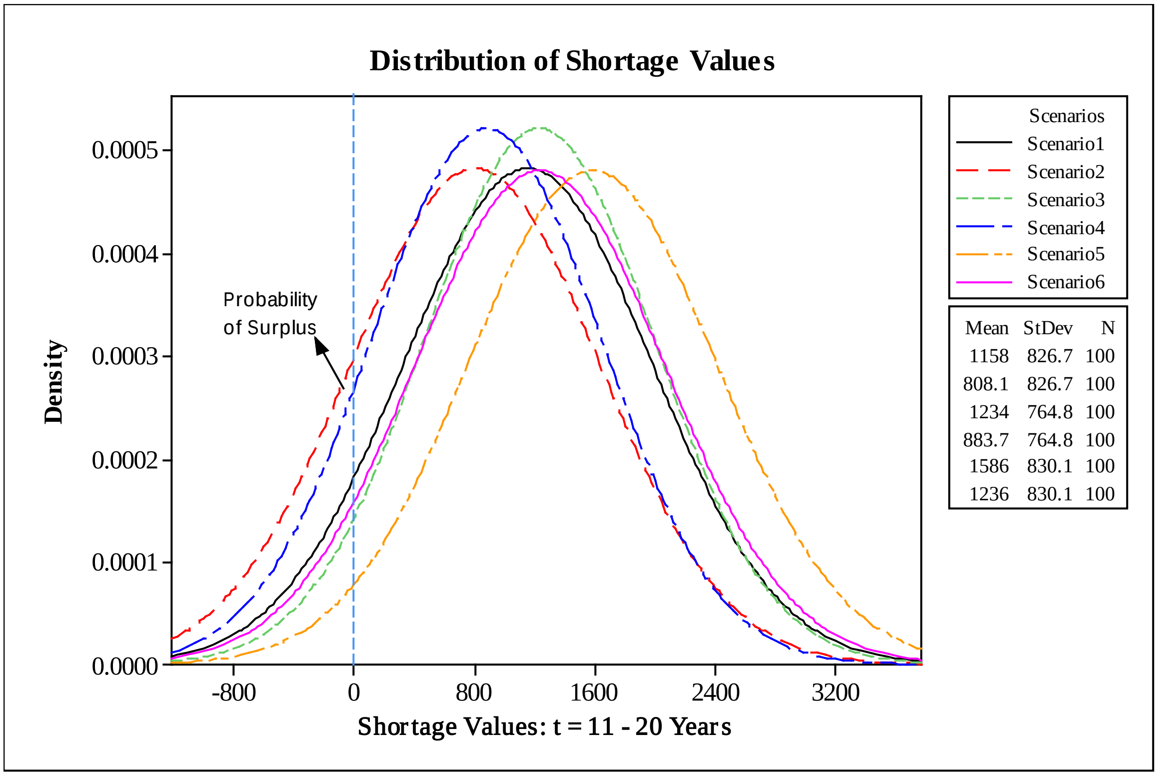


Figure 28. Comparison of the distribution of shortage values for the 11-20 years period

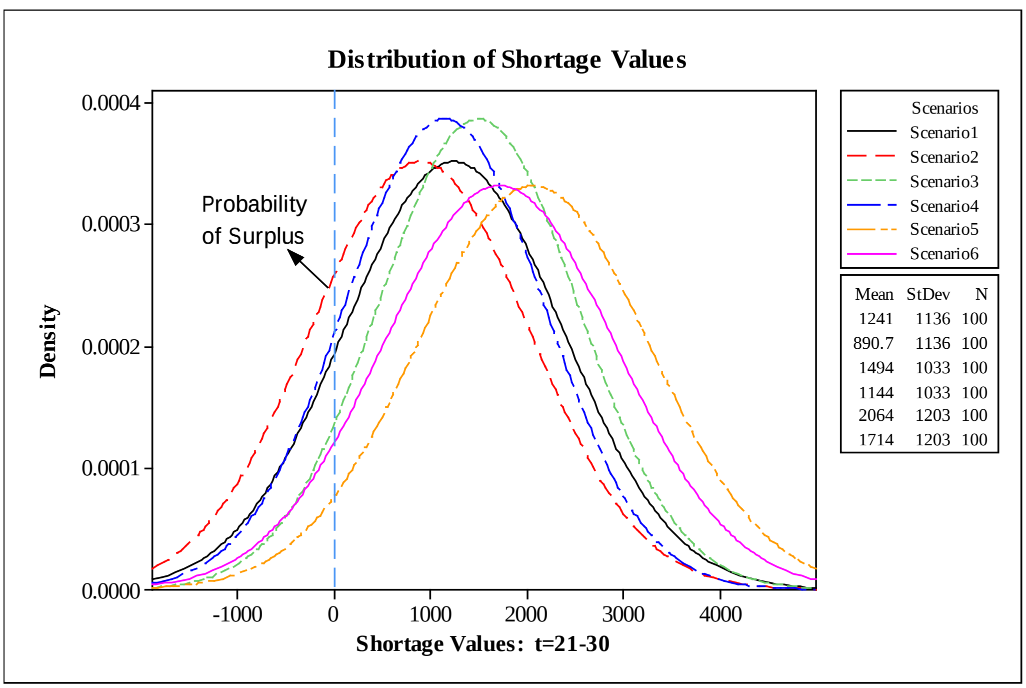
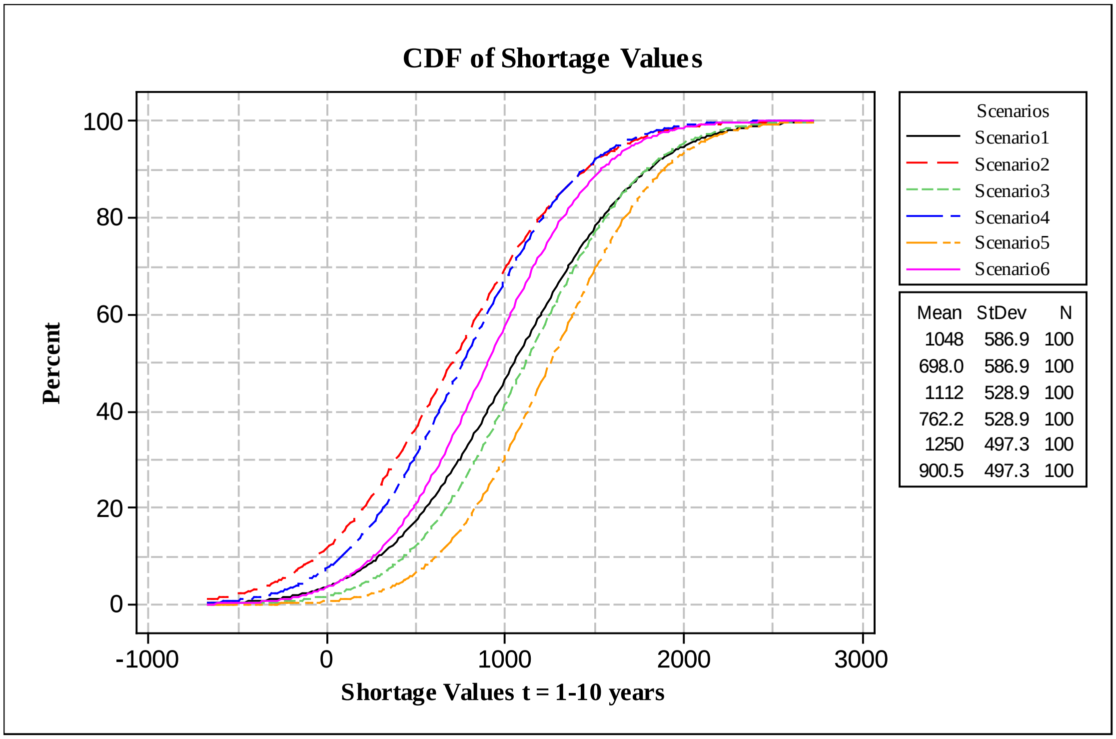


Figure 29. Comparison of the distribution of shortage values for the 21-30 years period



. Comparison of cumulative distribution function of shortage values for the 1-10 years period

