3-23-2018

A System Dynamics Innovation Diffusion Model Applied to Carbon Nanotube Manufacturing

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THESIS

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AFIT-ENS-MS-18-M-139

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AFIT-ENS-MS-18-M-139

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THESIS

Presented to the Faculty

Department of Operational Sciences

Graduate School of Engineering and Management

Air Force Institute of Technology

Air University

Air Education and Training Command

in Partial Fulfillment of the Requirements for the

Degree of Master of Science in Operations Research

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22 March 2018

AFIT-ENS-MS-18-M-139

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AFIT-ENS-MS-18-M-139

Abstract

The transition of advanced technologies from their nascent state to viable commercial entities is a critical step in assuring the United States' national technological superiority and support is often required to incubate such technological developments. We propose a spiral development to investigate the possible scenarios, underlying economics, and risk associated with scaling up carbon nanotube (CNT) production to a commercially viable scale. As the first stage of this proposed effort, this study characterizes the potential scenarios by which a CNT manufacturing company can generate positive annual net revenue and potentially be considered a competitive manufacturer of CNT products on an industrial scale. Subsequent stages of this effort will determine the potential risks associated with investing in the current CNT research and production efforts from a macro perspective. This study investigates the necessary adoption fractions, contact rates, production capacities, production costs, product prices, monetary support, and time necessary for the company of interest to be considered a commercially viable producer of CNT products. The subsidization required to generate varied profit margins is also explored. The application of system dynamics models determined to approximately represent the real diffusion and production of both CNT sheet and CNT yarn products generates insight regarding policy improvement for the company to achieve competitive commercial CNT production and provide an assessment of when CNT production may be profitable. This study should not be used as the basis for decision making due to the fact that the analysis is based on notional data and scenarios.

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To my family and friends, for their unwavering support.

To my God, with Whom all things are possible.

Acknowledgements

If I have seen further, it is by standing on the shoulders of giants.

– Sir Isaac Newton

I would like to thank the members of my committee, Dr. Richard Deckro and Dr. Brian Stone for their guidance throughout this process. I would also like to thank my family and friends, who remind me to just keep swimming.

Frances G. MacKinnon

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A SYSTEM DYNAMICS INNOVATION DIFFUSION MODEL APPLIED TO CARBON NANOTUBE MANUFACTURING

I. Introduction

1.1 Chapter Overview

This chapter introduces the research objectives, motivation, background, and methodology applied in this study. The transition of advanced technologies from their nascent state to viable commercial entities is a critical step in assuring the United States' national technological superiority. The purpose of this research is to gain insight into the possible methods by which a carbon nanotube (CNT) manufacturing company may scale up the current production of CNT products to an economically viable commercial scale. CNT technology is an increasingly desired area of research and development due to its unique properties and versatile applications in such areas as space vehicle design, power-generation, and substitution for scarce metals. CNTs are not necessarily a new technology but have been of significant interest in the last 25 years [19].

This study characterizes potential scenarios by which a company may achieve commercially viable CNT production in terms of CNT sheet and CNT yarn products. System dynamics is leveraged to develop various models with the primary motivation of discerning the possible scenarios by which a company may attain commercially viable production of CNT products and include: a CNT innovation diffusion system dynamics model, a technology-learning sub-model, and a technology-cost sub-model. Additional system dynamics models are developed to posture follow-on research, given clarifying information from the company of interest. Note that this analysis is notional due to the limited availability of specific information regarding the company of interest. However, this study provides insight insomuch as providing illustrative examples of analysis which may be conducted with adjusted assumptions per clarified information from the company.

1.2 Objective

The predominant objective of this thesis is to gain insight into the possible scenarios by which a CNT manufacturing company may produce ultimately profitably CNT products on a commercial scale. This objective is comprised of sub-objectives to more adequately satisfy the main objective. The main research questions of interest for this thesis objective include:

- What models should be applied or developed to analyze this company's CNT production process?
- What are the production capacity utilizations required for this company to produce CNT products at a desirable profit margin and desirable unit cost?
- At what adoption fraction is the company most profitable?
- At what contact rate of non-practitioners is this company most profitable?
- How much net revenue might this company produce in the future?
- How should the primary focus areas for this company be characterized to ensure minimized cost and maximized net revenue?
- Will Title III investment influence the future of this company?
- How does technology learning and experience aid in this company's development?

- What is the potential unit cost of this company's CNT products, given varied production capacity utilizations?
- What are the predominant applications of CNTs?
- What are the desirable properties of CNTs?
- What are the present and predicted markets for CNTs?
- Who are the predominant manufacturers of CNTs and is this company a competitive manufacturer?
- What are the subsequent steps for this research?

The questions listed are addressed through the following process:

- Determine the existing models which have been successfully implemented to determine the diffusion and production of technology.
- Develop a model to illustrate the potential unit costs of CNT product, given a desirable profit margin and capacity utilization.
- Develop a model which incorporates the adoption fraction of CNT products.
- Develop a model which incorporates the contact rate of non-practitioners of CNT products.
- Develop a model which will illustrate the potential net revenue of this company's CNT products.
- Conduct parametric sensitivity analysis to determine which focus areas may result in maximized net revenue and competitive manufacturing.
- Gain an understanding of Title III investment and the potential influence of Title III investment on the company's net revenue.

- Identify system dynamics models which illustrate the potential influence of technology learning and experience.
- Identify system dynamics models which illustrate potential unit cost of CNT products.
- Gain an understanding of CNT applications.
- Identify the desirable properties of CNTs and determine why CNT technology is attractive to consumers.
- Identify the predominant manufacturers of CNT products and determine if the company is a competitive CNT manufacturer.
- Characterize questions for future research.

This study includes models to assess both future supply and demand. By comparing predicted demand, as a function of adoption and existing consumers, with predicted supply, an assessment of when CNT production is profitable is estimated. The analysis and results of this initial study are notional and should not be used for decision making.

1.3 Motivation

The United States has a vested interest in maintaining technological superiority and CNT technology is no exception. CNT technology has been of high interest in the last 25 years in both the private and commercial sector[19]. Due to its unique properties, versatile applications, and incorporations into other existing technologies, CNTs are attractive technology [22]. CNTs may potentially be used in such areas as polymers as nano-fillers, LASER protection, optic, sensors, stealth technologies, Kevlar vests, bio-mechanical systems, and so forth [22]. It is thus imperative to gain insight into the direction of this versatile technology to better understand the commercial viability potential of CNTs.

1.4 Background

CNT technology is an increasingly desired area of research and development due to its unique properties and versatile applications in such arenas as the military, space vehicle design and development, and other applications [22]. CNTs are not necessarily a new technology, but have been of significant interest in the last 25 years. Although this study is limited in terms of available information, the following discussion characterizes the attributes of the company of interest.

Company Profile

The company of interest for this study is not disclosed. However, the following information is open-source and details the characteristics of this company. According to BCC [22], this company was originally founded in the early 2000s and currently holds several patents regarding CNT synthesis and CNT composites. This company has the potential to manufacture Multi-Walled Nanotubes (MWNT) and Single-Walled Nanotubes (SWNT) with specified chirality. According to LibreTexts [5], the chirality of a molecule refers to the mirror-image or non-superimposable characteristic of the molecule such that the mirror image of the molecule differs from the molecule itself. For example, a pair of hands is an example of chirality due to the fact that hands are non-superimposable images, according to Libretexts [5]. The CNT products generated by this company are produced in the form of sheets, yarn, and scrap by-products. This study primarily focuses on the production of CNT sheets and yarn due to available information. One of the predominant goals of the company is to increase production scale such that the company has the ability to produce millimeter-long CNTs with scalable industrial processes, according to BCC [22]. This company is unique due to an ability to produce strong, lightweight, and electrothermally conductive CNT yarn and sheets, according to BCC [22]. Recently, this company was awarded a military grant to produce CNT wires and cables to potentially replace copper material, due to the fact that CNT material is significantly lighter than copper material. According to BCC [22], "a third of the weight of a 15-ton satellite comes from copper wire, while a Boeing 747 has more than 135 miles of wire weighing 2 tons." Because of the potential to significantly reduce weight and thus reduce cost of satellites and other applications, CNT technology is attractive. BCC [22] indicates that the company has received various grants from interested parties for such applications as aerospace, EMI (electromagnetic interference) shielding, thermal management, and power-generation system enhancements. Per reports by BCC [22], this company "claims that delivering long lengths of CNT yarn further solidifies its position as the only U.S. commercial company to fabricate industrially relevant finished materials from CNTs." Additional information from the company regarding annual CNT product output is required to more accurately discern the level of competition posed by the company.

1.5 Methodology

This research leverages system dynamics and existing diffusion models to provide a framework to determine the potential net revenue and demand for CNT products manufactured by a specific company of interest. This study suggests that the target company is potentially postured to be commercially viable and a competitive manufacturer of CNT products, given achievement of assumed parameters of various phases of development posed by the company. However, additional clarification and explanation regarding the company's development is necessary to improve the accuracy of the results of this study.

1.6 Chapter Summary

Chapter I introduces the environment of the problem of interest, objectives, motivation, background, and methodology of this thesis. Chapter II encompasses a compiled literature review, which is leveraged as a basis for the development of the methodology presented in Chapter III and analysis presented in Chapter IV. Chapter III presents the methodology implemented to develop the system dynamic models determined to appropriately achieve the objectives outlined in Chapter I. Chapter IV presents the notional analysis conducted to address the research questions posed in Chapter I. Vetting of the model occurs throughout Chapter IV, insomuch as noting anticipated model behavior and also includes a model validation discussion. Chapter V provides a summary of the conclusions drawn from the analysis demonstrated in Chapter IV and provides recommendations for future research. This study is demonstrative in nature regarding potential analysis which may be conducted, given clarified dialogue with the company of interest and should thus not be utilized as a source of decision making.

II. Literature Review

Experience is an expensive school.

–Benjamin Franklin [26]

2.1 Chapter Overview

The purpose of this section is to compile and review previously conducted work in order to clarify the research questions identified in Chapter I. This section provides the foundation upon which the methodology in Chapter III and notional analysis in Chapter IV is conducted.

2.2 Technology Diffusion

The desire to accurately forecast the diffusion of new innovative technologies is of high interest today. Meade and Islam compiled a review of various developments made in the area of technology diffusion and the following discussion highlights relevant topics in their paper [19]. Some of the initial technology diffusion research strides occurred in the 1960s; the predominant research of interest was conducted by Fourt and Woodlock [11], Mansfield [14], Rogers [24], Chow [6], and Bass [3]. The works produced by these authors are sources of the majority of technology diffusion forecasting research. Six of the eight key models developed in 1970 are applied today to illustrate the diffusion of new technologies, primarily in consumer products. Gatigon, Eliashaberg, and Robertson [12] introduced the concept of considering various points of diffusion in various countries. Robinson and Lakhani introduced marketing variables into the known forecasting models [23]. Norton and Bass incorporated the concept of the diffusion of subsequent technologies [21]. Meade also incorporated new concepts for technology diffusion models to improve market development forecasting through the application of growth curves. Meade focused on statistical validity, model validity, and demonstrable forecasting validity and ability [19]. According to Meade [18], model validity refers to the technology of interest being adoptable and not just consumable while statistical validity refers to the model of interest being tested for significance. Meade [18] states that the demonstrable forecasting element refers to some level of forecasting uncertainty incorporated into the model. Mahajan and Peterson introduced the elements of time and space for forecasting technological substitution [17].

Mahajan, Muller, and Bass expanded upon the initial Bass model and illustrated the various methods by which a product should be marketed through the examination of diffusion models [16]. The goals of the collaboration between Mahajan, Muller, and Bass were to increase individual understanding of the diffusion process, utilize hazard model developments, explore the constraints of supply and distribution, and to model innovation launch [19].

An *S-curve* typically illustrates the cumulative diffusion of a technology into the market between the point at which an innovation is introduced to the market and the point of innovation saturation. Although the *S-curve* is generally accepted as the appropriate model to illustrate cumulative diffusion, there are opposing hypotheses as to why this is the case. Two opposing hypotheses include the assumption of a predominantly homogenous population of consumers and predominant heterogeneity of consumer population [19].

According to Bass [3], individuals within a population have a desire to innovate. Bass denotes this need to innovate by p, the coefficient of innovation. Bass also indicates that individuals have a need or desire to imitate other members of the population. Bass denotes this need to imitate by q, the imitation coefficient. Bass indicates that the probability that an individual adopts a particular innovation by time t is driven by the following:

$$p + qF(t). \tag{1}$$

The proportion of the population that adopts the technology is denoted by $F(t)$ at the certain time t. In the case of "pure innovation," according to Meade and Islam [19], in which $p > 0$ and $q = 0$, the technology diffusion follows a modified exponential curve. However, in the case of "pure imitation," in which $p = 0$ and $q = 0$, the technology diffusion follows a logistic curve [19].

Conversely, Rogers indicates that consumer populations are heterogeneous in terms of their desire to innovate [24]. Rogers suggests that technology adoption occurs over certain percentages of the population: 2.5% of innovation adopters include the innovators themselves, 13.5% of innovation adopters include the early adopters, 34% of innovation adopters include the early majority, 34% of innovation adopters include the late majority, and finally 16% of innovation adopters include the laggards [24]. Rogers further suggests that early adopters of innovations are typically of a higher tier socially and economically than later innovation adopters. Early adopters are also typically more educated than portions of the population which adopt innovations at a later point in time [24].

2.3 Technology Substitution

Although technology diffusion is a relevant topic for new and desirable technology, such as CNTs, it is possible that this technology will gradually substitute current technologies. According to Coleman, Khan, Blau, and Gun'ko [7, p1625], "no previous material has displayed the combination of superlative mechanical, thermal and electronic properties attributed to them." For example, current copper wiring in space vehicles may eventually be replaced by CNTs due to their relative lightness, conductivity, and other characteristics. It is therefore potentially useful to consider the forecast of CNT technology diffusion in terms of gradual substitution of current technologies. One approach includes a system dynamics modeling perspective to forecast technology substitution.

Kabir, Sharif, and Adulbhan [13] developed a systems dynamic model based on the Sharif-Kabir model [25] and the following discussion highlights elements of their research effort. The Sharif-Kabir model incorporates a method to alter the speed and direction of technology substitution predictions. Kabir, Sharif, and Adulbhan apply the Sharif-Kabir model with the addition of a multilevel substitution model with time dependent parameters.

Kabir, Sharif, and Adulbhan [13] illustrate the principles of multilevel substitution by suggesting the consideration of a market with n products at a certain time, t. Products subsequently enter the market in a defined order, P_1 to P_n, with P_n as the newest and most technologically advanced product available and P_1 as the initial and least technologically advanced product available on the market. A newer product substitutes an older product over time and thus the older product loses market share to the newer products [13]. To forecast market share of intermediate products, it is necessary to group products of interest into three groups: P_{old}, P_{new}, and P_i. P_{old} includes P_1 to P_{i-1}. P_{new} includes P_{i+1} to P_n. Kabir, Sharif, and Adulbhan [13] state that the market share of P_i is defined by the following:

$$f(P_i) = 1 - f(P_{old}) - f(P_{new}) \tag{2}$$

where $f(P_i)$ is the market share of product P_i at time t, $f(P_{old})$ is the market share of products P_{old} at time t, and $f(P_{new})$ is the market share of products P_{new} at time

t. Kabir, Sharif, & Adulbhan [13] suggest the use of the following model:

$$\ln(f/(1-f)) + \sigma(1/(1-f)) = C_1 + C_2 t \quad (3)$$

where f denotes the market share of the competing product. σ denotes the delay coefficient, $0 \leq \sigma \leq 1$. C_1 and C_2 are constants and t is a specific time. The delay coefficient, σ, is a constant that depends on the period being forecasted and is determined by the decision maker, according to Kabir, Sharif, & Adulbhan [13]. The following equation determines the rate of substitution of the the older product by the newer product:

$$df/dt = (f(1-f)^2)/(\sigma(f) + (1-f)) \quad (4)$$

The rate of substitution of a product lies on the following interval for a specific time t.:

$$C_2 = f(1-f)^2 df/dt \leq C_2 f(1-f)^2 \quad (5)$$

Equation 3 is made dynamic by the following:

$$(df(t))/dt = (\beta(t)f(t)[1-f(t)]^2)/(1-[(1-\sigma)f(t)]) \quad (6)$$

where $\beta(t)$ is the "instantaneous rate of change at time t" that makes C_2 a time dependent function. $f(t)$ denotes market share of the new product; σ denotes the delay coefficient; and t is time. Equation 5 can be integrated to determine the forecasting model once the functional form of $\beta(t)$ is determined [13].

Fisher-Pry Model

Substitution of older technologies by newer technologies is a crucial element in the grand scheme of consumerism. Historically, technology evolution is apparent and ongoing. For example, water-based paints were substituted for oil-based paints, plastic for wood flooring, and detergent for soap. Despite the rate of technology substitution, the end result typically encompasses the consumer's improved ability to perform a certain function, while the desired function does not change [8]. The following discussion highlights portions of the research conducted by Fisher and Pry [8]. The Fisher-Pry substitution model is based on three assumptions:

1. Many technological advancements can substitute other present technologies [8].

2. A technological advancement will eventually constitute the entire market for a specific need if substitution has occurred by at least a few percent [8].

3. The fractional rate of substitution by the new technology is proportional to the fraction of the market comprised of the previous technology [8].