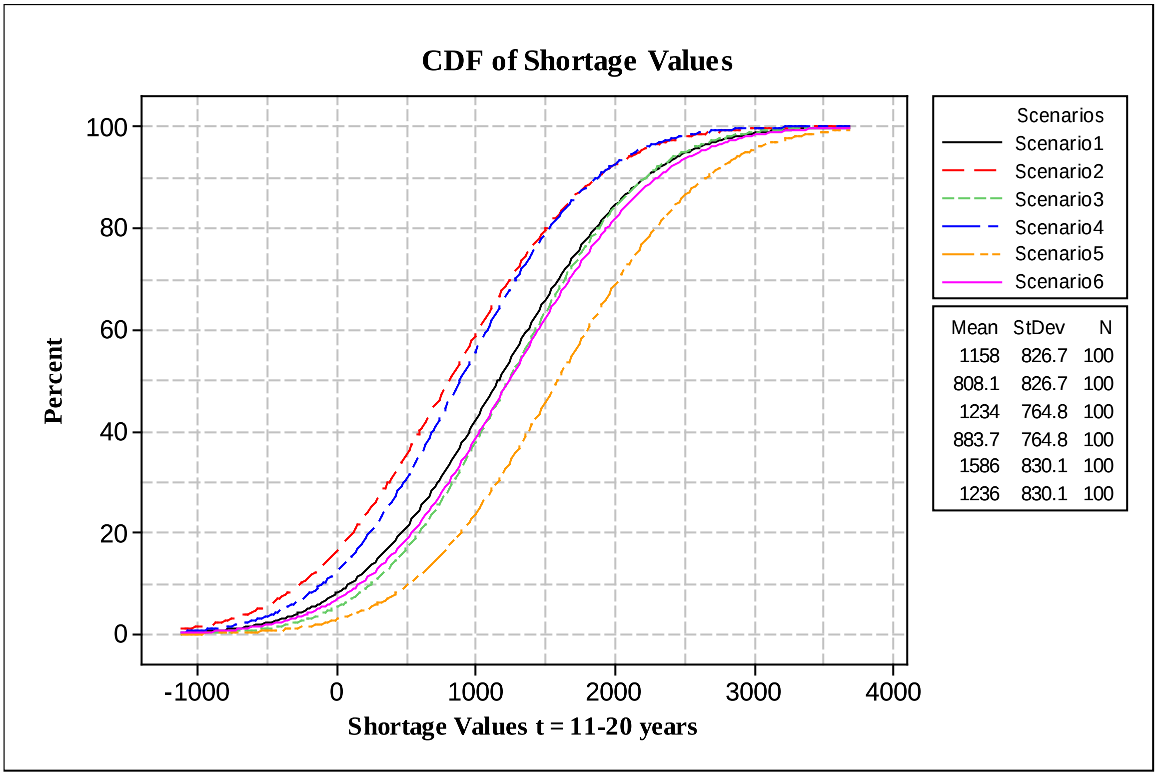


Figure 30. Comparison of cumulative distribution function of shortage values for the 11-20 years period

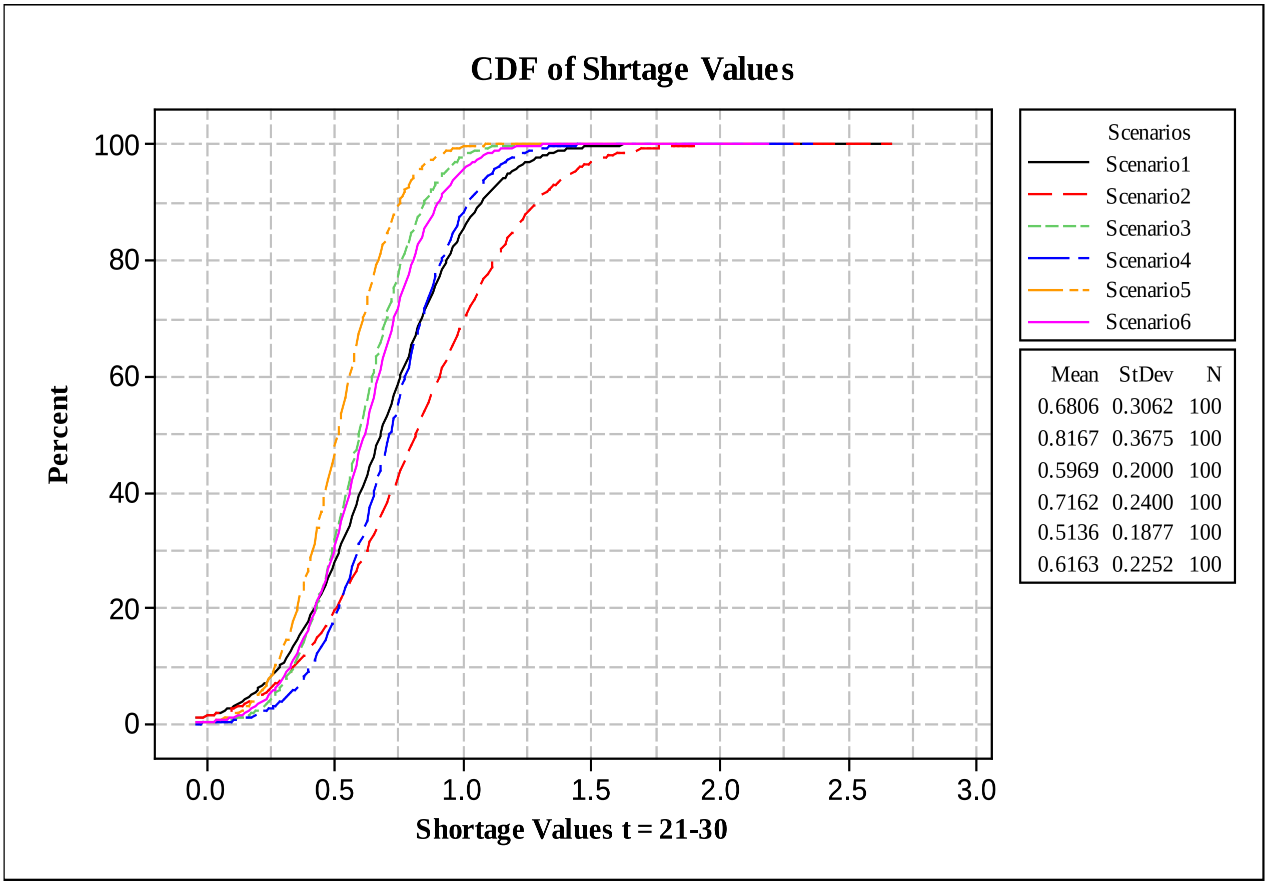


Figure 31. Comparison of the cumulative distribution function of shortage values for the 21-30 years period