The first assumption indicates that a newer technology is less developed than an older competing technology and thus the potential for improvement and cost reduction is greater for the new technology. The second assumption indicates the supposition that a slight increase in market percentage is an indication of economic viability and that the new technology will eventually substitute 100% of the competing older technology [8].

The Fisher-Pry model follows the assumption that the annual growth rate increment is constant. According to Fisher and Pry, substitutions typically follow an *S-curve* and follow exponential development [8]. The *S-curve* is characterized by two constants, according to Fisher and Pry [8]:

1. Early growth rate

2. Time when complete substitution is 50% complete

The fraction of the new technology present in the current market is given by the following equation:

$$f = (1/2)[1 + tan(h)\alpha(t - t_0)] \tag{7}$$

where, α denotes half the annual fractional growth in the early time period of the substitution and t_0 refers to the time when the new technology has successfully substituted 50% of the current market in terms of the old technology. To clarify, $f = 1/2$ when $t = t_0$ [8]. Fisher and Pry also indicate the necessity to characterize a technological substitution by the "takeover time," which is defined as the time it takes for a new technology to go from $f = 0.1$ to $f = 0.9$. The takeover time is inversely proportional to α and thus:

$$t = t_{0.9} - t_{0.1} = 2.2/\alpha \tag{8}$$

Fisher and Pry [8] indicate the more manageable form of equation (8) as follows:

$$f/(1 - f) = \exp 2\alpha(t - t_0) \tag{9}$$

This equation provides a method by which the data of substitution may be plotted on semilog paper as a function of time.

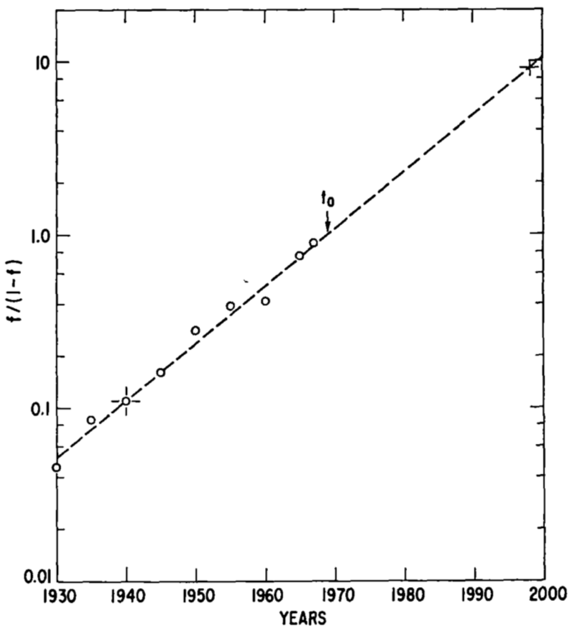

Figure 1. Fisher-Pry Substitution Model fit to U.S. Fiber Study

From [8]

Figure 1 originates from the Fisher and Pry paper in which the Fisher-Pry substitution model is fit to forecast the substitution of synthetic fibers for other fiber in the United States [8]. It is significant to note that the half substitution date, t_0, is labeled in Figure 1 at the point on the fitted line when $f/(1-f) = 1$, in 1969. The takeover time is calculated at 58 years between $f = 0.1$ in 1940 and $f = 0.9$ in 1998 [8].

The Fisher-Pry substitution model is an effective method to model the gradual substitution of one technology for others and is thus potentially applicable for subsequent research insomuch as modeling the substitution of CNTs for existing technologies, to include steel, copper, and so forth. As more data is available, the accuracy of the Fisher-Pry model when applied to CNT data may result in a more accurate forecast of the gradual substitution of CNTs for other technologies [8].

2.4 System Dynamics

Although an understanding of technology diffusion and substitution is relevant to this research effort, system dynamics is also a potentially useful tool to develop models and gain insight regarding complicated systems, such as CNT production. Forrester [9] is one of the predominant developers of system dynamics and applied such methodologies to industrial engineering efforts, mainly for the U.S. Navy, and much of his work is applied as the basis of the work conducted by Sterman [26].

> System dynamics is a perspective and set of conceptual tools that enable us to understand the structure and dynamics of complex systems. System dynamics is also a rigorous modeling method that enables us to build formal computer simulations of complex systems and use them to design more effective policies and organizations [26, p7].

System dynamics models are developed with particular annotation of variable relationships. Causal links, or arrows, indicate a relationship between two variables, according to Sterman [26]. Causal loop diagrams are useful methods of identifying interdependencies within a system dynamics model, according to Sterman [26]. The causal link arrows in a causal loop diagram are assigned polarity, positive (+) or negative (-), to indicate the effect on dependent variables by changes in independent variables. Positive feedback loops are referred to as reinforcing feedback loops (R) while negative feedback loops are referred to as balancing feedback loops (B). For example, Figure 2 illustrates a casual loop diagram of a simple system dynamics model with reinforcing and balancing feedback loops [27].

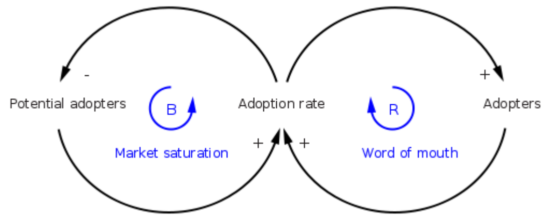

Figure 2. Feedback Loop

From [27]

In reinforcing feedback loops, an increase (or decrease) of a variable in the system induces a chain reaction of continued increase (or decrease) of that same variable. Balancing feedback loops represent the opposite case: as a variable increases (or decreases) the chain reaction causes other system variables to change and promote the opposite change in the initial variable. In Figure 2, the arrows have a plus or minus sign to indicate whether an increase in the variable next to the tail of the arrow causes an increase or decrease in the variable next to the arrow head. As illustrated in Figure 2, as the adoption rate increases, the number of adopters subsequently increases. Because the adoption rate is a function of the number of adopters, an increase in the number of adopters subsequently increases the adoption rate, which is an example of a reinforcing feedback loop. In addition, as the adoption rate increases, the number of potential adopters decreases, due to the fact that potential adopters transition to adopters per the adoption rate. This is an example of a balancing feedback loop. Stocks and flows are also crucial elements in a system dynamics model. Stocks are auxiliary variable which accumulate or deplete over time. Flows refer to the rates at which stocks accumulate or deplete. Stocks are typically represented by rectangles. Flows are typically annotated with arrows, or pipes, with specified valves, or rates [26]. Sources and sinks are annotated by clouds and are assumed to have infinite capacity within the model. A stock flows from a source and into a sink [26]. Auxiliary variables, constants, and data variables are also found in system dynamics models. The values of auxiliary variables are computed as a result of other variables in the model. Constants do not change during the simulation and data variables have values that change over time, although data variables do not depend on other model variables. Typically, data variables are applied as exogenous variables, variables whose values are not affected by system elements present in the systems dynamics model [26] [28]. System dynamics models have been developed to represent complex systems, particularly systems of technology diffusion. The following section characterizes two system dynamics models which illustrate the technology diffusion process.

Innovation Diffusion

According to Sterman [26], *S-shaped* growth patterns are anticipated in the diffusion and adoption of new technologies. It is useful to consider the growth of an idea or technology as an infectious disease spreading throughout a population. For example, the present practitioners of a technology *infect* a non-practitioner with the idea of using the technology. As the infection spreads, the population of practitioners increases as the *contagion* of the idea of using the new technology depletes the population of non-practitioners [26]. Sterman [26, p324] states that, "any situation in which people imitate behavior, beliefs, purchases of others, any situation in which people jump on the bandwagon, describes a situation of positive feedback by social contagion."

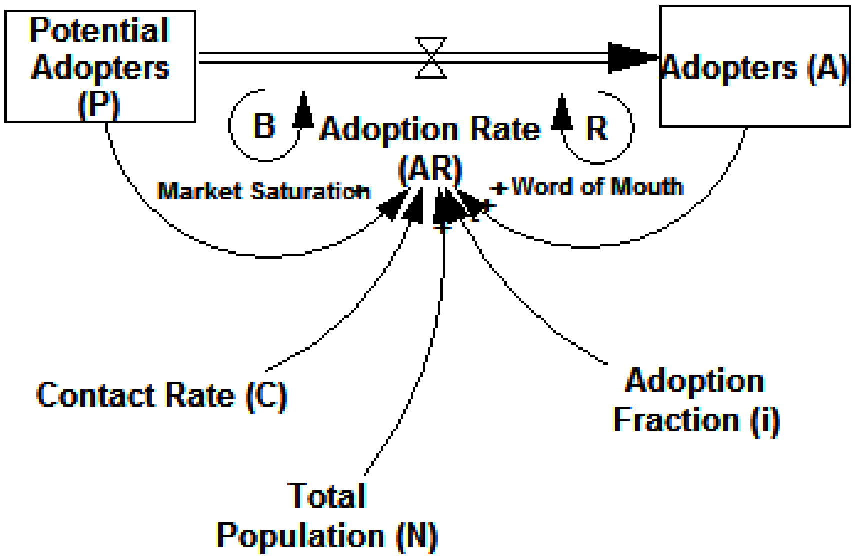

Figure 3. Innovation Diffusion Model

From [26, p325]

Figure 3 illustrates a modified case of innovation diffusion, according to Sterman [26, p325], and follows the social contagion example of the "spread" of using the technology as a result of a potential adopter coming into contact with an adopter or "infected" user of the technology at a specific rate per unit of time, denoted Contact Rate (C) in Figure 3. The percentage of contacts resulting in successful "infection" or adoption of the technology is denoted as the Adoption Fraction (i) in Figure 3. The following equations illustrate the relationships between variables in the Innovation Diffusion Model in Figure 3:

$$A = A_0 + \int AR \mathrm{d}t \tag{10}$$

where,

$$A_0 = \text{initial number of adopters}$$

$$AR = \text{adoption rate}$$

$$A = \text{number of adopters}$$

The potential adopters, P, is defined as follows:

$$P = N - A_0 - \int AR\mathrm{d}t \tag{11}$$

where,

$$N = \text{total population}$$

The adoption rate, AR, is defined as follows:

$$AR = c \times i \times P \times \frac{A}{N} \tag{12}$$

where,

$$C = \text{contact rate}$$

$$i = \text{adoption fraction}$$

Sterman [26] further states that the innovation diffusion model is an appropriate method of predicting innovation diffusion because it incorporates two necessary feedback components which are necessary for growth processes: the positive feedback loop, which generates the initial acceleration in growth, and the negative feedback loop, which generates the subsequent deceleration of growth [26]. Sterman suggests that any growth model necessitates a fractional growth rate that eventually declines to zero as the system gradually reaches carrying capacity. One of the faults of the innovation diffusion model is the lack of explanation for the initial number of adopters. Without an initial number of adopters in the innovation diffusion model, the model would lack initial contact between potential adopters and adopters and thus the subsequent growth behavior could be illustrated. This issue, also known as the startup problem according to Sterman [26], is rectified by the Bass diffusion model, which is discussed on the following section.

Bass Diffusion Model

The Bass diffusion model was developed by Frank Bass [3] in 1969 with the initial purpose of forecasting sales and diffusion of new technology innovations. The Bass diffusion model overcomes the startup problem of the innovation diffusion model and is one of the more popular growth models applied in marketing and technology management [26]. The Bass diffusion model provides a solution to the startup problem because it is designed with the assumption that potential technology adopters become aware of the new technology by external means, beyond that of contact with current adopters. Figure 4 illustrates the Bass diffusion model [26].

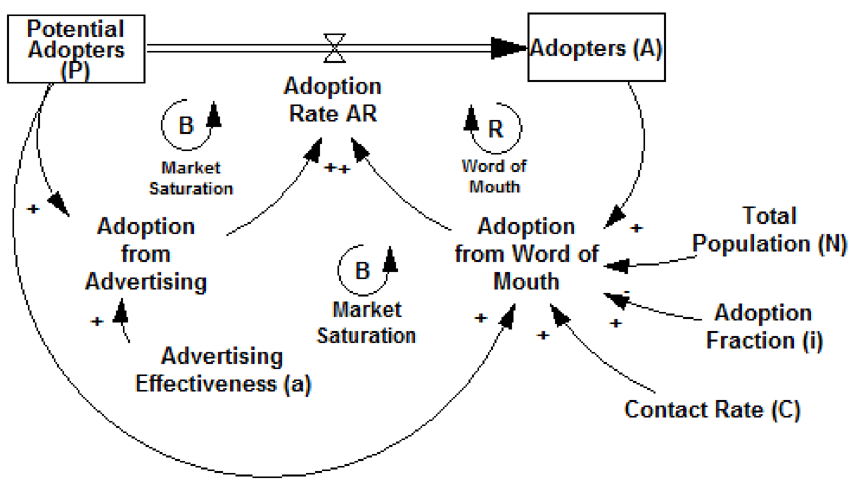

Figure 4. The Bass Diffusion Model

From [26, p333]

The sources of adoption in the Bass diffusion model are typically referred to as adoption from advertising and adoption from word of mouth. The adoption from word of mouth refers to the positive feedback loop found in the innovation diffusion model in which potential adopters become infected with the desire to adopt a technology as a result of contact with current adopters. The adoption from advertising refers to external sources of adoption, beyond that of contact with current adopters. The Bass diffusion model is designed with the assumption that the probability of successful adoption due to a potential adopter interacting with an adopter or advertisement is constant. The Bass diffusion model is also designed with the assumption that all potential adopters eventually adopt the technology and that adopters do not cease use of the product [3]. The Bass diffusion model does not take into account changes in consumer habits, according to Sterman [26]. The equations denoting the relationships between variables in the Bass diffusion model are similar to the innovation diffusion model equations previously discussed. The adoption rate, AR, in the Bass diffusion model is defined as follows:

$$AR = \text{Adoption from advertising} + \text{Adoption from Word of Mouth} \tag{13}$$

where,

$$\text{Adoption from advertising} = a \times P \tag{14}$$

$$a = \text{advertising effectiveness}$$

$$P = \text{potential adopters}$$

Advertising effectiveness is analogous with the adoption fraction which contributes to the adoption from word of mouth. Adoption from word of mouth is defined as follows:

$$\text{Adoption from Word of Mouth} = c \times \; i \times P \times \frac{A}{N} \tag{15}$$

The Bass diffusion model differs from the logistic diffusion model due to the fact that at time zero, in the Bass diffusion model, when there are no initial adopters of the technology, the sole contributing variable to adoption is the external adoption from advertising [26].

Model Validation

Although system dynamics provides insight regarding complex systems and problems, one of the underlying challenges of system dynamics is model validation. The following discussion illustrates how model testing is one element of the system dynamics model validation process. Sterman argues that model validity should not be solely based on how well a model fits historical data, given that fact that various diffusion models of different structure can produce different results but seemingly fit the historical data extremely well. According to Sterman,

> "the ability to fit historical does not, therefore, provide a strong basis for selecting among hypotheses about the nature or strength of different feedbacks that might be responsible for a system's dynamics [26, p330]."

Sterman also indicates that the predominant purpose of modeling is to gain insight into policy improvement. It is therefore beneficial for the model developer and the system subject matter expert develop improved confidence that the model will behave similarly to anticipated real world results. Sterman argues that fitting historical data may not provide insight into whether or not a model will successfully make accurate predictions. One of the major faults of the logistic model is an inability to illustrate anything but growth in the model. For example, demand of a product may decline in various years if the price dramatically increases and this phenomenon cannot be illustrated with a logistic model.

> "The utility of a model cannot be judged by historical fit alone but requires the modeler to decide whether the structure and decision rules of the model correspond to the actual structure and decision rules used by the real people with sufficient fidelity for the client's purpose [26, p331]."

However, fitting historical data should be considered as a valuable means by which model flaws may be identified and thus historical data fitting should not be neglected entirely. According to Forrester and Senge,

> “there is no single test to ‘validate’ a system dynamics model. Rather, confidence in a system dynamics model accumulates gradually as the model passes more tests and as new points of correspondence between the model and empirical reality are identified [10, p209].”

Forrester and Senge [10] state that the comparison of the system dynamics model with empirical reality provides a method of either confirming the validation of a model or determining the lack of validation of a model. Forrester and Senge [10, p414] also state that “model structure can be compared directly to descriptive knowledge of real-system structure; and model behavior may be compared to observed real-system behavior.” Forrester and Senge [10, p414] discuss several methods by which system dynamics model structure and behavior may be tested. Zagonel and Corbet [31] also discuss various methods by which confidence in the validity of system dynamics models may be gained through the categorization of various tests within five components of practice: system’s mapping, quantitative modeling, hypothesis testing, uncertainty analysis, and forecasting/optimization.

Table 1. Five Components of Modeling Practice

Loosely constrained ◄———► highly constrained

System's mapping	Quantitative modeling	Hypothesis-testing	Uncertainty analysis	Forecasting and optimization
Qualitative and inductive; involves drawing influence diagrams, CLDs, S&F diagrams, or any form of mapping or organization of the elements forming a system; attempts to get at the key causal interrelationships; focused upon identification of inter-organizational linkages and inter-dependencies	Quantitative and descriptive; involves formulation and simulation; largely system-focused; emphasizes S&F dynamics and the effects of delays; requires specification of the decision rules governing interrelationships; focused on representing and tracking consequences; sometimes rich in detail complexity	Quantitative and deductive; requires stating a hypothesis that explains dynamic behavior from the causal structure of the system; largely problem focused; emphasizes feedback-rich dynamics, learning, and exploration of the effect of changes in system structure; focused upon understanding and insight	Quantitative and exploratory; requires examining behavioral and quantitative sensitivity; emphasizes testing the robustness of the results produced from both quantitative modeling and hypothesis testing; focused upon uncertainty and risk, and identification of points of leverage for intervening in the system	Quantitative and predictive; within the range of the parameter space specified in the model, attempts to shed light on future behavioral patterns and the cross-sectional quantitative values of variables of interest, or to suggest optimal or robust solutions that maximize or "satisfice" particular utility functions

From [31, p6]

Table 1 illustrates the characteristics of the five components of modeling proposed by Zagonel and Corbet [31, p6]. The system's mapping component is considered to be qualitative, inductive and is also considered to be a useful method of of potentially gaining dynamic insights, according to Zagonel and Corbet [31]. The quantitative modeling component is similar to the system's mapping component and is primarily focused on gaining improved understanding of the stocks and flows within the system dynamics model. The hypothesis-testing component differs from the previously discussed components insomuch as focusing on the problem rather than the structure of the model. The hypothesis-testing component is developed with the motivation of determining whether or not the problem of interest is adequately addressed. The uncertainty analysis component encompasses determining how adversely an output of interest varies with variation of other variables within the model across realistic parameter ranges. The forecasting and optimization component comprises the determination of possible outputs in the future and achievement of various goals given variation of parameters across appropriate ranges. Forrester and Senge [10] maintain that the initial steps of validation begin as the model builder gains confidence in the model behavior, insomuch as discovering model behavior which is expected of the real system.

Forrester and Senge [10] also state that the process of validation extends beyond the developer of the model and into the broader "view of scientific knowledge as public knowledge [10, p414]." Because of the breadth of experience in the scientific community, a model may be viewed differently among personnel of various fields of study. For example, a scientist may determine that a model is "useful if it generates insight into the structure of real systems, makes correct predictions, and stimulates meaningful questions for future research," [10, p415]. Public and political leaders may determine that a model is useful given that it explains "causes of important problems and provides a basis for designing policies that can improve behavior in the future," according to Forrester and Senge [10, p415]. Forrester and Senge [10] state that the confidence in a system dynamics model increases as the model proves successful against various tests.

> "Validity is also relative in the sense that it can only be properly assessed relative to a particular purpose. It is pointless to try to establish that a particular model is useful without specifying for what purpose it is being used [10, p415]."

Structure-Verification Test

Forrester and Senge [10, p416] suggest that "verifying structure means comparing structure of a model directly with structure of the real system that the model represents." The structure-verification test falls under the system's mapping component of the five components of modeling proposed by Zagonel and Corbet [31]. This portion of testing involves verify 'face validity,' insomuch as a structural assessment of the model to determine whether or not the structure of the model is consistent with relevant descriptive system knowledge, according to Zagonel and Corbet [31]. In order for a model to successfully pass the structure-verification test, the model "must not contradict knowledge about the structure of the real system [31, p416]." The structure-verification test is initially conducted by the model developer, given the model developer's knowledge of the system. Forrester and Senge [10] state that the structure-verification test is then extended to external parties who did not initially contribute to the model development in order to clarify areas of improvement or alteration of the model to improve model fidelity.

Parameter-Verification Test

An interrelated test with the structure-verification test is the parameter-verification test, which entails the determination of the plausibility of model parameters conceptually and numerically corresponding to real life parameter values. The parameter-verification test may be considered to fall under the quantitative modeling component of the five components of modeling proposed by Zagonel and Corbet [31]. A parameter is considered to conceptually correspond to real life if the "parameters match elements of system structure," according to Forrester and Senge [10, p417]. A parameter is considered to numerically correspond to real life if the parameter ranges are close to the ranges of real life parameters.

Dimensional-Consistency Test

Forrester and Senge [10, p419] maintain that the dimensional-consistency test encompasses "dimensional analysis of a model's rate equations." The dimensional consistency test also falls under the quantitative modeling component of the five components of modeling proposed by Zagonel and Corbet [31]. Although Forrester and Senge [10] indicate the potential tedium of the dimensional-consistency test, it is a crucial test to ensure consistency within the system dynamics model and is "most powerful when applied in conjunction with the parameter-verification test," according to Forrester and Senge [10, p419].

Table 2. Twenty-Four Tests Organized by Five Components of Modeling

System's mapping	Quantitative modeling	Hypothesis testing	Uncertainty analysis	Forecasting & optimization
S #2a -- F&S Str #1a	1 - Face validity (structural assessment through *deductive* process)			
S #2b -- F&S Str #1b	2 - Validity of decision rules (*structural* focus)			
	S #2c -- F&S Str #1c	3 - Physical conservation		
	S #3 -- F&S Str #5	4 - Dimensional consistency		
	S #6	5 - Integration error		
	S #5a -- F&S Str #3	6 - Extreme conditions tests (*equations* focus)		
	S #4 -- F&S Str #2	7 - Parameter assessment		
	S #7a -- F&S Beh #1a	8 - Basic-behaviors reproduction		
	S #7 b-- F&S Beh #1b	9 - *Endogenous* behavior-reproduction tests		
	S #1a -- F&S Beh #7	10 - Boundary adequacy tests (*modes of behavior*)		
		S #7c -- F&S Beh #1c	11 - Qualitative *problem-behavior* test	
		S #1b -- F&S Str #4	12 - Boundary adequacy (*problem endogeneity*)	
		S #2d -- F&S Str #1d	13 - Validity of decision rules (*policy* focus)	
		S #10 -- F&S Beh #5	14 - Assessment of surprise behaviors	
		S #11a -- F&S Beh #8	15 - *Behavior* sensitivity analysis	
		S #5b -- F&S Beh #6	16 - Extreme condition tests (*model behaviors* focus)	
		S #8 -- F&S Beh #3	17 - Behavior anomaly tests (changed *assumptions* tests)	
		S #9 -- F&S Beh #4	18 - Family member (generalizability)	
		Quantitative sensitivity analysis - 19	S #11b -- F&S Beh #8	
		Policy sensititivity analysis - 20	S #s 1+11c -- F&S Pol #4	
		Boundary adequacy (*policy implications*) - 21	S #1c -- F&S Pol #3	
			Behavior correspondence - 22	S #7d -- F&S Beh #1d
			Behavior prediction - 23	F&S Beh #2
			Changed-behavior prediction - 24	F&S Pol #2
System's mapping	Quantitative modeling	Hypothesis testing	Uncertainty analysis	Forecasting & optimization

Test categories:
- Basic
- Intermediate
- Advanced

S - Sterman (2000); F&S - Forrester and Senge (1980); Str - Structure; Beh - Behavior; Pol - Policy implications

From [31, p12]

Table 2 illustrates the organization of the 24 tests proposed by Zagonel and Corbet [31, p12] to determine the relative confidence in the validity of a system dynamics model.

According to Sterman [26], the determination of whether or not a model is a robust means of determining likely system behavior is not solely based on how will the model results fit historical data or statistical testing, but is rather a value judgment made by both the client or subject matter expert and the model developer. Although the models are initially determined to be valid, additional clarification with the company is necessary to definitively determine whether or not the models developed are adequate representations of potential system behavior.

2.5 Carbon Nanotube Fabrication

Although comprehension of gaining confidence in a system dynamics models is an imperative element when developing predictive models, it is also imperative to understand the product of interest for the models developed. In this study, CNTs are the primary product of interest. Thus, the purpose of this section is to provide insight into the primary product of focus for this analysis: CNTs. The purpose of this section is to surmise that various techniques implemented to fabricate CNTs, which are highly desirable for nanotechnology applications due to their various valuable mechanical and electrical properties.

However, the incorporation of CNTs with nanotechnology faces serious challenges due to the intricate and problematic growth of CNTs, according to Zhang, Wei, and Ramanath [32]. The method of chemical vapor deposition (CVD) has been applied to increase the efficiency of the growth of CNT networks. The CVD method is a fairly robust method to produce massive amounts of CNT architectures. The CVD method requires a source of carbon as well as a metal catalyst with metallocene. The CVD method is attractive since it does not require prior catalyst deposition. In the CVD method, the growth of CNTs is site-selective on existing $SiO2/Si$ substrates [32]. Because the method of developing metal catalyst templates is no longer a requirement in this method, it is solely necessary to pattern the substrate silica on which the aligned CNTs will grow. This method is accomplished easily on the nanometer scale [32].

Arc Discharge

During the arc discharge process, the CNTs self-assemble in the presence or absence of a catalyst. The chemical vapor required for the arc discharge process is generates by an arc discharge between two carbon electrodes [22].

Laser Ablation

The laser ablation process occurs inside an oven at 1,200°C. A laser is implemented to vaporize a graphite target inside the oven to generate a hot vapor plume. Small carbon molecules and atoms condense to form large clusters as the vaporized species cools. The clusters grow into single-wall carbon nanotubes (SWCNT). The SWCNT can diffuse through or over the surface of the catalyst particles [22].

Chemical Vapor Deposition

The chemical vapor deposition (CVD) process requires an energy source to transfer energy to a gaseous carbon molecule. This energy transfer causes the molecule to become reactive atomic carbon. Energy sources may include plasma or a resistively heated coil. The gaseous carbon molecule may include methane, carbon monoxide, or acetylene. The resulting reactive carbon molecule diffuses toward a heated substrate. The substrate is coated with a catalyst which may include Ni, Fe, or CO. The molecule binds to the catalyst and CNTs are formed. This delicate process occurs only when precise environmental factors are controlled [22].

Flame Synthesis

The flame synthesis process is potentially cost-effective for the growth of CNTs in bulk quantities and is a relatively new growth method. A fuel-rich flame is defined as a "high-temperature environment suitable for CNT formation in the presence of metal catalysts [22, p69]." The increased temperature required for this process occurs with combustion of a portion of the hydrocarbon gas. The residual fuel acts as the required hydrocarbon reagent. CNTs developed through flame synthesis have unique characteristics including low density and high surface areas. These properties are attractive due to the enhancement of the adsorption properties of the CNTs [22].

2.6 Carbon Nanotube Properties

CNTs are composed of graphitic cylinders measured at a few nanometers in diameter which maintain unique electronic properties. It is interesting to consider CNT behavior as quantum wires, nonlinear electronic elements, and transistors. One particularly interesting composition of CNTs is referred to as the "bucky shuttle," according to Kwon, Tomanek, and Iijima [15]. CNTs assemble in the form of the "bucky shuttle" under specific conditions [15].

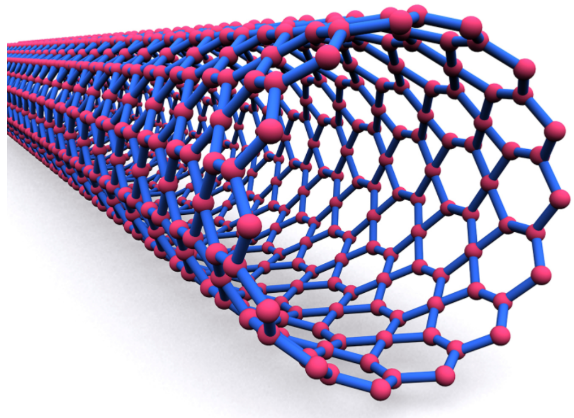

Figure 5. Carbon Nanotube Structure

From [29]

Figure 5 illustrates the structure of CNTs on the nanoscale [29]. CNTs are 1-2 nm (nanometer) in diameter and are comprised of a number of layers of carbon atoms in a cylindrical shape. Single-walled carbon nanotubes (SWCNTs) are composed of a single layer of carbon atoms. Multi-walled carbon nanotubes (MWCNTs) are composed of multiple concentric tubes of carbon atoms and are typically $\geq$ 1 mm (millimeter) in length and 20 nm in diameter. CNTs are possibly one of the strongest known fibers due to their high tensile strength. CNTs are 100 times stronger than steel while having one-sixth the weight. CNTs are also typically desirable due to other traits including high surface area, conductivity, potentially high molecular absorption, and electronic properties [2].

2.7 Carbon Nanotube Applications

CNT applications presently being explored include polymer composites, electron field emitters, electromagnetic shielding, batteries, super capacitors, hydrogen storage and structural composites. The majority of applications requires mass-production of CNTs and thus the progression from research and development to commercial production is currently of interest [2]. Table 3 illustrates some of the applications of CNTs today.

Table 3. CNT Applications

Application	Description
Scanning Microscope Tips	Point of contact with nanoscale sample
Nanosensor	Ultrahigh-sensitivity sensing element
Batteries/supercapacitors	Paper-thin, lightweight, flexible, high-efficiency batteries
Field emission devices	Compact X-ray devices, flat-panel displays, specialty lighting
Drug Delivery Systems	Used to target and deliver therapy; also possess useful antioxidant properties
Semiconductors	CNTs grown on-chip can increase clock speed and reliability
Printed electronics	Potential applications include low-cost RFID tags
Memory	Could replace DRAM, SPAM, and flash memory with a universal memory design
Hydrogen storage	Mobile hydrogen storage
Conductive fibers	Smart textiles
Ultracapacitors	Ultracapacitor electrodes made from vertically aligned nanotubes

From [22]

CNTs and other hollow nanoparticles are predominantly leveraged commercially as filler materials in various polymer nanocomposites. Beyond CNT use in nanocomposites, other commercial applications are limited small quantities of CNTs applied in the fabrication of canning microscope probes, nanosensors, and this form-factor supercapacitors [22].

2.8 Carbon Nanotube Market

Table 4 illustrates the increase the worldwide commercial MWNT capacity and revenue from 2014 to 2019 [22]. The net revenues are calculated with the base price of

$100.00 per kilogram, or $0.10 per gram, for commodity grade MWNT, as illustrated in Table 4, according to BCC [22].

Table 4. Global MWNTs Tier 1 Companies Market by Capacity and Revenue

Capacities/Revenues	2014	2015	2016	2017	2018	2019
Global production capacities (tons)	1,445	1,485	2,385	2,995	3,395	4,195
Global Revenues ($M)	143.6	147.0	223.5	270.1	270.1	270.1

From [22, p448]

Although Table 4 indicates an increasing trend in global production capacity, it is difficult to assume a consistent increase with high fidelity given the challenge of customer acceptance of CNTs as a financially competitive material or a substitutive material. In comparison with the global CNT market, Table 5 indicates the current U.S. Commodity-Grade MWNTs Tier 1 Companies, according to BCC [22].

Table 5. U.S.Commodity-Grade MWNTs Tier 1 Companies Market

Company(Location/Capacity/Price/Revenue	2014	2015	2016	2017	2018	2019
CNano Technology Ltd. (U.S./China)	225	225	225	375	375	375
Hyperion Catalysis International (U.S.)	100	100	100	100	100	100
Hythane Co. (U.S.)/Eden Energy (AU)	40	40	100	100	100	100
Total Production Capacities (ton)	365	365	365	575	575	575
Benchmark price ($/kg)	100	100	100	75	75	75
Total Revenues ($ millions)	36.5	36.5	36.5	43.1	43.1	43.1

From [22, p457]

Additional information from the company regarding annual CNT product output is required to more accurately discern the level of competition posed by the company. Table 5 lists various CNT manufacturing companies and indicates that the benchmark price varies from $100.00 per kilogram, or $0.10 per gram, to $75.00 per kilogram, or $0.07 per gram, between 2014 and 2019. Subsequent analysis will determine if the company is producing CNTs at a competitive price and production rate.

2.9 Chapter Summary

This chapter reviews the history of technology diffusion, technology diffusion models, and technology substitution models. This chapter also suggests possible CNT applications, CNT properties, and CNT fabrication methods. This chapter provides information regarding the CNT global and North American markets. This section also provides an explanation for the role system dynamics plays in the development of technology diffusion models. This collective literature review postures the subsequent development of the methodology and analysis of this study.

III. Methodology

Essentially, all models are wrong, but some are useful.

–George E. P. Box

3.1 Chapter Overview

This chapter presents the methodology implemented to achieve the objectives outlined in Chapter I. In this study, we apply system dynamics with estimated and assumed parameter inputs, to determine the potential point and scenario in which the company may achieve commercial viability in terms of producing both CNT sheets (product A) and CNT yarn (product B). Based on notional scenarios, system dynamics models are developed through the utilization of Vensim, a commercial software developed for the purpose of system dynamics modeling and simulation. It should be noted that the methodology is implemented with limited information regarding the company of interest and additional information from the company is necessary to implement a more accurate methodology and determine the actual company viability.

3.2 The Model

The models were designed in Vensim, a commercial software product used to build and simulate system dynamics models. The initial system dynamics models developed to study the manufacturing and market diffusion of CNTs in this study were developed by Maj Brian B. Stone [28] and include five sub-models: cash-flow sub-model, manufacturing sub-model, sales revenue sub-model, expenses sub-model, and product demand sub-model. Although these models are potentially applicable for future analysis, given the limited information for this study, the following models were solely implemented for the notional analysis of this study: the CNT innovation diffusion model, technology learning sub-models, and the technology cost sub-models. See Appendix A for tables of variables, variable types, units, and equations for the CNT innovation diffusion model, technology learning sub-models, and the technology cost sub-models. Two sets of the technology learning and technology cost sub-models are developed for the purpose of analysis of both CNT sheet and CNT yarn products. Although these models were developed with previously discussed assumptions and limitations, as this research evolves, the models may be modified with clarification from the company regarding the initial assumptions and limitations in order to improve confidence in model performance. CNT sheet and CNT yarn products are identified in the models as product A and product B, respectively. A third scrap product, labeled product C, is derived from the scrap material produced as a result of manufacturing CNT sheets and CNT yarn. Because specific information regarding the scrap material was not available, the analysis in this study does not incorporate the scrap product. However, as this research evolves, the sub-models can be modified to incorporate the scrap product. Note that the technology learning and technology cost sub models incorporate shadow variables, which are denoted with gray font. A shadow variable is a variable which is incorporated from another model. Some of the CNT innovation diffusion model variables appear as shadow variables in both the technology learning and technology cost sub-models.