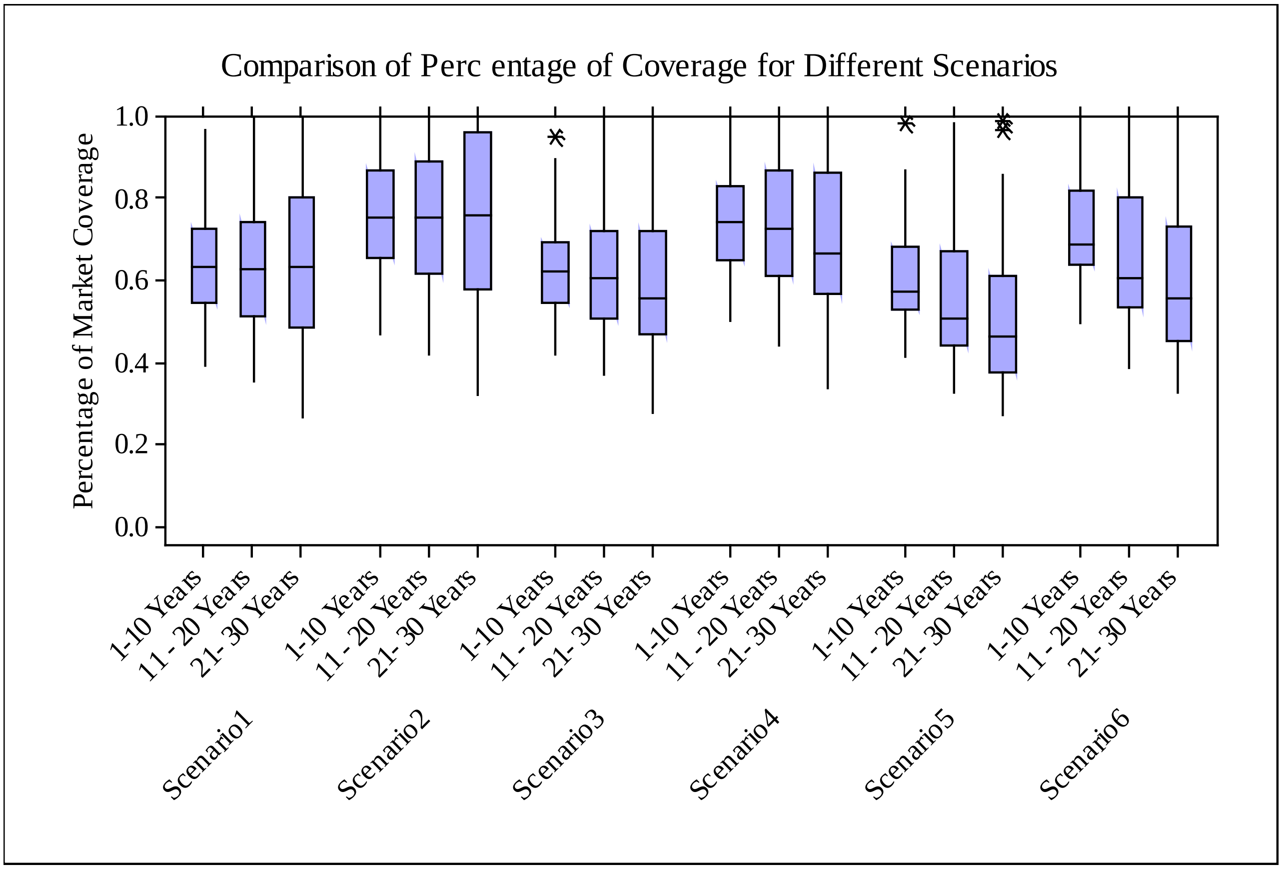


Figure 32. Comparison of percentage of coverage for different scenarios

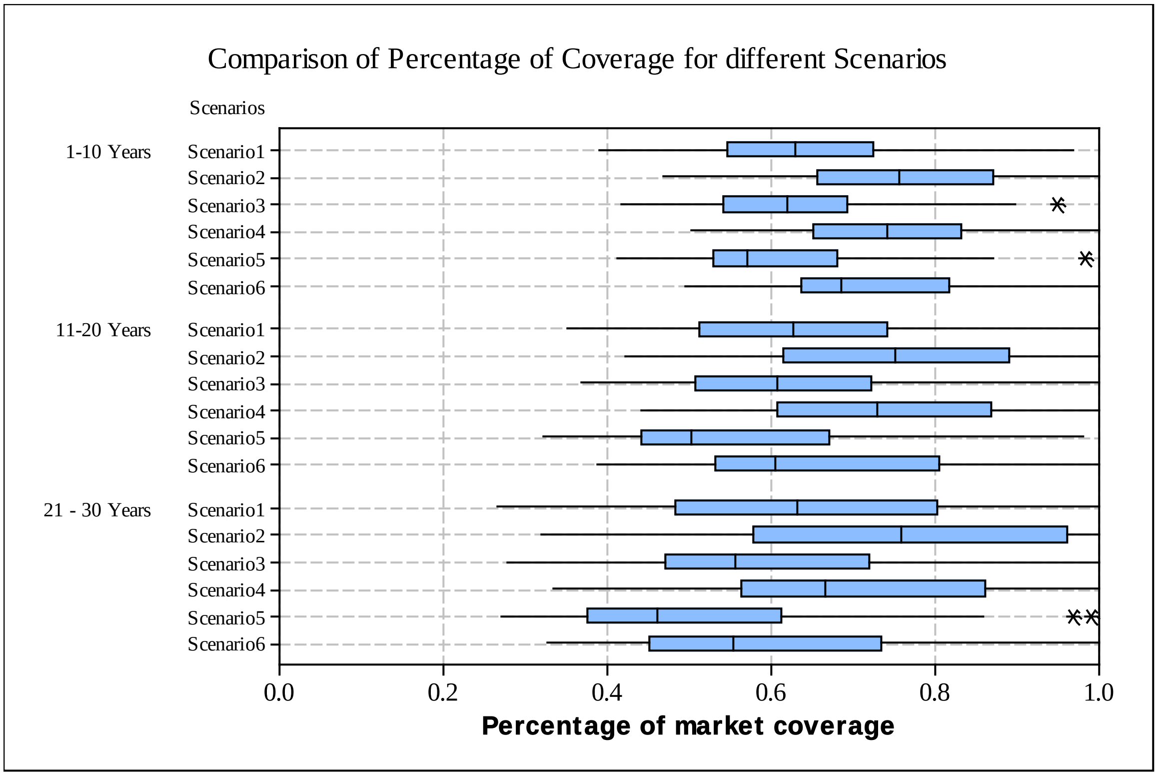


Figure 33. Comparison of percentage of coverage for different scenarios by year

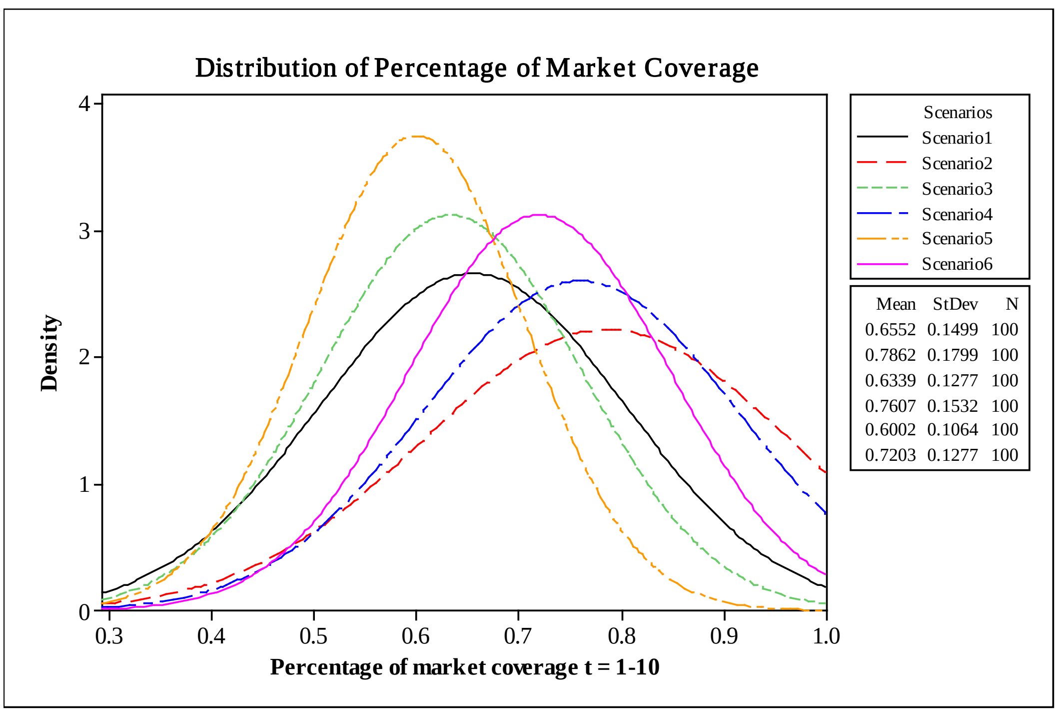


Figure 34. Comparison of the distribution of percentage of market coverage for 1-10 years

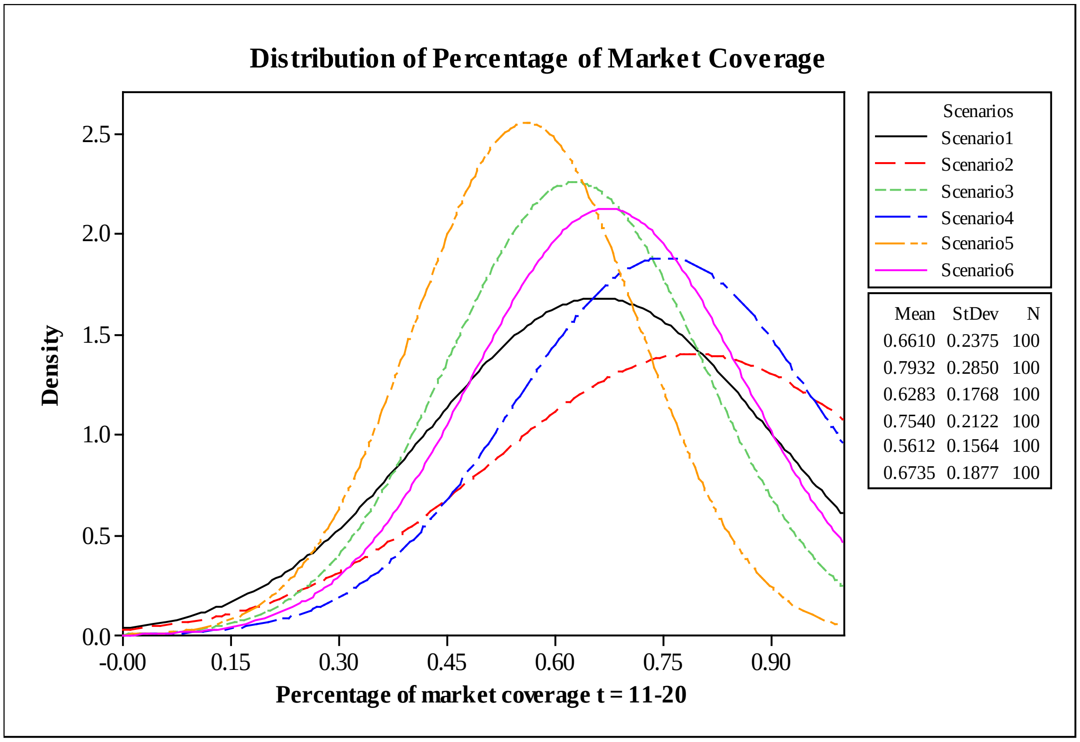


Figure 35. Comparison of the distribution of percentage of market coverage for 11-20 years

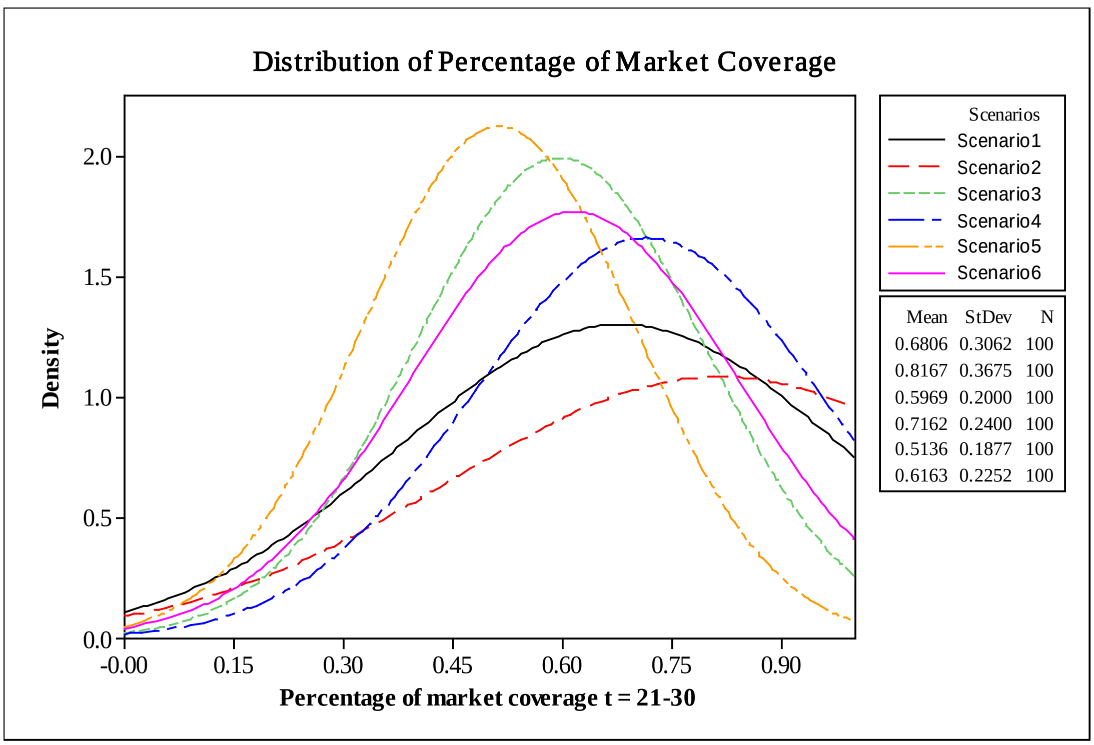


Figure 36. Comparison of the distribution of percentage of market coverage for 21-30 years