Cash Flow Sub-Model

The cash flow model for the technology manufacturer shows the relationships between investment, additional income, sales revenue, and expenses for the company manufacturing the new technology [28]. The stock variable is working capital, which is defined as the summation of profits, investments, and additional income. The auxiliary variable is manufacturing profit. The flow variables are additional income per period, income unrelated to manufacturing, and investments, from private and government sources. Exogenous variables to the cash flow sub-model are sales revenue, from the sales revenue sub-model, production expenses, from the expenses sub-model, and operating expenses, from the expenses sub-model. The cash flow sub-model is shown to the left of the dashed line in Figure 6.

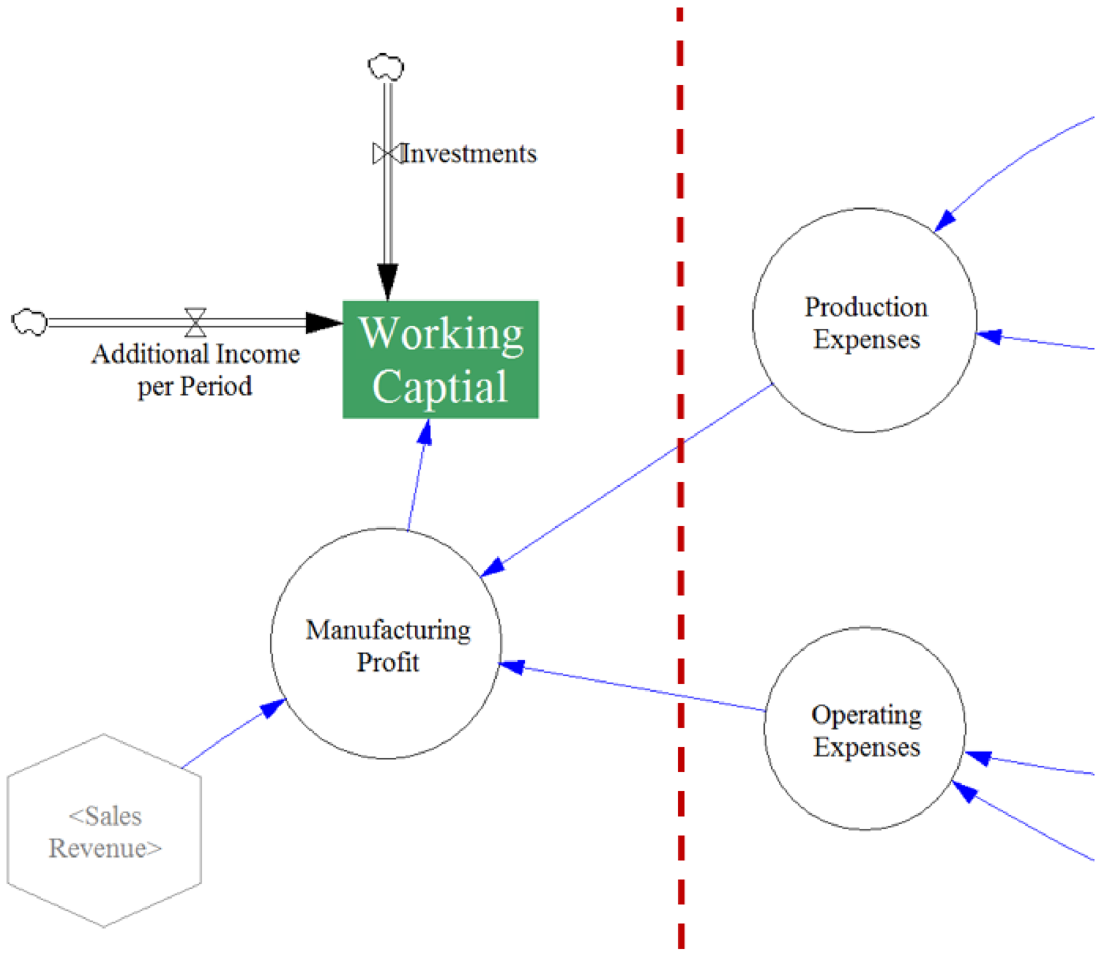

Figure 6. Cash Flow Sub-Model

From [28]

Making manufacturing profit a separate variable allows the model to track profits per period and provides insight into the profitability of the manufacturing process independent of investments and other income.

Manufacturing Sub-Model

The manufacturing sub-model involves the relationships between the amount of available plant space, the number of CNT manufacturing machines, for product both CNT sheet, product A, and CNT yarn, product B, the amount of machine downtime, and the production capacity for products A and B [28]. The stock variables are the facility size, the number of machines, the amount of machine downtime, and the production capacity for product A and B. The data variables are the production rate for each machine type. The flow variables are the square feet renovated in the plant, the change in downtime for each machine type, and the purchases of each machine type. The manufacturing sub-model is shown in Figure 7.

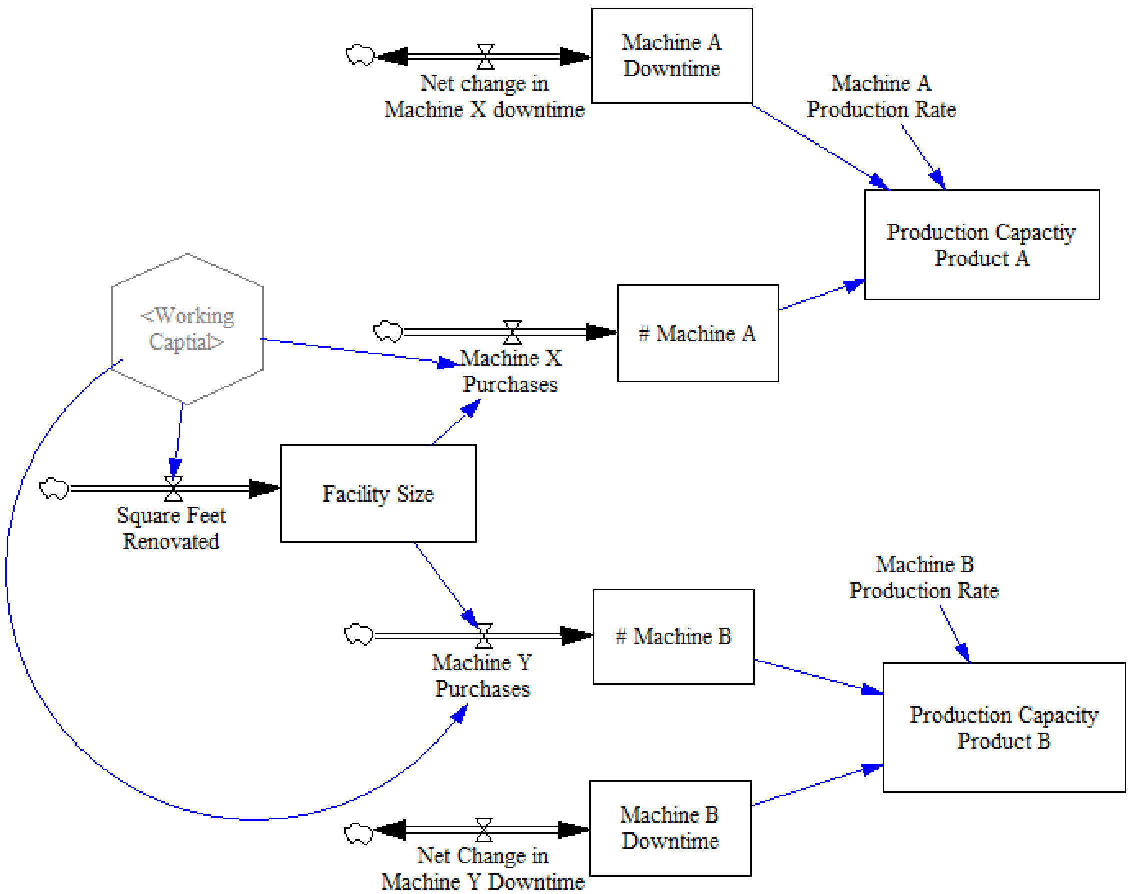

Figure 7. Manufacturing Sub-Model

From [28]

The exogenous variable to the manufacturing sub-model, although not exogenous to the full model, is the working capital stock variable from the cash flow sub-model. The production capacity stock variables for products A and B are exogenous variables in the sales revenue sub-model. Working capital and production capacity are part of the reinforcing feedback loop that occurs when an increase in the facility size and the number of machines causes an increase in production capacity, which increases sales revenue, which increases working capital, which can be used to increase facility size and the number of machines [28].

Sales Revenue Sub-Model

The sales revenue sub-model shows the relationships between the following variables: production rate for product A, CNT sheets, and B, CNT yarn, and C, scrap product; the inventory for product A, B, and C; the sale price for product A, B, and C; and the sales revenue of products A, B, and C. A unique aspect of the technology being modeled is that there are two types of sales [28]. The first is standard customer sales for existing product lines using standard formulas and dimensions. The second is called R&D sales, which are typically ordered by government entities for one-time purchases that usually require customized adjustments to the standard production formulas or product dimensions. As a final note, product C is a by-product of products A and B and is therefore modeled somewhat differently. The stock variables are the inventory for Products A, B, and C. The dynamic variables are the number of standard and R&D customers for products A and B, the revenue from products A, B, and C, the standard price for products A, B, and C, the R&D price for products A and B, and the overall sales revenue. The data variables are the target production rates for products A and B, the proportion of customers that make R&D purchases for products A and B, the average amount of product A and B purchased by R&D customers, and the average amount of product A and B purchased by standard customers. The rate variables are production rates for products A, B, and C, the standard sales rates of products A, B, and C, and the rate of R&D sales for products A and B.

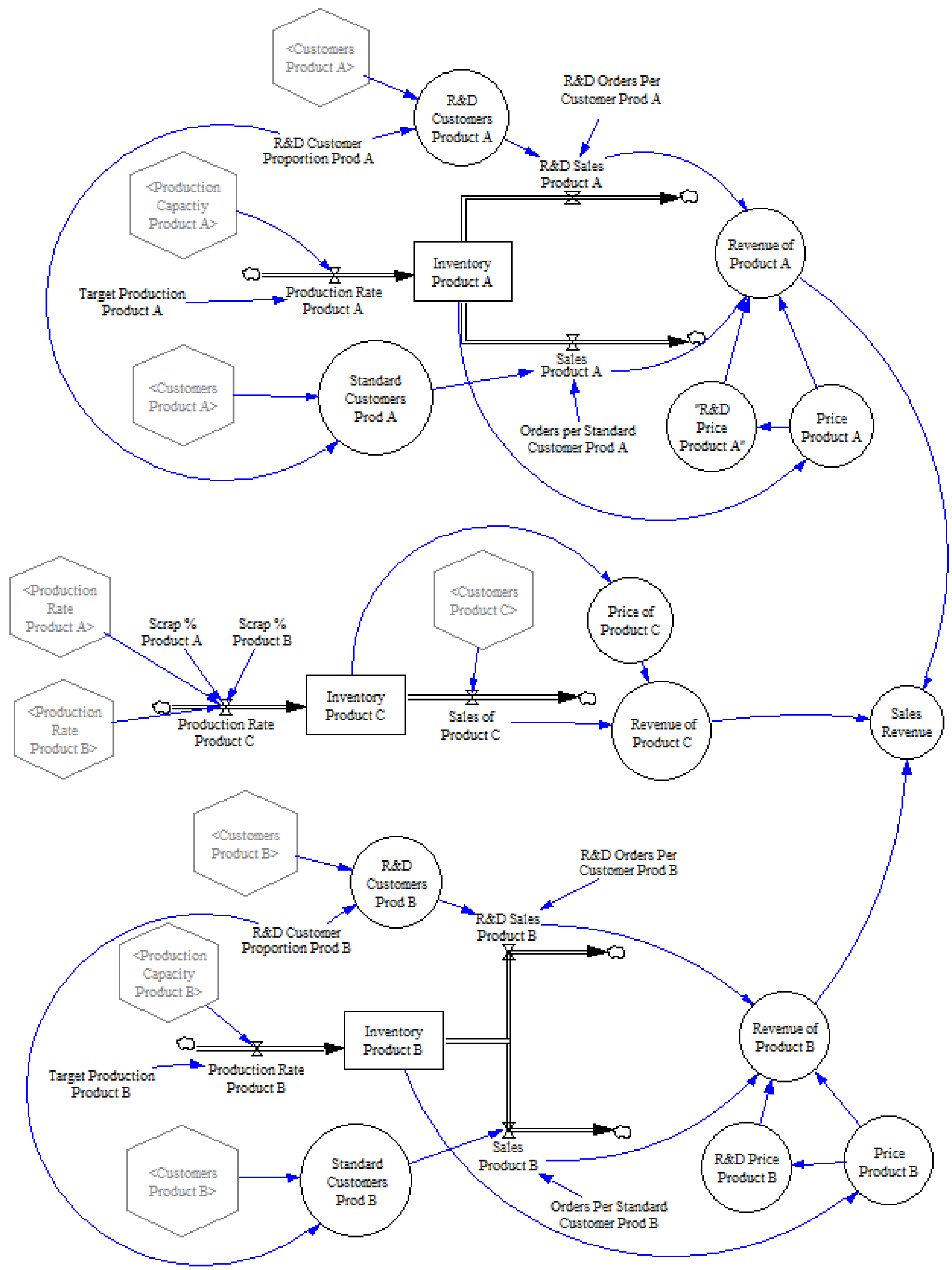

Figure 8. Sales Revenue Sub-Model

From [28]

Exogenous variables to the sales revenue sub-model include the production capacity for products A and B, and the number of customers for products A, B, and C. The sales revenue sub-model is shown in Figure 8. The portion for product B has been omitted since it is identical to the model for product A. As mentioned in the previous section, production capacity and sales revenue are part of the reinforcing feedback loop that promotes a continued increase in working capital. The number of customers for products A, B, and C are also part of a reinforcing feedback loop that occurs when an increase in sales revenue causes an increase in production capacity, which attracts more customers who require higher-volume production. This results in a further increase in sales revenue [28].

Expenses Sub-Model

The expenses sub-model shows the relationships among the plant, equipment, and personnel variables and the operating expenses [28]. The stock variables are the number of overhead employees and the number of employees involved with manufacturing. The auxiliary variables are the energy costs from operating the machines, the HVAC (Heating, Ventilation, and Air Conditioning) costs, the overall energy costs, the overall employee wages, the variable costs of products A and B, the overall plant expenses, the overall production expenses, and the overall operations expenses. The data variables include the raw material costs for products A and B, the average wages paid to overhead and manufacturing equipment operators, the facility fixed cost, such as maintenance, rent, and so forth, and the cost per square foot for refreshing the air on the manufacturing floor. The expenses model is shown in Figure 9.

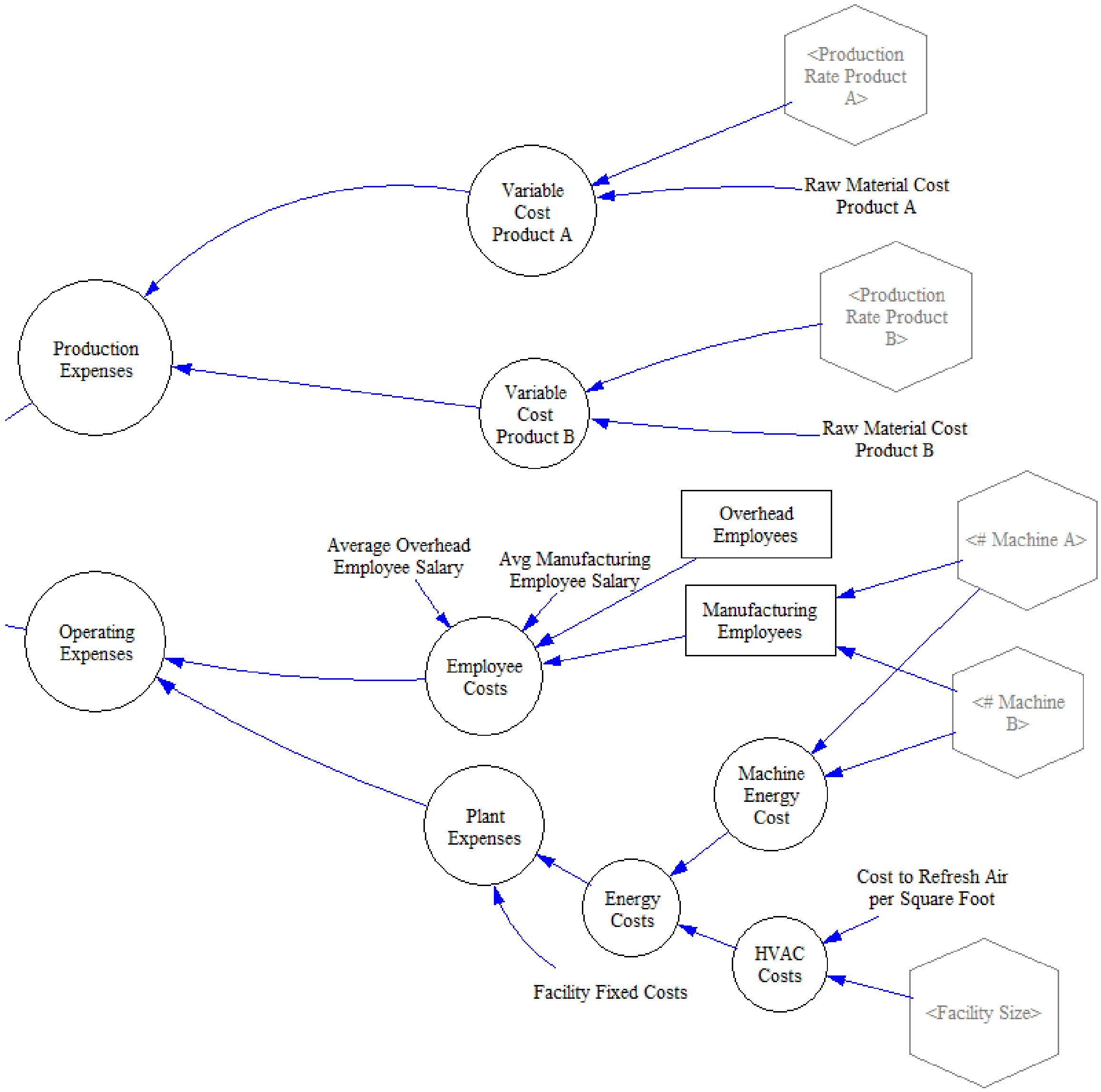

Figure 9. Expenses Sub-Model

From [28]

The exogenous input variables to the expenses sub-model are, the facility size, from the manufacturing sub-model, the number of machines producing product A and B, from the manufacturing sub-model, and the production rates for products A and B, from the Sales Revenue Sub-Model. The production expenses and operation expenses auxiliary variables are inputs to the cash flow sub-model. The production and operating expenses are part of a balancing feedback loop that occurs when an increase in working capital causes an increase in the number of machines and the facility size, which increases the production and operating expenses, which causes a decrease in working capital [28].

Product Demand Sub-Model

The product demand sub-model illustrates how advertising, word-of-mouth, production capacity, and product price influence the number of customers for product A, or CNT sheets, product B, or CNT yarn, and product C, or scrap material produced by CNT sheets and yarn [28]. This model is based on a modification of the traditional Bass diffusion model for technology [3]. The stock variables in the product demand sub-model include the total population, the potential customers for each product, and the customers for each product. The dynamic variables are the fraction of the population willing to adopt each product, the number of people willing to adopt each product, the number of people who adopt from advertising for each product, the number who adopt from word-of-mouth for each product, the probability of contacts with adopters for each product, the degree of social contacts among the adopters, and the number of contacts with adopters for each product. The data variables are the reference price of each product, the contact rate for the potential adopters, the advertising effectiveness, and the adoption fraction for each product. The flow, or rate, variables are the net population increase and the adoption rates for each product. The product demand Sub-model is shown in Figure 10.

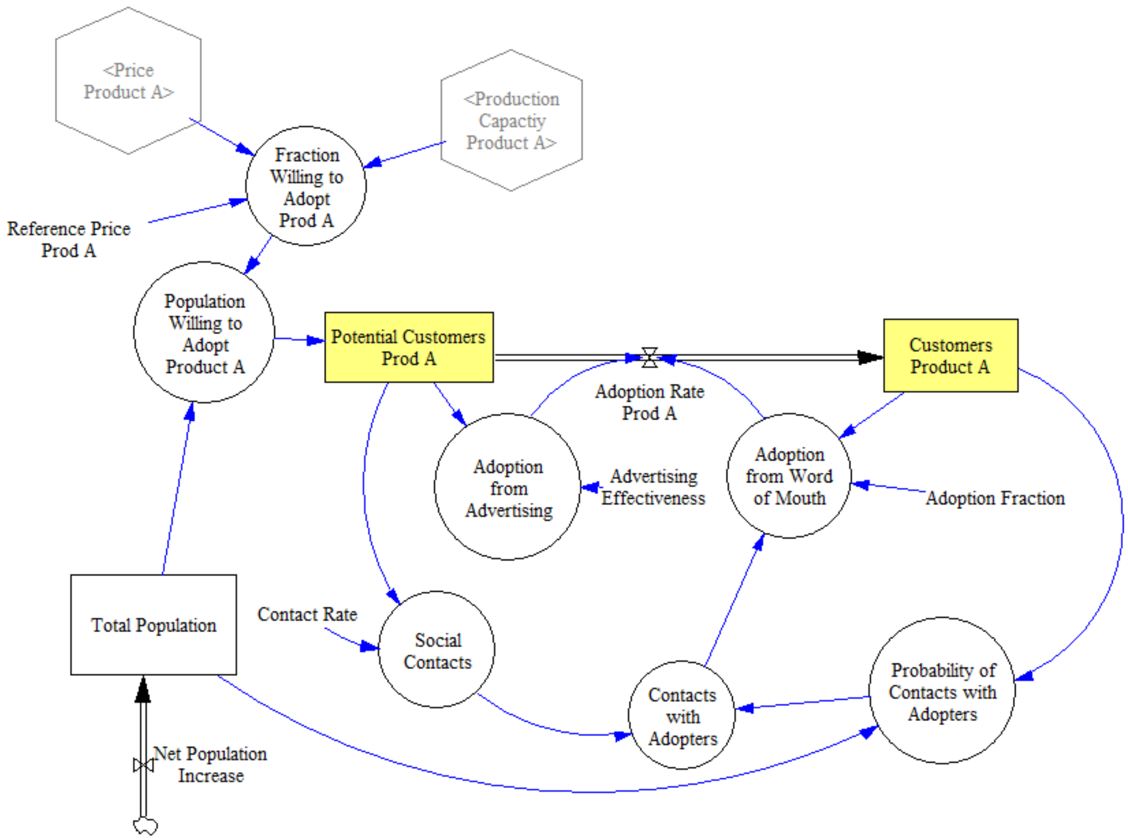

Figure 10. Product Demand Sub-Model

From [28]

Note that only the demand model for product A is shown, as the models for products B and C are identical. The product demand sub-model is part of two feedback loops. There is a reinforcing feedback loop where an increase in customers for the products causes an increase in sales revenue, which causes an increase in working capital, which can be used to build more production capacity. An increase in production capacity increases demand for the new technology which increases customers for the products. There is a balancing feedback loop where an increase in customers for the technology causes an increase in sales, which causes a reduction of the inventory, which causes an increase in the price of the product, which decreases the number of potential customers [28].

CNT Innovation Diffusion Model

The CNT innovation diffusion model is the primary model used in this analysis. In this model, the rate of transition by which non-practitioners become practitioners of a technology is the driving force which contributes to the rate of diffusion of a technology. According to Sterman [26], potential adopters do not immediately adopt a new technology; rather the adoption occurs gradually with time. The adoption rate depends on the following:

1. Current number of practitioners
2. Current number of potential adopters
3. The effectiveness of practitioners convincing non-practitioners to become practitioners
4. The contact frequency between practitioners and non-practitioners

It is often helpful to consider the analogy of practitioners of a technology as "infected" or "predatory" individuals with the desire to use the technology of interest while the non-practitioners are the "uninfected" or "prey" who have not yet adopted the technology of interest. The population is comprised of the "non-practitioners" and "practitioners." Of the "non-practitioners" population, a percentage transition to "non-practitioner contacts" at a rate of "contact rate." The predatory "practitioners" come into contact with the prey of "non-practitioners" as a result of "practitioner prevalence," which is the percentage of practitioners within the total population. As the practitioner prevalence increases, and the "non-practitioner contacts" increase, the "practitioner with non-practitioner contacts" increases. As non-practitioners come into contact with practitioners, also known as "practitioner with non-practitioner contacts," a percentage of contacts, also known as "adoption fraction," actually become "infected" with the desire to adopt the technology and thus result in successful adoption of the technology, also known as "adoptions."

The rate of successful adoption of the technology is a driving force behind the "production rate," or the rate at which technology is produced by the company. "Production rate" is also influenced by the "product per adoption," or the amount of product purchased by a new adopter, "product per practitioner," or the amount of product required by a preexisting practitioner, and the "production capacity," or the maximum amount of product possible generated in a given time period, in this case one year. The "cumulative amount" corresponds to the cumulative generation of product and depends on the rate of production. The "sales revenue" depends on the "product price," or market price of the product, as well as the "production rate." As the "production rate" increases, the "sales revenue increases." The "cumulative revenue" corresponds to the cumulative revenue generated by "sales revenue." Similarly, "cumulative production cost" corresponds to the cumulative cost of product generation and is dependent on the "cost," or generation cost, of one unit of product. "Cost" is the also dependent on the "production rate." The "net revenue" of a product is the result of the difference between "cost" and "sales revenue." The overall net revenue is the result of the summation of each product's net revenue.

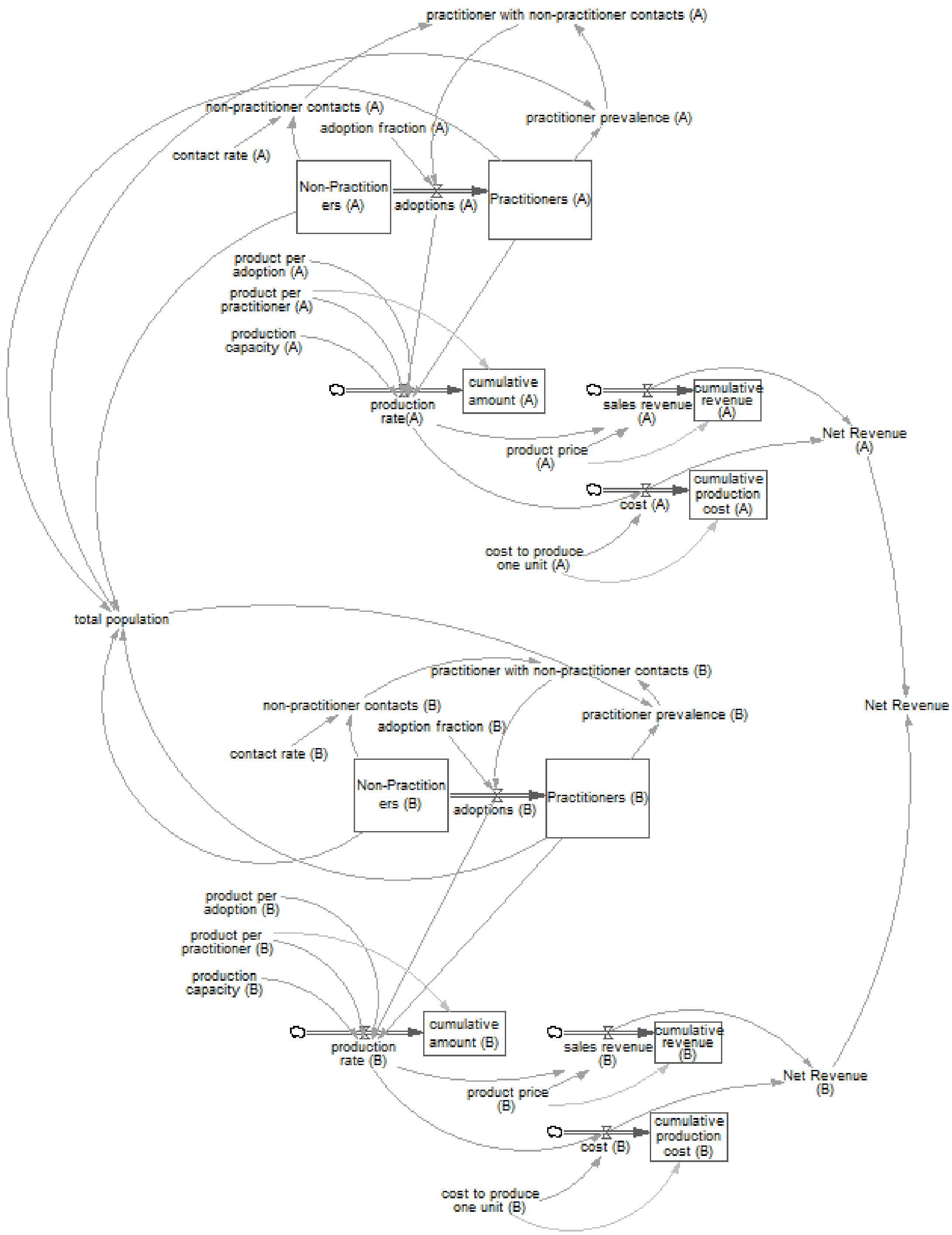

Figure 11. CNT Innovation Diffusion Model

As illustrated in Figure 11, this model incorporates the interaction of two products.

This model is modified based on diffusion models found in the Vensim User Guide [30] and the innovation diffusion model discussed by Sterman [26]. Product A corresponds to CNT sheets and product B corresponds to CNT yarn. The adoption and diffusion of both products follows the previous explanation of variable interaction. This model is designed with the motivation of determining the potential net revenue of the company in terms of the two primary products of interest. The total population N is defined as follows:

$$N = N_{aa} + N_{na} + N_{ab} + N_{nb} \tag{16}$$

where,

$$N_{aa} = \text{number of practitioners of product A (CNT sheets)}$$

$$N_{aa} = \text{number of non-practitioners of product A (CNT sheets)}$$

$$N_{ab} = \text{number of practitioners of product B (CNT yarn)}$$

$$N_{ab} = \text{number of non-practitioners of product B (CNT yarn)}$$

The following equations are applicable to both CNT sheets and CNT yarn portions of the model. The relationship between non-practitioners and practitioners is defined as follows:

$$N_a = N_{ao} + \int R_a \cdot \mathrm{d}t \tag{17}$$

where,

$$N_a = \text{number of practitioners}$$

$$N_{ao} = \text{initial population of practitioners}$$

$$R_a = \text{adoption rate}$$

The adoption rate, R_a, is defined as follows:

$$R_a = A_f \times P_c \tag{18}$$

where,

$$A_f = \text{adoption fraction}$$

$$P_c = \text{practitioner with non-practitioner contacts}$$

Practitioner with non-practitioner contacts, P_c, is defined as follows:

$$P_c = NP_c \times \theta_p \tag{19}$$

where,

$$NP_c = \text{non-practitioner contacts}$$

$$\theta_p = \text{practitioner prevalence}$$

Non-practitioner contacts, NP_c, is defined as follows:

$$NP_c = R_c \times N_n \tag{20}$$

where,

$$R_c = \text{contact rate}$$

$$N_n = \text{non-practitioners}$$

Production rate, R_p, is defined as follows:

$$R_p = R_a \times \beta_a \times \beta_p \times \kappa \tag{21}$$

$$\beta_a = \text{product per adoption}$$

$$\beta_p = \text{product per practitioner}$$

$$\kappa = \text{production capacity}$$

The cumulative amount, C, is the cumulative total amount of product produced and is defined as follows:

$$C = N_{ao} \times \beta_p + \int R_p \cdot \mathrm{d}t \tag{22}$$

The cumulative revenue, C_r, is the cumulative revenue generated over time and is defined as follows:

$$C_r = N_{ao} \times \omega_p \int S_R \cdot \mathrm{d}t \tag{23}$$

where,

$$\omega_p = \text{product price}$$

$$S_r = \text{sales revenue}$$

The sales revenue rate, S_r, is defined as follows:

$$S_r = R_p \times \omega_p \tag{24}$$

The cumulative production cost, C_c, is defined as follows:

$$C_r = N_{ao} \times \omega_c + \int C_t \cdot \mathrm{d}t \tag{25}$$

where

$$\omega_c = \text{cost to produce one unit}$$

The cost rate, C_t, is defined as follows:

$$C_t = R_p \times \omega_c \tag{26}$$

The net revenue, N_r, of each product is defined as follows:

$$N_r = S_r + C_t \tag{27}$$

The overall net revenue, N, is defined as follows:

$$N = N_{ra} + N_{rb} \tag{28}$$

where,

$$N_{ra} = \text{CNT sheet net revenue}$$

$$N_{rb} = \text{CNT yarn net revenue}$$

Technology Learning Sub-Model

The technology learning sub-models applied in this study are based on the technology learning sub-models developed by Ahmadian [1]. According to Ahmadian [1], as experience in terms of production increases, the unit cost of a new technology decreases over time. In this case, technology learning is a function of cumulative production of a new technology. The "Learning A" and "Learning B" variables are incorporated in the technology learning sub-models for each individual CNT product with the motivation of incorporating the learning variable as a shadow variable in the subsequent technology cost sub-model. The technology learning sub-models for CNT sheets and CNT yarn have identical equations and variable relationships. Ahmadian [1] states that the following equations define the variables in the technology learning sub-model:

$$\delta_p = q_p \times R_p + q_a \times R_a \tag{29}$$

where,

$$\delta_p = \text{production per year}$$

$$q_p = \text{product per practitioner}$$

$$q_a = \text{product per adoption}$$

$$R_a = \text{number of adoptions}$$

$$R_p = \text{number of practitioners}$$

The cumulative production, Q, is defined as follows:

$$Q = Q_i + \int \delta_p \cdot \mathrm{d}t \tag{30}$$

where,

$$Q_i = \text{initial production experience}$$

The “Learning A” and “Learning B” variables in each technology learning sub-model correspond with the learning index, which illustrates the influence of technology learning on unit cost. Subsequent analysis of the technology learning sub-model will illustrate that as technology learning increases, the unit cost of the new technology decreases. Technology learning index, L_c, is defined by the following, according to Ahmadian [1]:

$$L_c = \left(\frac{Q}{Q_i}\right)^{S_L} \tag{31}$$

where the learning exponent, S_L, is defined as:

$$S_L = \frac{Ln(E_c)}{Ln(2)} \tag{32}$$

and where E_c, the progress ratio, is defined as the strength of learning in reducing unit cost of the technology. Figure 12 and Figure 13 depict the technology learning sub-models developed for this study.