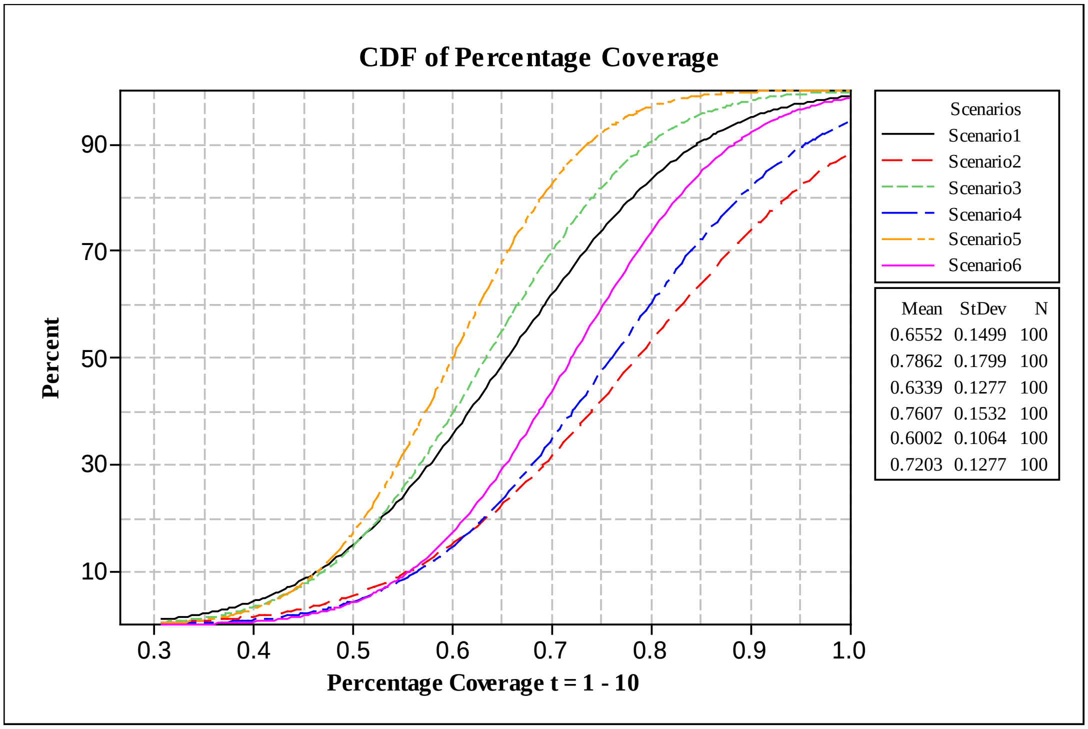


Figure 37. Comparison of the cumulative distribution of percentage of market coverage for 1-10 years

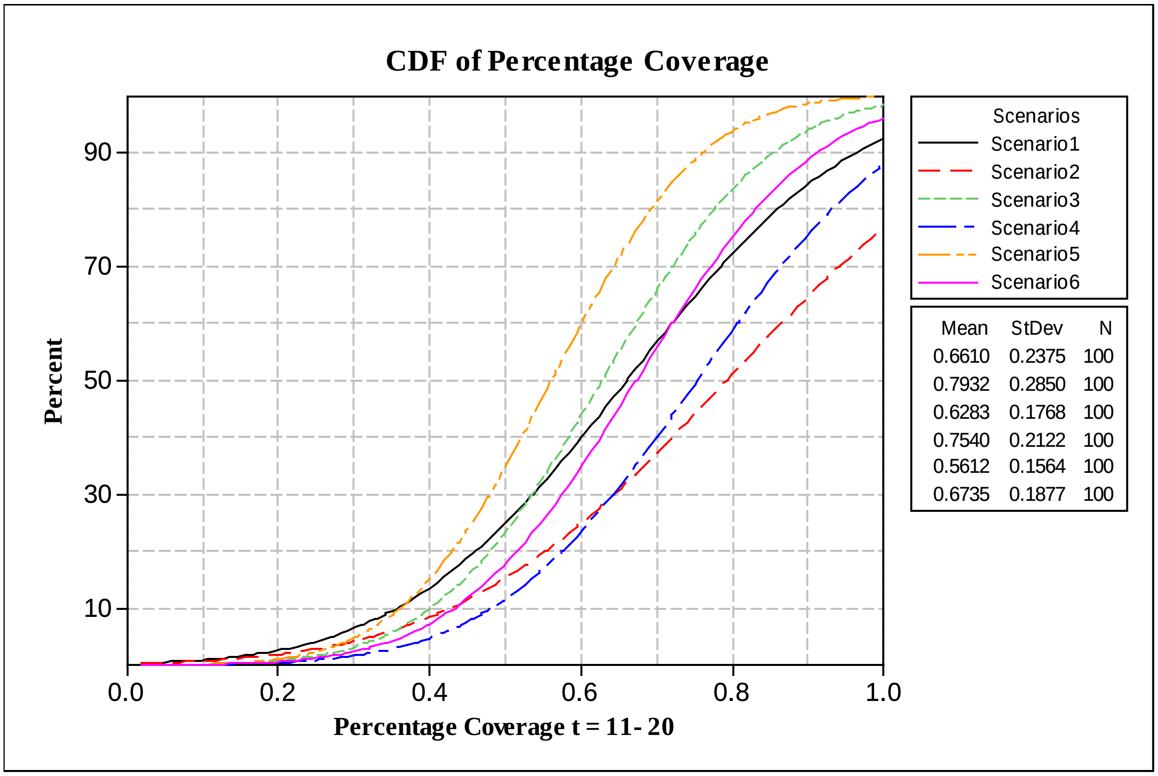


Figure 38. Comparison of cumulative distribution of percentage of market coverage for 11-20 years

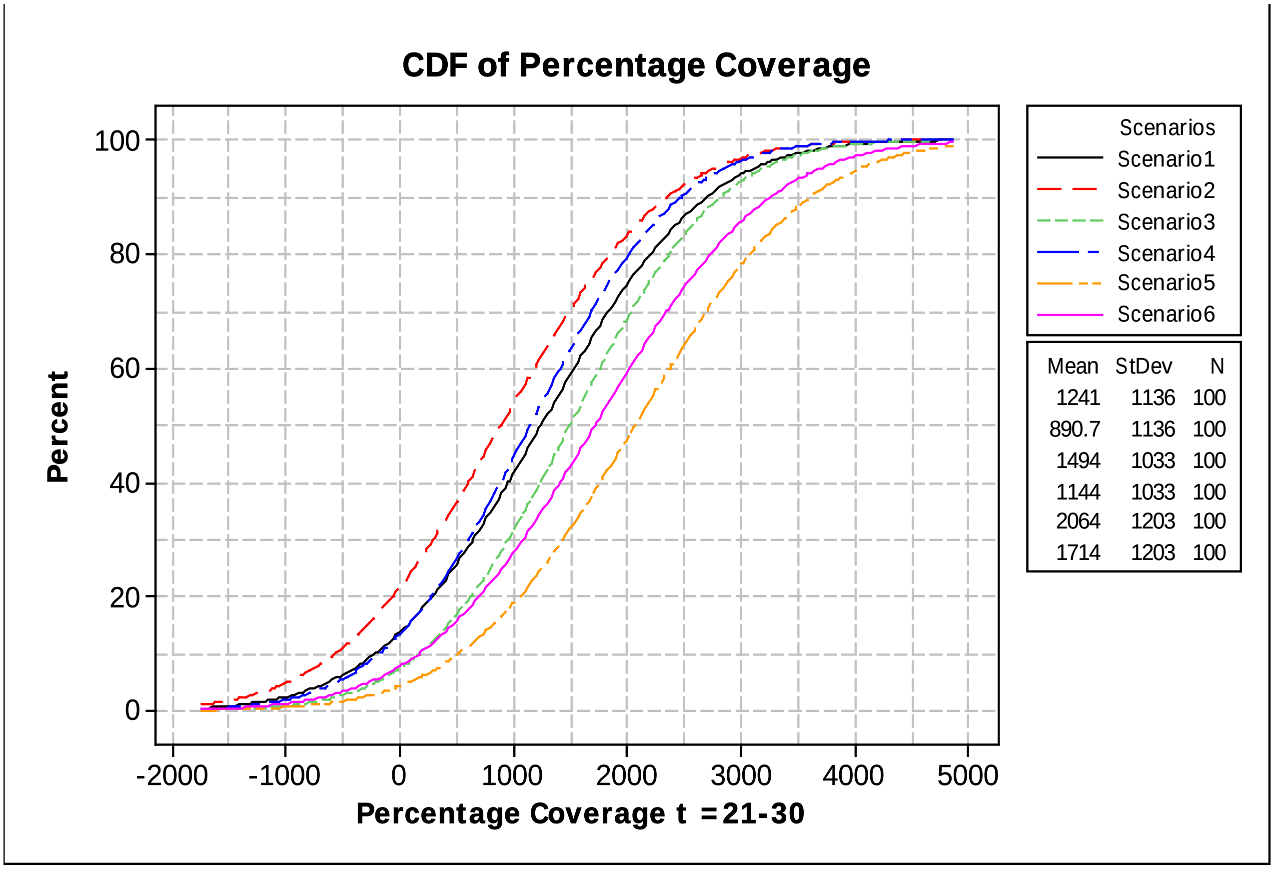


Figure 39. Comparison of cumulative distribution of percentage of market coverage for 21-30 years

5.5 Conclusion

In this chapter we proposed a location allocation model which chooses the optimal locations among suitable locations by maximizing the customer demand coverage so it chooses locations such that all or the greatest amount of estimated customer demand is within a specified impedance cutoff. Also, the model captures the hydrogen demand uncertainty and measures the risk of having hydrogen fuel shortage in future. The model is based on the capacitated Maximal Covering Location Problem (MCLP) and in order to measure the risk of having hydrogen fuel shortage in the future, the Geometric Brownian Motion (GBM) was used to model the uncertainty of the demand.