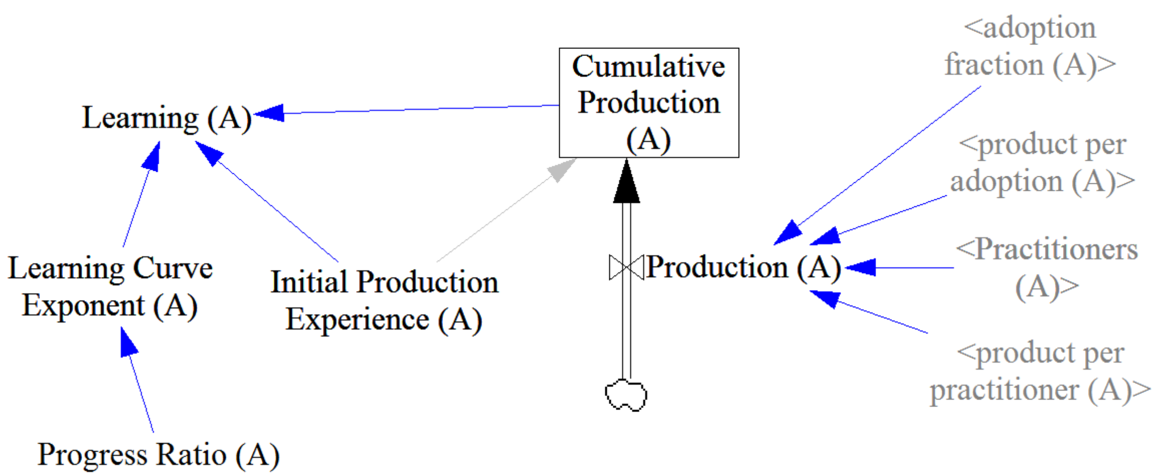

Figure 12. Technology Learning Sub-Model: CNT Sheets

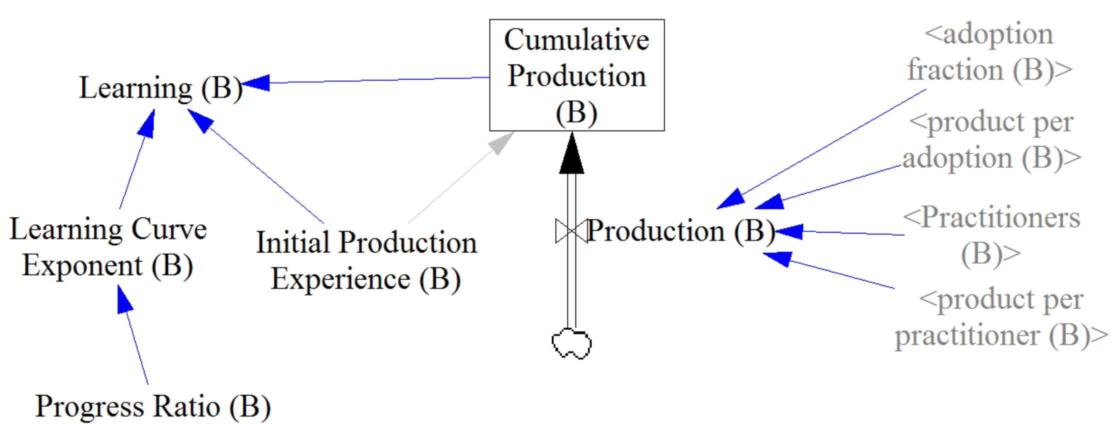

Figure 13. Technology Learning Sub-Model: CNT Yarn

Technology Cost Sub-Model

The technology cost sub-models applied in this study originate from the technology cost sub-models developed by Ahmadian [1]. Ahmadian [1] indicates that the total cost of a unit of product is comprised of both the variable and fixed costs of the product. Fixed costs may include rent paid by the company for the manufacturing space, employee salaries, and equipment cost. Variable costs may include other expenses which vary, according to the total amount of product produced by the company. As the production rate increases, the variable cost also increases while the fixed costs are independent of the production rate. Because the variable and fixed costs are not explicitly known, the ratio of fixed to variable costs is assumed to be 1. As additional information is made available, different scenarios may be analyzed with varying variable and fixed cost ratios. The purpose of the technology cost sub-model is to determine the variation in unit cost, given variation in capacity utilization. Ahmadian [1] defines the initial variable cost of the product as follows:

$$C_{vi} = \frac{P_i}{1+\mu_d} \times \frac{1}{1+\gamma} \tag{33}$$

where,

$$C_{vi} = \text{initial variable cost}$$

$$P_i = \text{initial price}$$

$$\mu_d = \text{desired profit margin}$$

$$\gamma = \text{fixed to variable cost ratio}$$

According to C.C.D. Consultants Inc [4], the profit margin is defined as the ratio of gross profit to revenue. In this model, a 10% desired profit margin is selected for both CNT sheet and CNT yarn technology cost sub-models for the purpose of this notional analysis. As more data becomes available, this value may be altered to analyze different scenarios at varied desired profit margins. Initial fixed cost, C_{fi}, is defined as follows:

$$C_{fi} = \frac{P_i}{1 + \mu_d} \times \frac{\gamma}{1 + \gamma} \tag{34}$$

Unit variable cost, C_{vu}, is defined as follows:

$$C_{vu} = C_{vi} \times L_c \tag{35}$$

Unit fixed cost, C_{fu}, is defined as follows:

$$C_{fu} = C_{fi} \times L_c \tag{36}$$

Unit cost, C_u, is defined as follows:

$$C_u = C_{vu} + \frac{C_{fu}}{\lambda} \tag{37}$$

where,

$$\lambda = \text{capacity utilization}$$

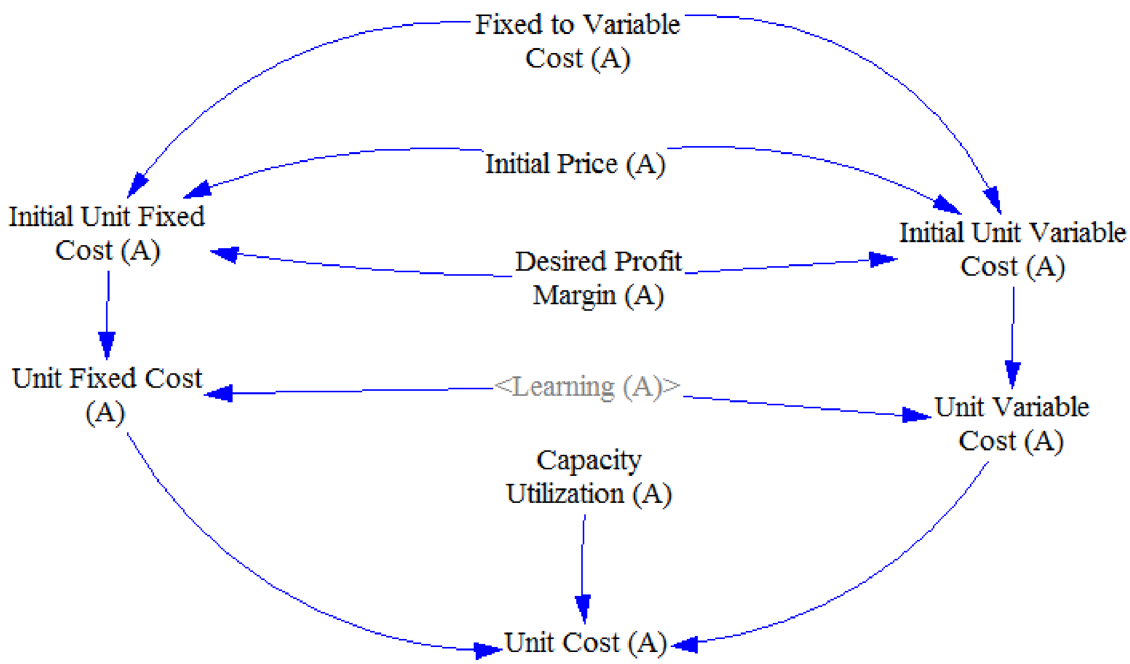

Figure 14. Technology Cost Sub-Model: CNT Sheets

Figure 14 and Figure 15 depict the technology learning sub-models developed for this study. Note that product A refers to CNT sheets and product B refers to CNT yarn.

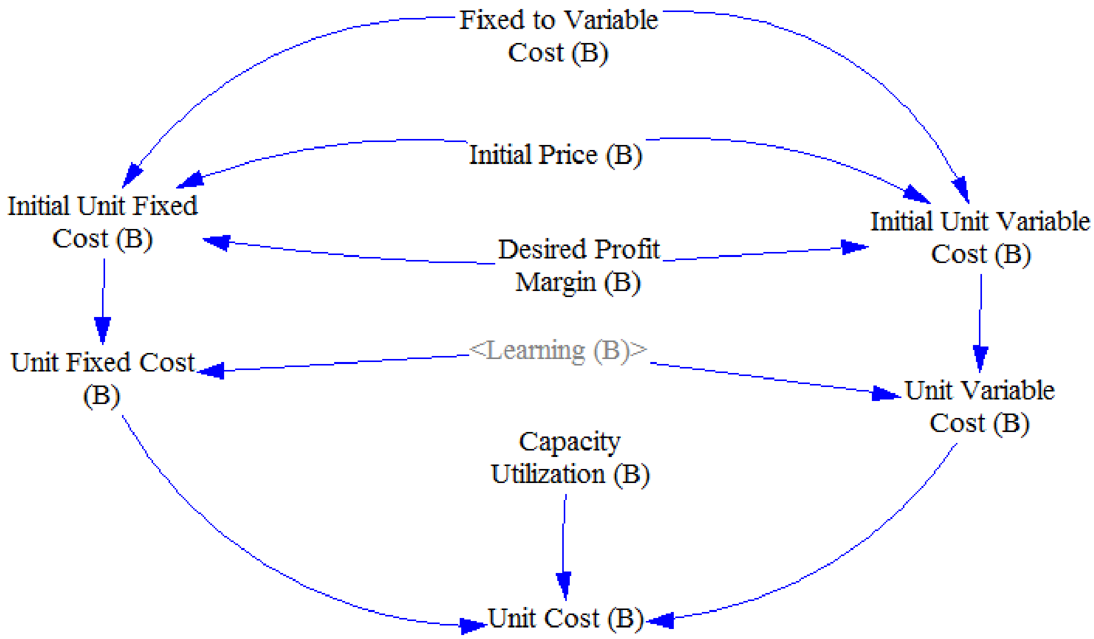

Figure 15. Technology Cost Sub-Model: CNT Yarn

Following Ahmadian[1], it is anticipated that as the capacity utilization increases, the unit cost of the technology decreases. This result is confirmed in subsequent analysis of the technology cost sub-models for both CNT sheet and CNT yarn product. The Technology-Cost sub-models are identical in terms of model structure and variable relationships for both for CNT sheet and CNT yarn products.

3.3 Model Settings

Each scenario of posed company development is run from 2017 to 2060 with a time step of one year. The purpose of this length of time is to illustrate the expected model behavior over time. The company achieved an annual output of one ton of CNT product per year in 2016. In order to derive a price of CNT product in 2016, the following notional relationships are applied:

$$2016 \text{ sales revenue}(\$) = \$4,180,432.00 \tag{38}$$

$$1 \text{ metric ton} = 1{,}000{,}000 \text{ grams} \tag{39}$$

$$\$4.18 = \text{price per gram in 2016} \tag{40}$$

Because we assume that sales revenue is comprised of the two predominant CNT products, yarns and sheets, it is assumed in the subsequent illustrative analysis that $4.18 per gram is the present and future price of CNT product for the company. This price is applied for subsequent analysis. Because the amount of CNT product per adoption and product per practitioner is assumed to be 1,000 grams, and that 1,000,000 grams of CNT product were produced in 2016, the number of customers total in 2016 is estimated as follows:

$$\text{product per adoption and practitioner} = 1{,}000 \text{ grams} \tag{41}$$

therefore for the purpose of this illustrative analysis,

$$2016 \text{ customers total} = 1{,}000 \text{ customers} \tag{42}$$

Due to the assumption that each product was sold in equal amounts, it is assumed that the amount of initial practitioners for each product is 500 customers. The number of non-practitioners for each product for this illustrative analysis is assumed to be 1,000,000 customers. As more information regarding the customer base is made available, these parameters may be adjusted in the model as required. We are aware that the company desires to develop commercial products. However, this illustrative analysis focuses solely on CNT sheet and CNT yarn products.

3.4 Assumptions and Limitations

The assumptions and limitations of this study include the following summary:

- The company of interest is primarily motivated to generate as much net revenue as possible at the fastest rate possible.
- The company is primarily a manufacturer of two products: CNT sheets and CNT yarn, although we are aware that the company aims to produce commercial products beyond raw CNT material.
- The company generated 1 ton of CNT products total in 2016.
- The company had approximately 1,000 customers in 2016.
- The company has achieved Phase I of their company development plan.
- The contact rate for each non-practitioner is on average 25 contacts per year.
- The initial number of non-practitioners is 2 million customers.
- The adoption fraction is 1% of the non-practitioner and practitioner contacts.
- CNT yarn and CNT sheets have equivalent contact rates, adoption rates, product per practitioner, and product per adoption.
- The company will continue to receive an average annual title III investment.
- Production cost per gram of CNT sheets and CNT yarn include variable and fixed costs.

- The fixed to variable cost ratio per product is 3, per Ahmadian [1].
- Sales revenue is calculated in terms of CNT sheets and CNT yarn.
- The company is able to fill all annual orders, given that the annual capacity is not exceeded.
- This model will forecast company outputs until 2060.
- Commercial viability is defined as the point at which the company of interest makes a profit at any point in time in terms of CNT products.
- Although CNT products are currently made to order with acute specifications, the price earned per CNT product sold is assumed to be $4.18 for this illustrative analysis.

These assumptions may be altered or relaxed with future extensions of the models and are made in order to demonstrate model applications.

3.5 Company Phases

This model incorporates products A, or CNT sheets, products B, or CNT yarn, and the relative contribution of both products to the annual net revenue. The company of interest is considering the implementation of three phases with the motivation to increases annual net revenue. The company provided characterizations of each phase in terms of production capacities and cost of producing one gram of CNT sheet and CNT yarn products. The phase parameters serve as base scenarios for this illustrative analysis.

1. Phase I

Improve and replicate existing reactor technology to increase factory output 10 times for yarn and 4 times for sheet and design of a next generation automated production scale reactor. Deliverables are: demonstration in production of output from current technology that achieve these output goals; and completion of engineering designs for the next generation reactor. Table 6 illustrates the primary objectives of Phase I proposed by the company.

Table 6. Phase I Objectives

Production-Related Metric	Milestones
Sheet Volume Capacity	0.8 metric tons per year
Sheet Average Cost	$2.45 per gram
Yarn Volume Capacity	0.1 metric tons per year
Yarn Average Cost	$18.11 per gram

2. Phase II

Introduce scaled and multiple reactor systems to increase factory capacity by an additional 20 times for yarn and 4 times for sheet and prototyping critical subsystems for the next gen production reactor. Deliverables are: demonstration of in production of systems that achieve these output goals; and demonstration of working critical subsystem prototypes for the next generation reactor. Table 7 illustrates the primary objectives of Phase II proposed by the company.

Table 7. Phase II Objectives

Production-Related Metric	Milestones
Sheet Volume Capacity	3 metric tons per year
Sheet Average Cost	$1.00 per gram
Yarn Volume Capacity	2 metric tons per year
Yarn Average Cost	$1.00 per gram

3. Phase III

Based on the success of Phase II, the goal of Phase III is to design and build a continuous production reactor to operate at 50 to 100 times the current production rates. The deliverable is a demonstration of a completed fully functional, continuous reactor that achieves kilogram per hour output. Although Phase III details are not explicitly available for this study, for the purposes of this illustrative analysis, Phase II objectives are considered the baseline objectives and the following parameters are assumed to coincide with Phase III objectives:

Table 8. Phase III Objectives

Production-Related Metric	Milestones
Sheet Volume Capacity	150 metric tons per year
Sheet Average Cost	$1.00 per gram
Yarn Volume Capacity	200 metric tons per year
Yarn Average Cost	$1.00 per gram

Note that the achievement of Phases I, II, or III does not make the company a competitive CNT manufacturer in terms of production capacity. The reader is reminded that the lowest production capacity of U.S. commodity-grade MWNTs tier 1 companies was 365 tons annually, according to BCC [22]. This is substantially higher than the highest posed annual production capacities of Phase III at 150 tons of CNT sheet and 200 tons of CNT yarn products.

3.6 Chapter Summary

This chapter illustrates the methodology applied to achieve the objectives outlined in Chapter I by means of the research and information compiled in Chapter II. This section provides explanation regarding the development of the sub-models which may be useful in determining the potential outputs for the company of interest. The CNT innovation diffusion model is the predominant model applied for subsequent analysis while the remaining models may be implemented for future research and analysis regarding the probable behavior of the company of interest.

IV. Analysis

Einstein's theory of relativity has not been proven correct; it stands because it has not been disproven, and because there is shared confidence in its usefulness.

–Forrester and Senge [10, p415]

4.1 Chapter Overview

The purpose of this chapter is to identify and illustrate the analysis conducted to address the research questions outlined in Chapter I. Lacking detailed company information, a series of scenarios, some derived from available company data, were executed to demonstrate the models' applications and capabilities. Note that throughout the analysis, portions of the results are identified as anticipated due to the research compiled in the literature review in Chapter II. The purpose of noting anticipated results is to illustrate the vetting of the model in terms of confirming expected model behavior. Recall that the structure-verification test encompasses the "face validity" or structural consistency with the real system. Parameter-verification entails the determination of model parameters corresponding to real life parameters. According to Sterman [26], noting expected model behavior is an imperative element in vetting and confirming confidence in model performance.

4.2 Company Phases: Scenarios

The purpose of this section is to illustrate the potential outcomes for the company, assuming the achievement of Phases I, II, and III, given the target costs of production and production capacities. The objectives outlined for Phases I, II, and III are input as parameter values in the subsequent analysis. Table 9 illustrates the notional model settings for subsequent analysis. Note that discount rates are not applied in this analysis.

Table 9. Phase Settings

Variable (A=sheets; B=yarn)	Phase I	Phase II	Phase III	Units
contact rate A	25	25	25	1/year
adoption fraction A	0.01	0.01	0.01	dmnl
product per adoption A	1,000	1,000	1,000	unit/person
product per practitioner A	1,000	1,000	1,000	unit/(person*year)
production capacity A	800,000	3M	150M	unit/year
product price A	$4.18	$4.18	$4.18	dollar/unit
cost to produce one unit A	$2.45	$1.00	$1.00	dollar/unit
initial practitioners A	500	500	500	person
non-practitioners A	1,000,000	1,000,000	1,000,000	person
contact rate B	25	25	25	1/year
adoption fraction B	0.01	0.01	0.01	dmnl
product per adoption B	20	20	20	unit/person
product per practitioner B	1,000	1,000	1,000	unit/(person*year)
production capacity B	100,000	2M	200M	unit/year
product price B	$4.18	$4.18	$4.18	dollar/unit
cost to produce one unit B	$18.11	$1.00	$1.00	dollar/unit
initial practitioners B	500	500	500	person
non-practitioners B	1,000,000	1,000,000	1,000,000	person

It should be noted that "person" is synonymous with "customer" and that the term "unit" is synonymous with "gram" in Table 9. The term "dmnl" refers to a dimensionless variable. The factors in Table 13 may be altered with with precise data from the company when it is available. The factors in Table 9 are applied for the demonstrative analysis of this study. In addition, note that product A corresponds to CNT sheets and product B corresponds to CNT yarn in Table 9. See Appendix A for a table of model terms and equations.

Phase I Results

The purpose of this section is to illustrate the potential outcomes of the notional parameters of the Phase I parameters proposed by the company. Phase I results for CNT sheets, product A, indicate model behavior which coincides with expected behavior of the CNT innovation diffusion model according to Sterman [26]. The initial amount of non-practitioners in this notional scenario is 1,000,000 customers and reaches the minimum of 926,500 customers. This is expected behavior given that the number of non-practitioners gradually decreases until all potential non-practitioners become practitioners of the new technology. Similarly, the practitioners A, practitioners of CNT sheets, behavior follows behavior expected of practitioners, which is to increase as the number of non-practitioners decreases, according to Sterman [26] and Bass [3]. The adoptions A also follows the expected bell-curve of adoptions with an initial exponential increase and finally an exponentially decrease in the number of adoptions per year. This is expected behavior of the CNT innovation diffusion model, according to Bass [3], since the amount of non-practitioners is decreasing over time. The sales revenue A also increases over time since the practitioners A also increases over time. However, the cost A also increases as the number of practitioners increases. The net revenue of CNT sheets gradually increases from $973,100.00 in 2017 and finally plateaus at $1.38 million, beginning in 2020, per the assumptions of this notional scenario. This plateau in CNT sheet net revenue coincides with the year that production rate capacity of 800,000 units per year is achieved, which is assumed per the CNT sheet production capacity proposed by the company for Phase I.

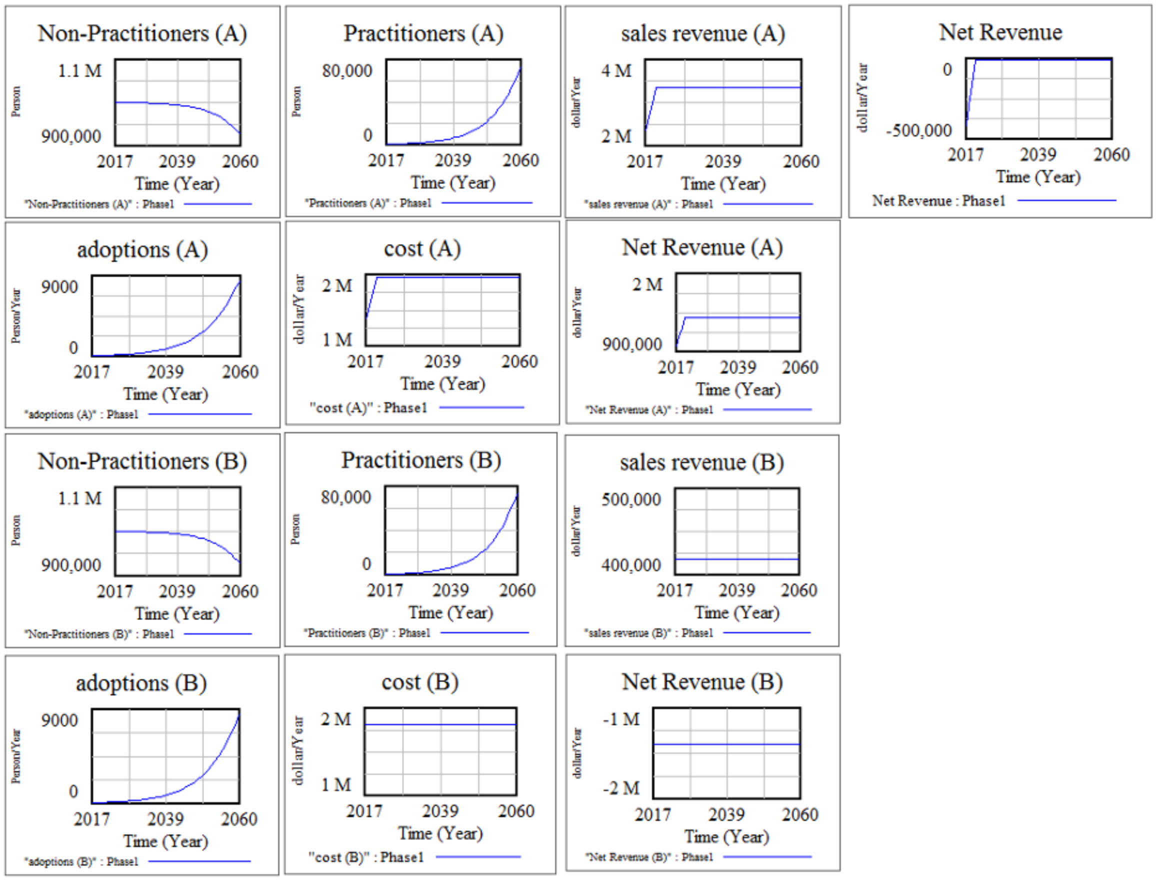

Figure 16. Phase 1 Results

Phase I results for CNT yarn, product B, also indicate model behavior which coincides with expected behaviors of diffusion models. The initial amount of non-practitioners is 1,000,000 customers and reaches the minimum of 926,500 customers. This is expected behavior of non-practitioners to eventually become practitioners over time. Similarly, the practitioners B, practitioners of CNT yarn, behavior follows behavior expected of practitioners to increase as the number of non-practitioners decreases. The adoptions B also follows the expected bell-curve of adoptions with an initial exponential increase and finally an exponential decrease observed in the number of adoptions per year, according to Sterman [26] and Bass [3]. This is expected behavior since the amount of non-practitioners is decreasing over time. CNT yarn generates -$1.39 million from 2017 to 2060, per this notional analysis and model parameters. This consistent CNT yarn net revenue is anticipated due to the fact that the maximum production rate of 100,000 units per year, which is assumed per the CNT sheet production capacity proposed by the company for Phase I, is reached beginning in 2017 and continued to be reached through 2060. Although the net revenue gradually increases from a minimum value of -$419,900.00 in 2017, the maximum net revenue reached and maintained is -$9,000.00, beginning in 2020. This is the anticipated result given that the cost to produce product B, CNT yarn, is $18.11 per gram of CNT product while the assumed price is $4.18 per gram of CNT product. Because the company is losing $13.93 per gram of CNT yarn sold in this notional scenario, it is evident that effort must be made in decreasing the cost of production per gram of CNT yarn produced. Because this notional example indicates potential negative net revenue, subsequent analysis includes the notional scenarios of Phases II and III.

Phase II Results

Phase II results for CNT sheets, product A, also indicate model behavior which coincides with expected behaviors of diffusion models. The initial notional amount of non-practitioners is 1,000,000 customers and reaches the minimum of 926,500 customers in this illustrative scenario. This is expected behavior given that the number of non-practitioners gradually decreases until all potential non-practitioners become practitioners of the new technology. Similarly, the practitioners A behavior follows behavior expected of practitioners to increase as the number of non-practitioners decreases. The adoptions A also follows the expected bell-curve of adoptions with an initial exponential increase and finally an exponentially decrease in the number of adoptions per year. This is expected behavior since the amount of non-practitioners is decreasing over time. The sales revenue A also increases over time since the practitioners A also increases over time. However, the cost A also increases as the number of practitioners increases.

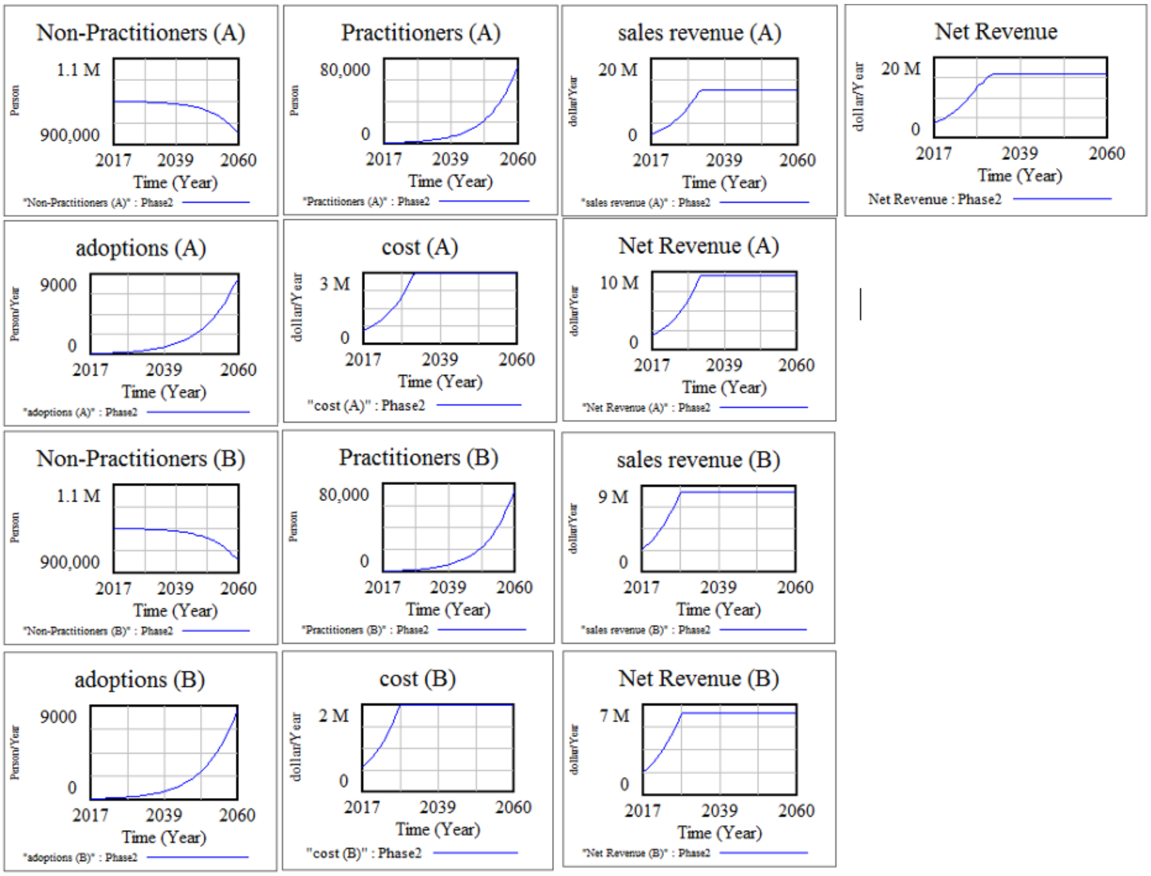

Figure 17. Phase 2 Results

The net revenue of CNT sheets gradually increases from $1.78 million in 2017 and finally plateaus in at $9.54 million, beginning in 2032. This plateau in CNT sheet net revenue coincides with the year that production rate capacity of 3 million units per year is achieved, which is assumed per the CNT sheet production capacity proposed by the company for Phase II. Phase II results for CNT yarn, product B, also indicate model behavior which coincides with expected behaviors of diffusion models. The initial amount of non-practitioners is assumed to be 1,000,000 customers and reaches the minimum of 926,500 customers. This is expected behavior of non-practitioners to eventually become practitioners over time. Similarly, the practitioners B behavior follows behavior expected of practitioners to increase as the number of non-practitioners decreases. The adoptions B also follows the expected bell-curve of adoptions with an initial exponential increase and finally an exponentially decrease in the number of adoptions per year. As anticipated, according to Sterman [26] and Bass [3], the amount of non-practitioners is decreasing over time. Unlike the results of Phase I, the net revenue of CNT yarn begins at a minimum value of $1.78 million in 2017 and finally plateaus in 2028 at $6.36 million. This plateau in CNT sheet net revenue coincides with the year that production rate capacity of 2 million units per year is achieved, which is assumed per the CNT yarn production capacity proposed by the company for Phase II. This notional scenario of Phase II of company development results in a minimum net revenue of $6.44 million in 2017 and plateaus at $15.9 million, beginning in 2032. Because the total cost of producing CNT yarn in Phase II is set at $1.00 per gram. Because of the selling price of $4.18 per gram, the company is able to generate profit of $3.18 for each gram of CNT yarn sold. Phase II is thus a more beneficial scenario for the company than the Phase I scenario.

Phase III Results

The purpose of this section is to illustrate the notional scenario of Phase III implementation, given the success of Phase II achievement. Phase III results for CNT sheets, product A, also indicate model behavior which coincides with expected behaviors of diffusion models. The initial amount of notional non-practitioners is 1,000,000 customers and reaches the minimum of 926,500 customers in this notional example. This is expected behavior given that the number of non-practitioners gradually decreases until all potential non-practitioners become practitioners of the new technology, according to Sterman [26] and Bass [3]. Similarly, the practitioners A behavior follows behavior expected of practitioners to increase as the number of non-practitioners decreases. The adoptions A also follows the expected bell-curve of adoptions with an initial exponential increase in the number of adoptions per year. This is expected behavior since the amount of non-practitioners is decreasing over time. The sales revenue A also increases over time since the practitioners A also increases over time. However, the cost A also increases as the number of practitioners increases. Per the notional Phase III parameters, a minimum net revenue of $3.57 million occurs in 2017 and a maximum net revenue of $524.9 million occurs in 2060. Note that the net revenues generated in the notional scenarios for Phases II and III are identical from 2017 to 2027. However, the first difference occurs in 2028 when Phase II generates a net revenue of $12.89 million and Phase III generates $13.05 million. This difference in net revenue is anticipated because the maximum production capacity of 2 million units per year, per the assumed Phase II parameters, is achieved in 2028. However, the assumed production capacity for CNT yarn for Phase III is assumed to be 200 million units per year and thus the anticipated difference in net revenue occurs in 2028.