Chapter 6- Concluding Remarks and Future work

In the final chapter, conclusions and a number of potential future researches are reviewed. Two main problems (questions) have been addressed in this work: (1) how to design and plan a sustainable regional infrastructure for hydrogen fuel supply chain network under uncertain demand; and (2) in what capacity and location the infrastructure will need at the macro and micro levels.

We introduced a multi-period optimization model taking into account the stochasticity and the effect of uncertainty in hydrogen production, storage and usage in macro view (U.S. county level).We developed a spatially aggregated demand model to estimate the potential demand for fuel cell vehicles based on different household attributes such as income and education among others.

We also proposed a Geographic Information System (GIS)-based Multi-Criteria Decision Making (MCDM) tool which finds the suitable locations for a hydrogen fueling station by considering factors such as land availability, air quality, and energy source availability. The results were used to choose the optimal locations for the location allocation model by maximizing the customer demand coverage.

We also developed a location allocation model which identifies the optimal locations among suitable locations by maximizing the customer demand coverage based on the capacitated Maximal Covering Location Problem (MCLP). Also, the model captured the hydrogen demand uncertainty and measured the location risk of having hydrogen fuel shortage in future. In this dissertation we also propose a life cycle assessment (LCA) and economic assessment model to compare different waste to energy methods for transportation use. In addition, we provide a number of potential future researches that can directly be done towards this thesis.

6.1 Comparison of centralized, distributed and off-grid hydrogen production

Hydrogen production could be centralized, decentralized or a mixture of both. While generating hydrogen at centralized primary energy plants promises higher hydrogen production efficiency, difficulties in high-volume, long range hydrogen delivery makes electrical energy distribution attractive within a hydrogen economy. On the other hand, small regional plants or even local filling stations could generate hydrogen. While hydrogen generation efficiency for decentralized is lower than that for centralized hydrogen generation, losses in hydrogen delivery can make such a scheme more efficient. The proper balance between centralized and decentralized productions is one of the important issues in the hydrogen economy.

6.2 Real option model

It is useful to develop a real option model to investigate the value of investment opportunity such as construction of hydrogen infrastructure which is able to handle the multiple uncertainties from market, political and technological aspects. A well-functioning hydrogen economy requires two major investments. The first investment is the construction of a hydrogen infrastructure, in which hydrogen is produced, stored delivered and sold to consumers at hydrogen fueling stations. The second investment is the production and retail of fuel cell vehicles. It's not possible to have a huge investment on hydrogen infrastructure without fuel cell vehicles being available on a large scale. Likewise, a fuel cell vehicle manufacturer will only produce hydrogen cars if fueling stations are available throughout a large area. In this thesis our focus was more on the first investment given that demand for fuel cell vehicles can be estimated by our proposed model (section 3.3.4).

Building hydrogen infrastructure (production plants, storage facilities and delivery modes) is very expensive and needs significant investment with substantial risks. Given the size of the resources committed in the investments and the long investment period before realizing profits, it is necessary to employ an adequate valuation method to maximally explore the value of the investment.

Traditionally, project valuation has been used through a simple valuation framework called Net Present Value (NPV) approach, where the risk is considered undesirable. It penalizes the present value of the risky cash flows with discount factor that represents the time value of money and aversion attitude of risk. Uncertainties will thereby increase the firm's opportunity costs and raise the threshold rate of required return, which will induce investors to reject the risky projects. The attractiveness of option is on that it enables the investors to pay a small amount of money, in the control of profits loss, to explore the potential strategic value of the investment opportunity. As a result, investors can make more informed decisions, taking into account learning factors and managerial flexibility, which will always place the investor in a favorable position. Dealing with uncertainty is the key to real option. It can help quantify management's ability to adapt its future plans to capitalize on favorable investment opportunities or to respond to undesirable development in a dynamic environment by cutting its losses.

6.3 Enhancement of Geographic Information System (GIS)-based Multi-Criteria Decision Making (MCDM) and GIS-based location allocation tools

This tool can be extended by having more real data regarding micro level data of locations such as land availability, air quality, energy source availability. Both (GIS)-based Multi-Criteria Decision Making (MCDM) and GIS-based location allocation model can be integrated into single framework/App to find suitable and also optimal locations for hydrogen fueling stations.

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Appendix A

A.1. Emissions (Data sources were accessed on September 2012 [5, 12, 17])

A.1.1. Incineration air emissions

Air Emission and energy use were calculated Based on UK Department for Environment, Food and Rural Affairs report [12] and Zaman [5].

All the values were calculated based on total MSW of NY, NJ and PA multiply to emission rate (kg/ton):

Nitrogen oxides:
59500 (ton/day) x 1.6 (kg/ton) =95200 kg/day

Particulates:
59500 (ton/day) x 0.038 (kg/ton) =2261kg/day

Sulfur dioxide:
59500 (ton/day) x 0.042 (kg/ton) =2499 kg/day

Hydrogen chloride:
59500 (ton/day) x 0.058 (kg/ton) =3451 kg/day

Hydrogen fluoride:
59500 (ton/day) x 0.001 (kg/ton) =59.5 kg/day

VOC (volatile Organic Compounds):
59500 (ton/day) x 0.008 (kg/ton) =476 kg/day

Cadmium:
59500 (ton/day) x 0.000005 (kg/ton) =0.297 kg/day

Nickel:
59500 (ton/day) x 0.00005 (kg/ton) =2.975 kg/day

Arsenic:
59500 (ton/day) x 0.000005 (kg/ton) =0.297 kg/day

Mercury:
59500 (ton/day) x 0.00005 (kg/ton) =2.975 kg/day

Dioxins and furans:
59500 (ton/day) x 0.0000004 (kg/ton) =0.0238kg/day

Polychlorinated biphenyls:
59500 (ton/day) x 0.0000001 (kg/ton) =0.005 kg/day

Carbon dioxide:
59500 (ton/day) x 1000 (kg/ton) =59500000 kg/day

A.1.2. Plasma Gasification air emissions

Air Emission and energy use were calculated Based on UK Department for Environment, Food and Rural Affairs report [12] and Zaman [5].

All the values were calculated based on total MSW of NY, NJ and PA multiply to emission rate (kg/ton):

Nitrogen oxides:
59500 (ton/day) x 0.780 (kg/ton) =46410 kg/day

Particulates:
59500 (ton/day) x 0.012 (kg/ton) =714 kg/day

Sulfur dioxide:
59500 (ton/day) x 0.052 (kg/ton) =3094 kg/day

Hydrogen chloride:
59500 (ton/day) x 0.032(kg/ton) =1904 kg/day

Hydrogen fluoride:
59500 (ton/day) x 0.034 (kg/ton) =2023 kg/day

VOC (volatile Organic Compounds):
59500 (ton/day) x 0.011 (kg/ton) =654.5 kg/day

Cadmium:
59500 (ton/day) x 0.0000069 (kg/ton) =0.41 kg/day

Nickel:
59500 (ton/day) x 0.00004 (kg/ton) =2.38 kg/day

Arsenic:
59500 (ton/day) x 0.00006 (kg/ton) =3.57 kg/day

Mercury:
59500 (ton/day) x 0.000069 (kg/ton) =4.1 kg/day

Dioxins and furans:
59500 (ton/day) x 0.00000004 (kg/ton) =0.00238kg/day

Carbon dioxide:
59500 (ton/day) x 1000 (kg/ton) =59500000 kg/day

A.1.3. Anaerobic Digestion air & water emissions

Air Emission and energy use were calculated Based on UK Department for Environment, Food and Rural Affairs report [12] and Zaman [5]

A.1.3.1 Air Emissions

All the values were calculated based on total MSW of NY, NJ and PA multiply to emission rate (kg/ton):

Nitrogen oxides:
59500 (ton/day) x 0.188 (kg/ton) =11186 kg/day

Sulfur dioxide:
59500(ton/day) x 0.003 (kg/ton) =178.5 kg/day

Hydrogen chloride:
59500 (ton/day) x 0.00002 (kg/ton) =1.19 kg/day

Hydrogen fluoride:
59500 (ton/day) x 0.000007(kg/ton) =0.41 kg/day

Cadmium:
59500(ton/day) x 0.000001(kg/ton) =0.059 kg/day

Nickel:
5950059500(ton/day) x 0.0000003 (kg/ton) =0.017 kg/day

Arsenic:
59500(ton/day) x 0.0000005 (kg/ton) =0.029 kg/day

Mercury:
59500(ton/day) x 0.0000006 (kg/ton) =0.035 kg/day

Carbon dioxide:
Based on data reported by the EPA and the East Bay Municipal Utility District [17] for methane production rates – 3,300 ft^3 CH_4/wet ton – and volumetric composition – 64% CH_4 and 36% CO_2 – methane and carbon dioxide production were calculated as follows:

59500tons x 3,300 ft^3 CH_4/ton = 196350000 ft^3 CH_4 – which is 64% of total biogas

Therefore, the other 36% of biogas (CO_2) is given by:

64/196278548.4 = 36/x where x = 110446875 ft^3 CO_2;
110446875 ft^3 CO_2 x 28.32 L/ft^3 x 1.842 g/L x 1 ton/10^6 g = 5760ton CO_2

A.1.3.2 Emissions to water

Nitrogen:
59500(ton/day) x 0.01 (kg/ton) =595 kg/day

COD, Chemical Oxygen Demand:
59500(ton/day) x 0.1 (kg/ton) =5950 kg/day

BOD, Biological Oxygen Demand:
59500(ton/day) x 0.025 (kg/ton) =1487 kg/day

A.2. Input-Output (Energy) (Data sources were accessed on September 2012 [6, 5, 15, 19, 22])

A.2.1. Incineration energy consumption & generation:
Based on Finnveden [6] energy start-up is 77.8 kWh/ton so total requirement for 59500(ton/day) is:

59500(ton/day) x 77.8 (kWh/ton) =4629 MWh

Based on Circeo [22] energy generation (electricity) is 544 kwh/ton so in our study total energy generation from incineration process is:

59500(ton/day) x 544 (kWh/ton) =32368 MWh

A.2.2. Plasma Gasification energy consumption & generation:

Based on Ducharme [15] energy start-up is 355 kWh/ton so total requirement for 59500(ton/day) is:

59500(ton/day) x 355 (kWh/ton) =21122.5 MWh

Based on Ducharme [15] energy generation is 808 kWh/ton so in our study total energy generation from incineration process is:

59500(ton/day) x 808 (kWh/ton) =48076 MWh

Note that the classic gasification energy generation is around 685 kwh/ton [5]

A.2.3. Anaerobic Digestion energy consumption & generation:

A.2.3.1 Digester Energy Requirements

59500tons x 10^6 g/ton x 1 mL/1.034 g x 1L/1000 mL x 1 m^3/1000 L = 57520 m^3 of MSW produced per day

Using data from Biogas Prediction and Design of a Food Waste to Energy System for the Urban Environment [19]:

- Mixing:

  Energy required for mixing 30 m^3 = .735 kW; therefore, to mix the additional 57520 m^3 of waste added to the digester 33.82 additional MWh are needed per day

  0.735 kW/30 m^3 x 57520 m^3 x 24 hours/day =33.82 MWh/day

- Heating

  Energy required for heating 30 m^3 = 200 W (heating load) + 1.2 kW (hot water pump) = 1.4 kW; therefore, to heat the additional57520 m^3 of waste added to the digester 64.42 additional MWh are needed per day

  1.4 kW/30 m^3 x 57520 m^3 x 24 hours/day = 64.42 kWh/day

- Digestate Processing – Screw Press

  Energy required for processing the digestate from 30 m^3 = 2.2 kW (screw press) + 0.735 kW (recirculation pump) + 100 W (sulfur removal) = 3.035 kW; therefore, to heat the additional 57520 m^3 of waste added to the digester 139.66 additional MWh are needed per day

  3.035 kW/30 m^3 x57520 m^3 x 24 hours/day = 139.66 MWh/day

- Process Control

  Energy required for controlling 30 m^3 = 200 W; therefore, to control the additional 57520m^3 of waste added to the digester 9.203 additional MWh are needed per day

0.200 kW/30 m^3 x 57520 m^3 x 24 hours/day = 9.2 MWh/day

Total Energy Used for waste per day = 33.8 MWh + 64.4 MWh + 139.6 MWh + 9.2 MWh = ***247.1 MWh/day***

As mentioned in Air emission for anaerobic digestion, the amount of methane produce from 59500tons is 196278548 ft^3 CH_4

A.3. Life Cycle Networks

A.3.1. 1. Incineration (CML 2 method)

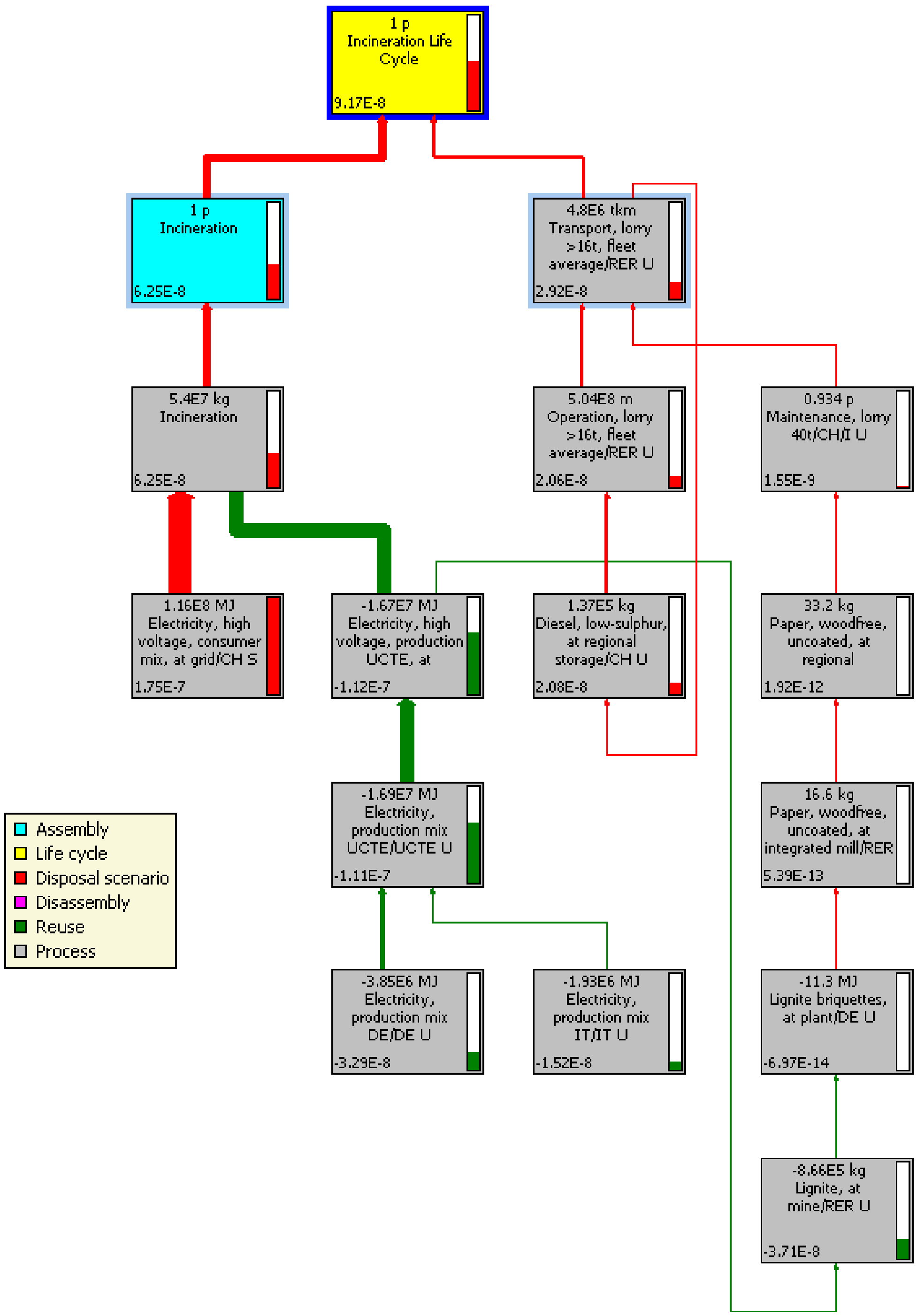

Figure 40. Life Cycle for Incineration (CML 2 method)

A.3.1.2. Incineration (Eco-indicator 99(E))

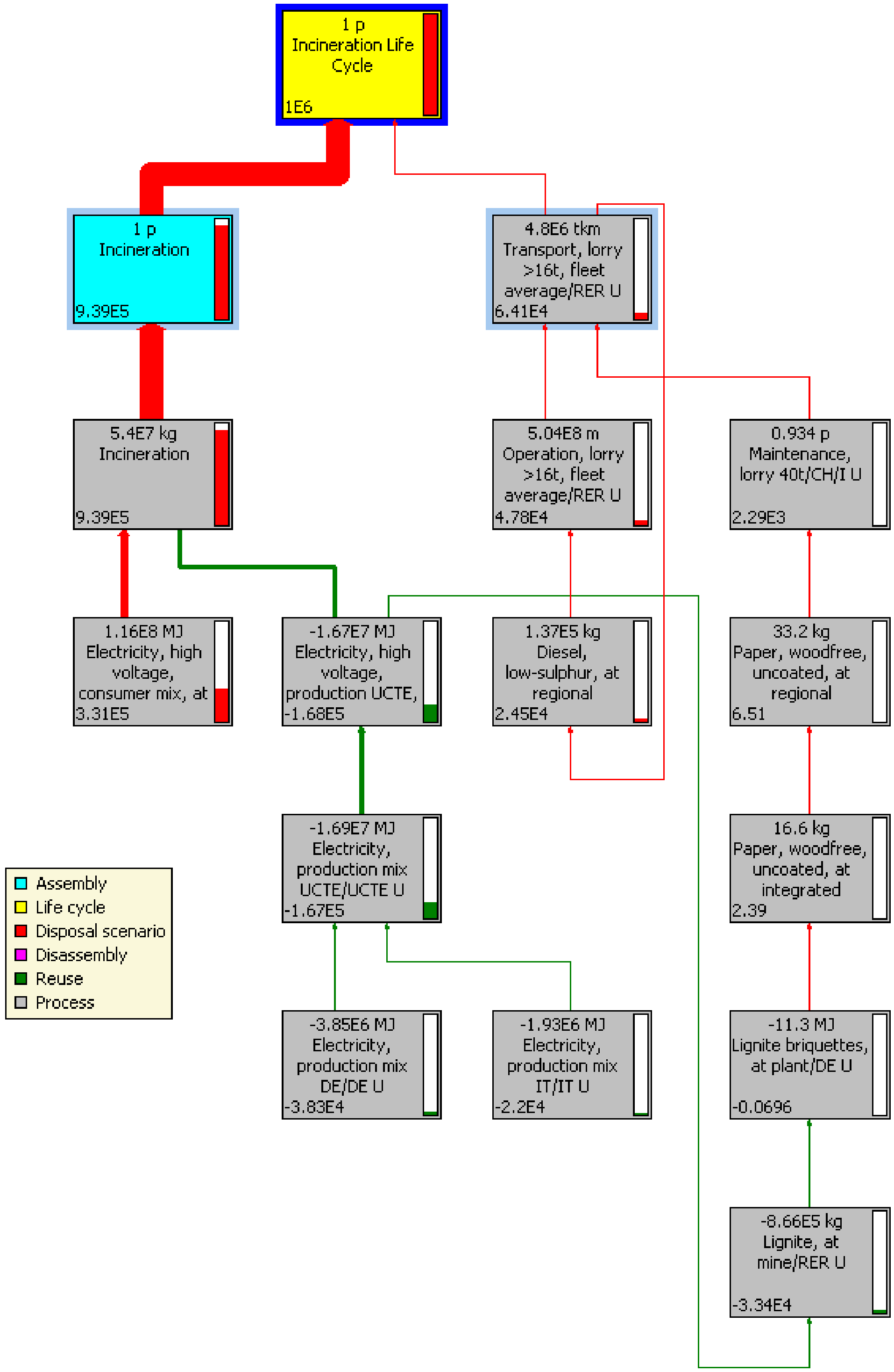

Figure 41. Life Cycle for Incineration (Eco-indicator 99(E))

A.3.2. 3. Plasma Gasification (CML 2 method)

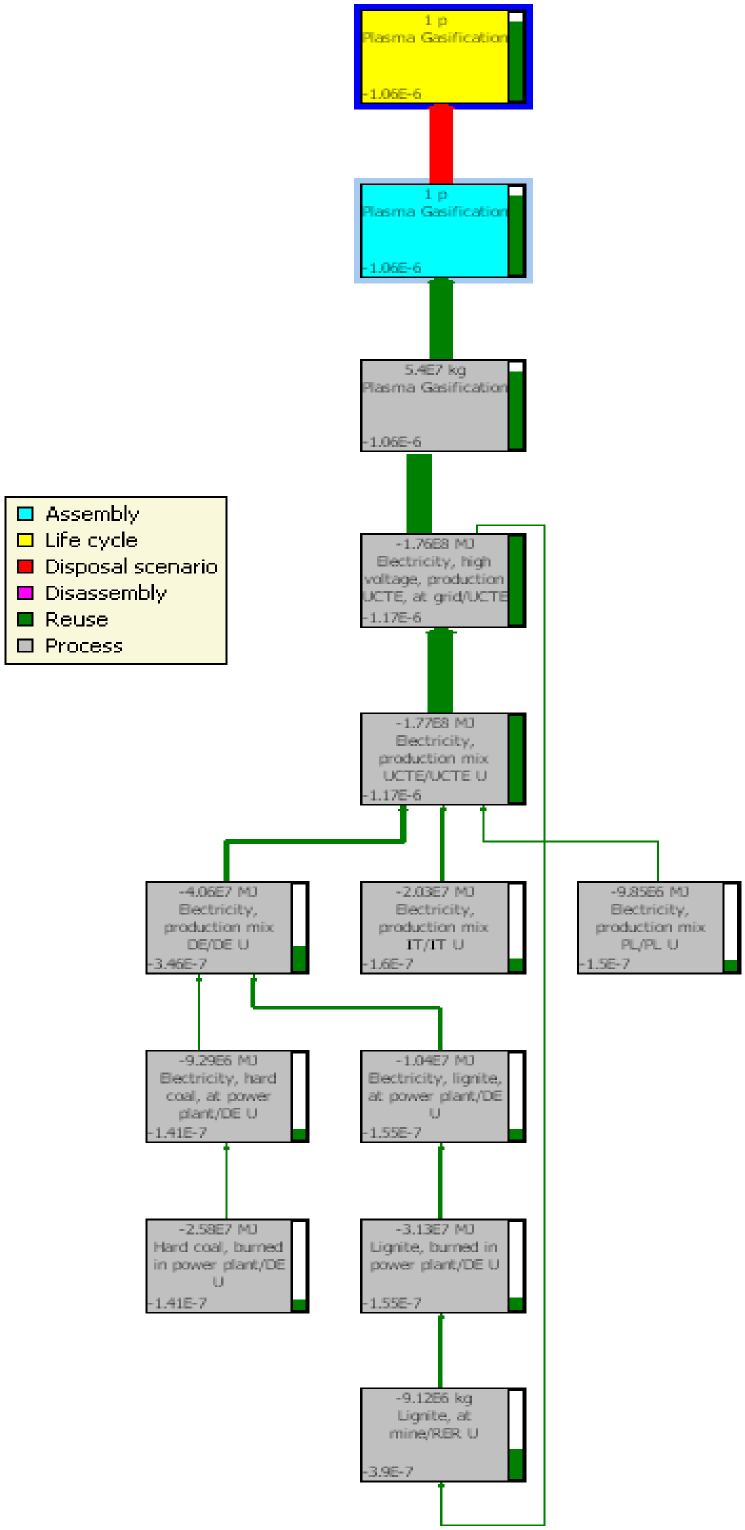

Figure 42. Life Cycle for Plasma Gasification (CML 2 method)

A.3.2.b Plasma Gasification (Eco-indicator 99(E))

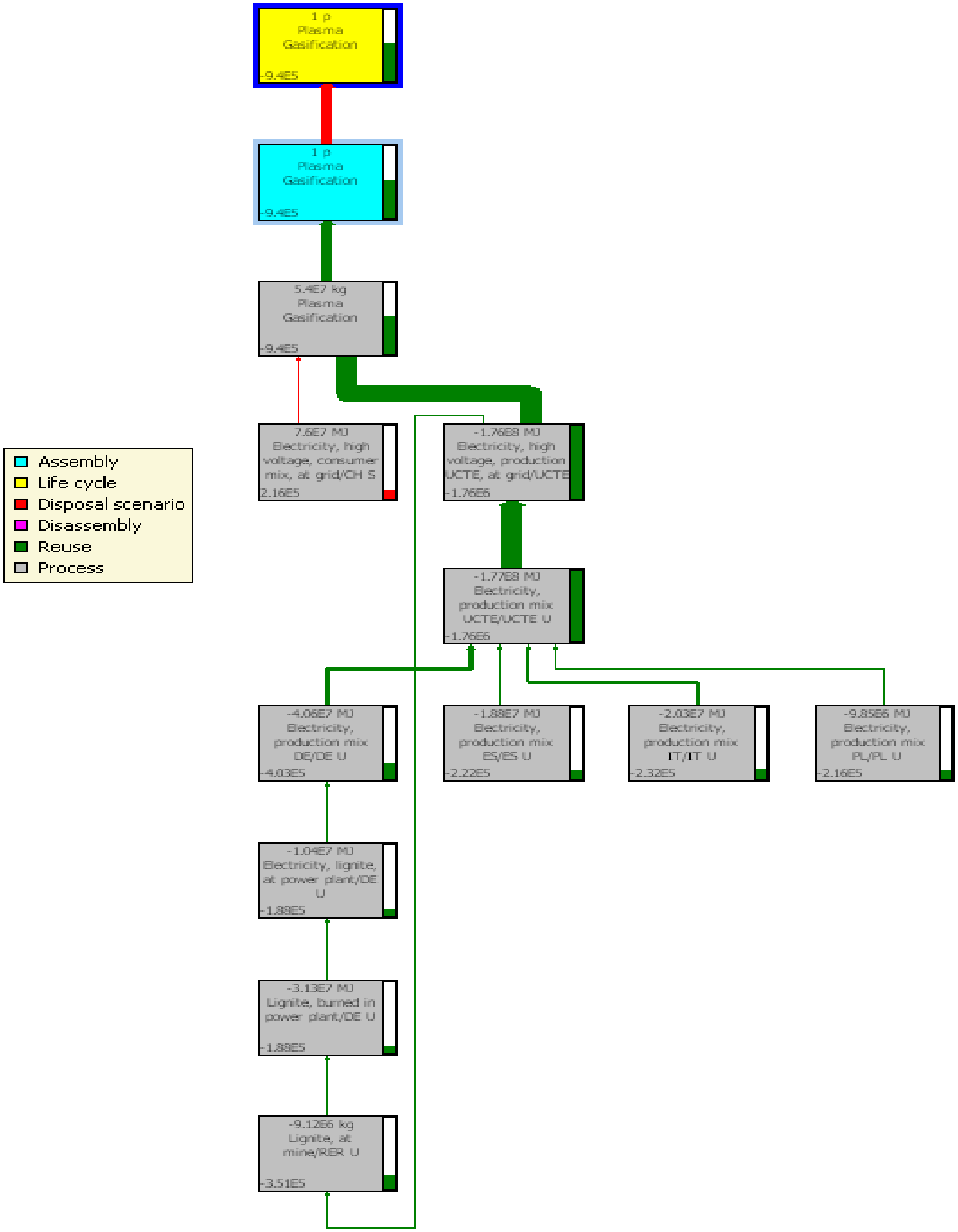

Figure 43. Life Cycle for Plasma Gasification (Eco-indicator 99(E))

A.3.3.a. Anaerobic Digestion (CML 2 method)

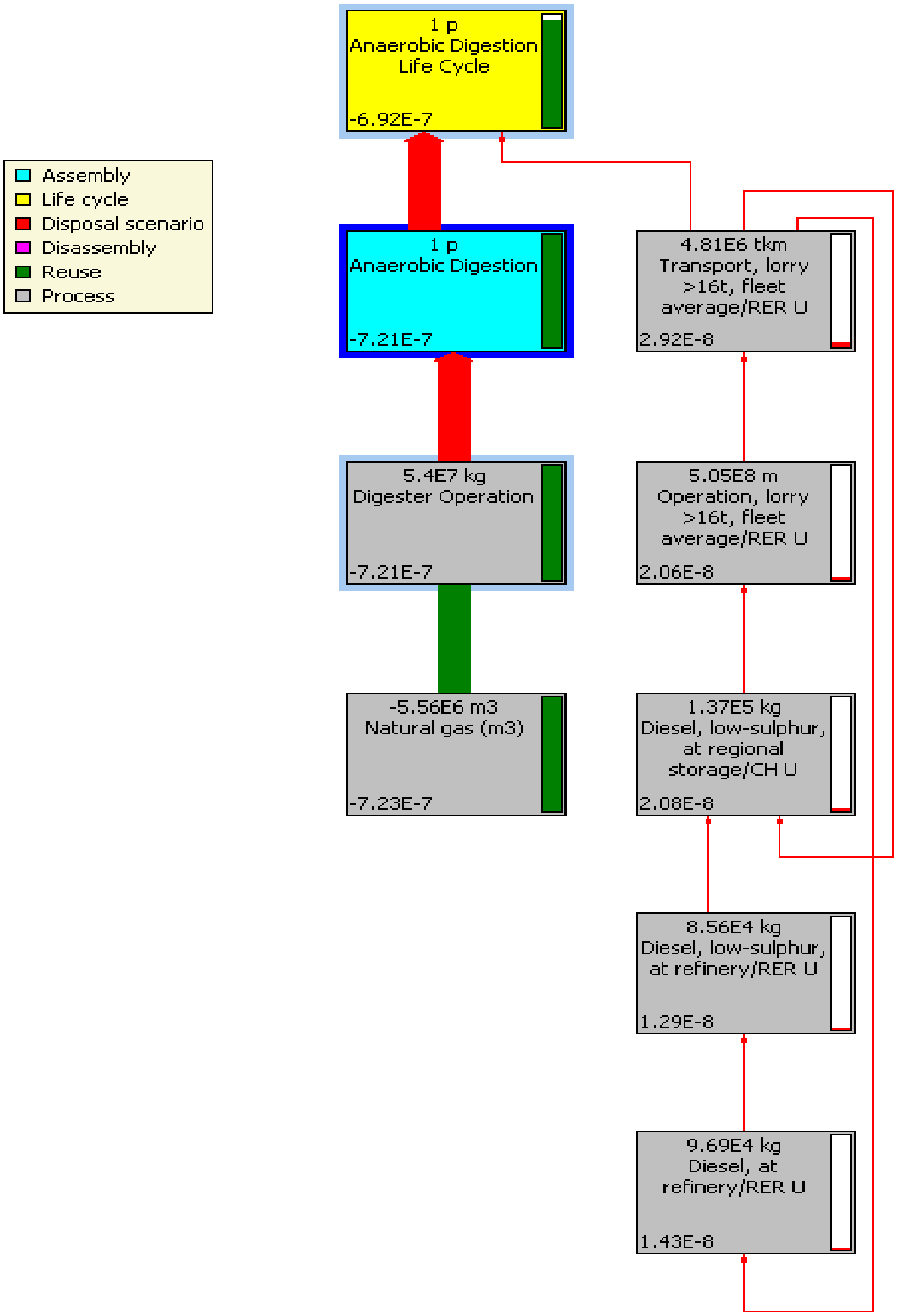

Figure 44. Life Cycle for Anaerobic Digestion (CML 2 method)

A.3.2.b. Anaerobic Digestion (Eco-indicator 99(E))

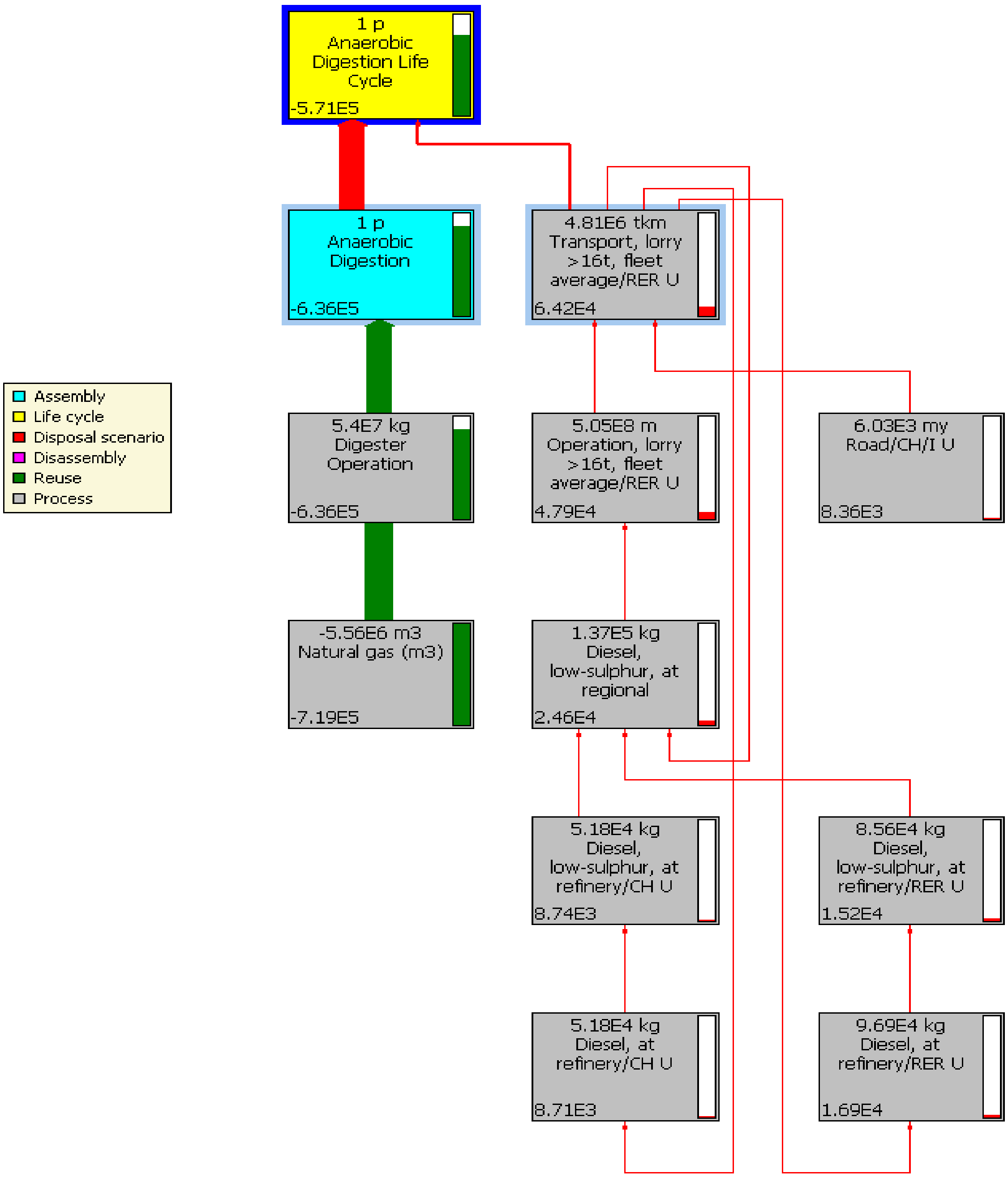

Figure 45. Life Cycle for Anaerobic Digestion (Eco-indicator 99(E))

A.4. Waste Scenarios

Incineration: Based on DEFRA [12] only 20 percent were disposable so waste transportation km per ton for disposed material is:

50 miles x 11.89 ton x 1.61 (miles/km) =957.145 t/km

Incineration: Based on DEFRA [12] only 20 percent were disposable so waste transportation Km per ton for disposed material is:

50 miles x 11.89 ton x 1.61 (miles/km) =957.145 t/km

Plasma Gasification:

Also same value from incineration was used for plasma gasification.

Anaerobic Digestion:

Assumed 50 percent of the amount of input is disposable [94] which becomes

50 miles x2 9739.17 ton x 1.6 (miles/km) =957.145 t/km