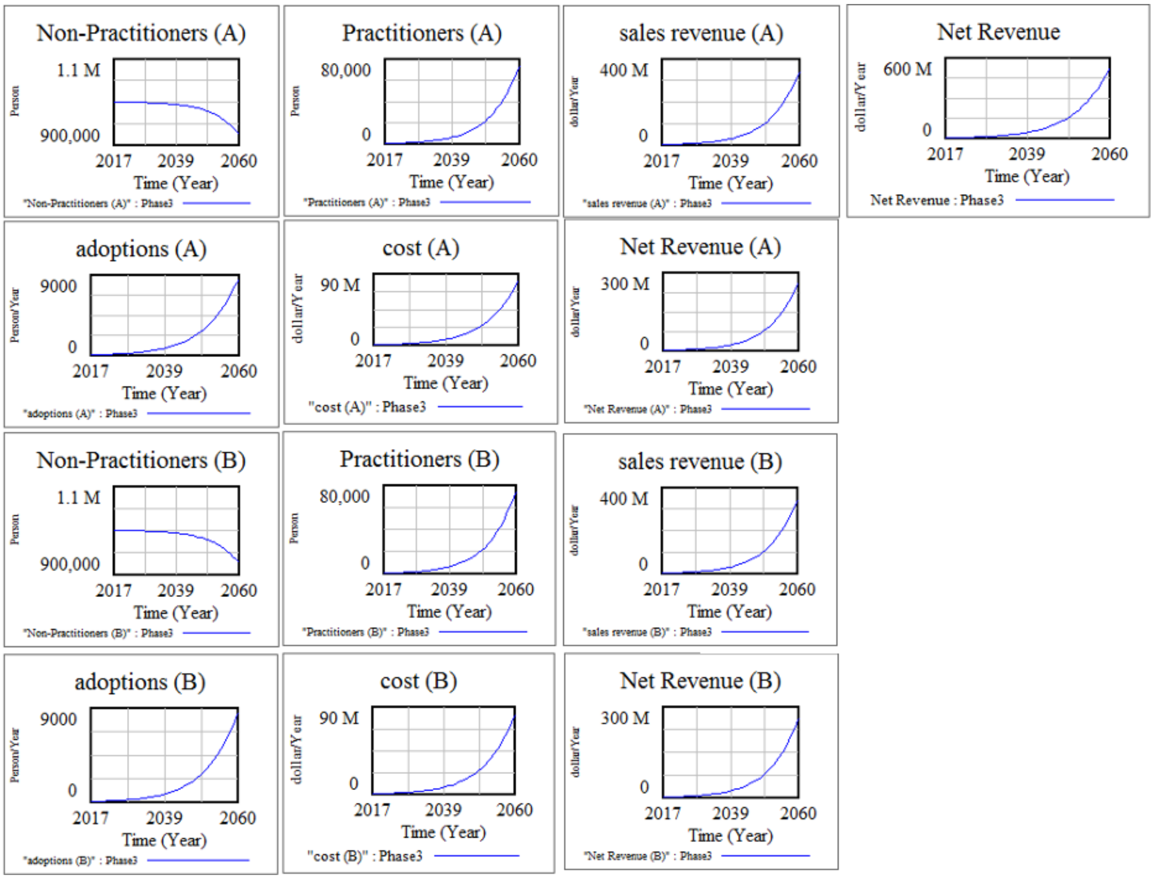

Figure 18. Phase 3 Results

In this notional scenario, the net revenues of CNT sheets and CNT yarn gradually increase from $1.78 million in 2017 and finally reaches maximum values of $262.5 million in 2060. Phase III net revenue results do not reach a plateau value because the production capacities, per the assumed production capacities posed by the company for Phase III of company development, of each product are not reached. Phase III results for CNT yarn, product B, also indicate model behavior which coincides with expected behavior of diffusion models. The initial amount of non-practitioners is 1,000,000 customers and reaches the minimum of 926,500 customers. This is expected behavior of non-practitioners to eventually become practitioners over time. Similarly, the practitioners B behavior follows behavior expected of practitioners to increase as the number of non-practitioners decreases. The adoptions B also follows the expected bell-curve of adoptions with an initial exponential increase and finally an exponentially decrease in the number of adoptions per year. This is expected behavior since the amount of non-practitioners is decreasing over time, according to Sterman [26] and Bass [3].

Phase Comparisons

Phases I, II, and III produce different results in terms of sales revenue, production cost, and net revenue. Because the adoption fraction is held constant at 1% and the contact rate is held constant at 25 contacts per year in this illustrative analysis, the amount of non-practitioners, practitioners, and adoptions are identical among Phases I, II, and III. This is illustrated in Figure 19.

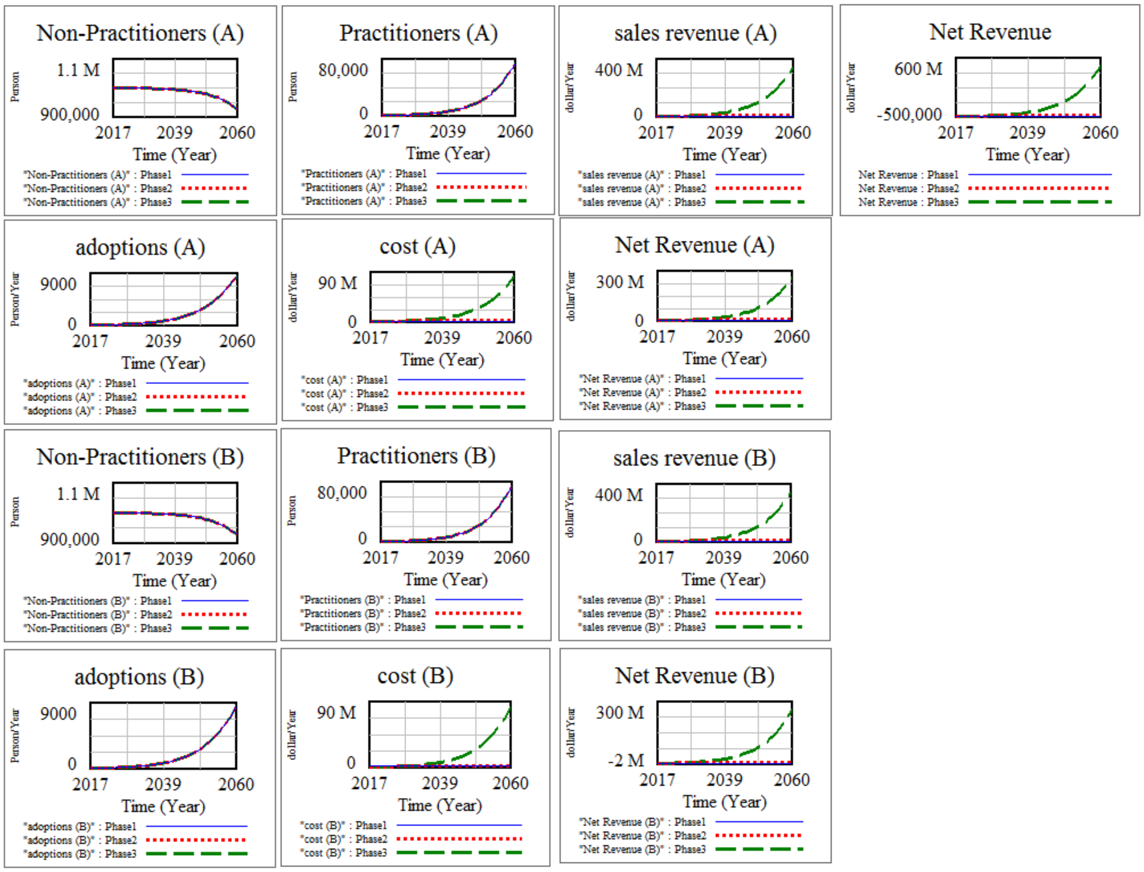

Figure 19. Phase Results Comparison

Figure 20 illustrates the differences in net revenue produced by CNT sheet and CNT yarn products between Phases I, II, and III. Note that Phases II and III produce identical net revenue until 2028, at which point in time Phase II potentially generates \$12.89 million and Phase III potentially generates -\$13.05 million in net revenue.

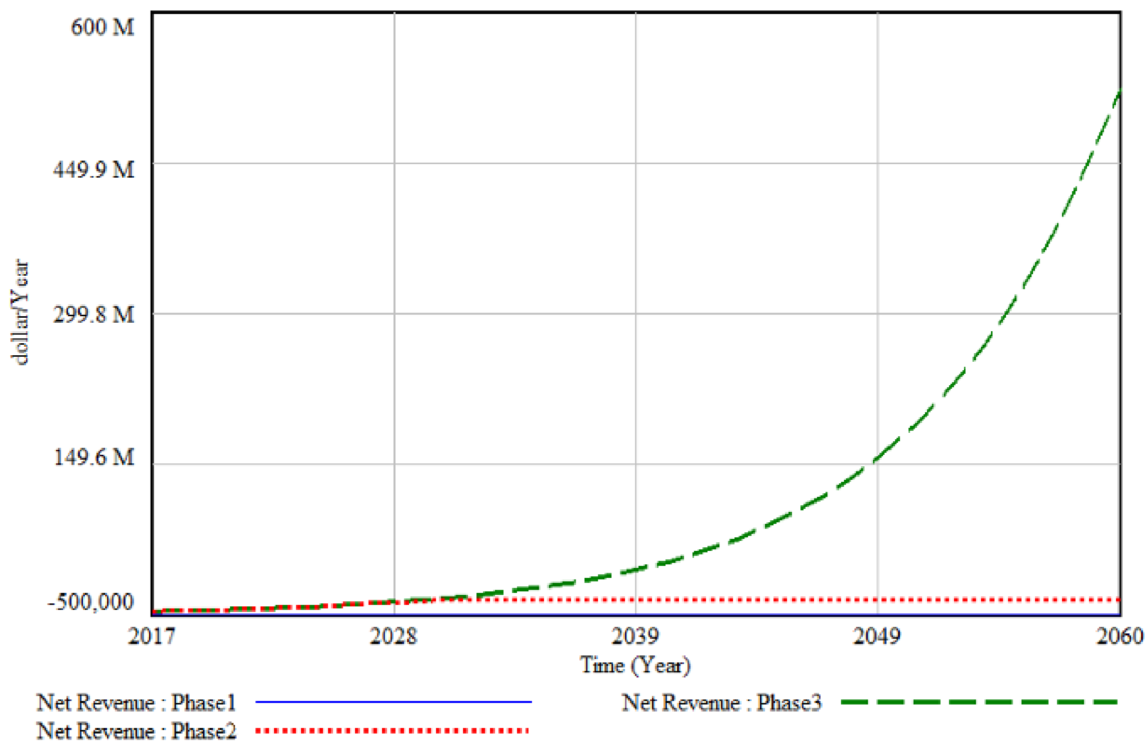

Figure 20. Phase Net Revenue Comparison

Table 10 illustrates the difference between Phases I, II, and III in terms of net revenue potentially generated by CNT sheet and CNT yarn products between 2018 and 2060, given the scenarios' notional values. Note that Phase II and Phase III potentially generate identical minimum net revenues of $3.57 million while Phase I potentially generates a minimum net revenue of -$419,900.00.

Table 10. Phase Comparison: Minimum and Maximum Net Revenues

Phase	Minimum Net Revenue	Maximim Net Revenue
I	-$419,900.00	-$9,000.00
II	$3.57M	$15.9M
III	$3.57M	$524.9M

The disparity between net revenue among Phases I, II, and III is predominantly due to the alteration in cost of production per gram of CNT sheets and CNT yarn.

Because CNT sheet product cost of production in Phase I is assumed to be \$2.45 per gram and the production cost CNT yarn is set at \$18.11 per gram, Phase I results in higher net revenue loss than Phases II and III, in which the cost of production for both CNT sheet and CNT yarn products is assumed to be \$1.00 per gram. In conclusion, Phase I, II, and III notional scenarios illustrate that potential net revenue increases as cost to produce product decreases and that increase in production capacities results in increased potential net revenue. This analysis indicates that the achievement of Phase I parameters are not beneficial to the company in terms of generating positive net revenue. Because Phases II and III result in positive net revenue, due to the assumed decrease cost in producing one gram of CNT product and increased production capacities, Phases II and III achievement should be of primary focus for the company. The reader is reminded that this analysis is notional and that elicitation of precise data will result in potentially more accurate results.

Subsequent Phase Implementation

The purpose of this section is to illustrate the impact of subsequent implementation of the Phase II of development posed by the company. This portion of notional analysis was conducted with the following assumptions:

1. The company decreases CNT sheet production cost by 25% annually until Phase II CNT sheet cost of $1.00 per gram is achieved

2. The company decreases CNT yarn production cost by 25% annually until Phase II CNT yarn cost of $1.00 per gram is achieved

3. The company increases CNT sheet production capacity by 25% annually until Phase II CNT sheet production capacity of approximately 3 million grams is achieved

4. The company increases CNT yarn production capacity by 25% annually until Phase II CNT yarn production capacity of approximately 2 million grams is achieved

This portion of analysis also illustrates the points in time at which various target profit margins are achieved. Phase I prices and capacities for CNT yarn and CNT sheets are applied as the starting parameters in this portion of notional analysis. Table 11 indicates the parameter values in this portion of analysis. The remaining parameters are held constant at the initial Phase I parameter values.

Table 11. Subsequent Phase II Implementation Values

Year	Sheet Cost	Yarn Cost	Sheet Capacity (grams/year)	Yarn Capacity (grams/year)
2017	$2.45	$18.11	800000	100000
2018	$1.84	$13.58	1000000	125000
2019	$1.38	$10.19	1250000	156250
2020	$1.03	$7.64	1562500	195312.5
2021	$1.00	$5.73	1953125	244140.625
2022	$1.00	$4.30	2441406.25	305175.7813
2023	$1.00	$3.22	3051757.813	381469.7266
2024	$1.00	$2.42	3051757.813	476837.1582
2025	$1.00	$1.81	3051757.813	596046.4478
2026	$1.00	$1.36	3051757.813	745058.0597
2027	$1.00	$1.02	3051757.813	931322.5746
2028	$1.00	$1.00	3051757.813	1164153.218
2029	$1.00	$1.00	3051757.813	1455191.523
2030	$1.00	$1.00	3051757.813	1818989.404
2031	$1.00	$1.00	3051757.813	2273736.754

Table 12 illustrates the results of subsequent implementation of Phase II parameters from initial Phase I parameters. The percent profit margin values indicate the revenue necessary to generate the relative target profit margin.

Table 12. Subsequent Phase II Implementation Results

Year	Net Revenue	1% Profit	5% Profit	10% Profit	25% Profit	50% Profit
2017	-$419,900	$3,220,890	$3,348,450	$3,507,900	$3,986,250	$4,783,500
2018	$305,600	$2,890,620	$3,005,100	$3,148,200	$3,577,500	$4,293,000
2019	$1,054,000	$2,600,043	$2,703,015	$2,831,730	$3,217,875	$3,861,450
2020	$1,846,000	$2,339,867	$2,432,535	$2,548,370	$2,895,875	$3,475,050
2021	$2,486,000	$2,322,697	$2,414,685	$2,529,670	$2,874,625	$3,449,550
2022	$3,185,000	$2,348,250	$2,441,250	$2,557,500	$2,906,250	$3,487,500
2023	$3,990,000	$2,391,680	$2,486,400	$2,604,800	$2,960,000	$3,552,000
2024	$4,916,000	$2,460,360	$2,557,800	$2,679,600	$3,045,000	$3,654,000
2025	$5,998,000	$2,546,210	$2,647,050	$2,773,100	$3,151,250	$3,781,500
2026	$7,259,000	$2,661,350	$2,766,750	$2,898,500	$3,293,750	$3,952,500
2027	$8,745,000	$2,801,639	$2,912,595	$3,051,290	$3,467,375	$4,160,850
2028	$10,230,000	$3,248,160	$3,376,800	$3,537,600	$4,020,000	$4,824,000
2029	$11,970,000	$3,800,630	$3,951,150	$4,139,300	$4,703,750	$5,644,500
2030	$14,040,000	$4,459,150	$4,635,750	$4,856,500	$5,518,750	$6,622,500
2031	$16,510,000	$5,245,940	$5,453,700	$5,713,400	$6,492,500	$7,791,000

Figure 21 illustrates the results of gradual implementation of Phase II and the net revenues necessary to achieve target profit margins.

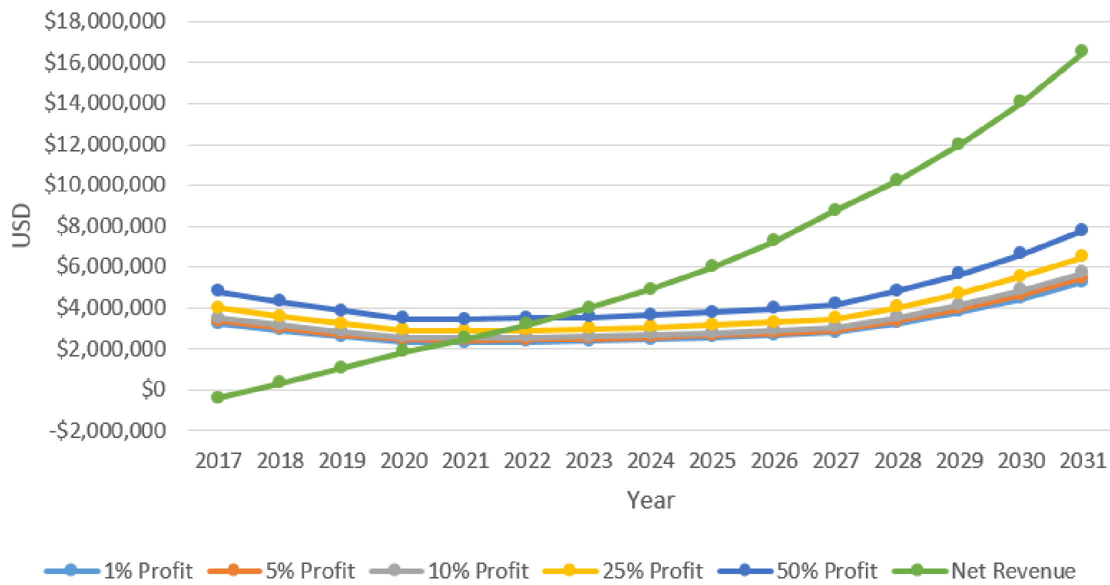

Figure 21. Subsequent Phase II Implementation

The 1% and 5% target profit margins were achieved in 2021. The 10% and 25% target profit margins were achieved in 2022. The 50% target profit margin was achieved in 2023. This portion of analysis illustrates that a decrease in production cost and increase in production capacity impacts the potential net revenue of the company and that higher target profit margin achievement necessitates greater implementation time.

Price Decrease

The purpose of this section is to illustrate the possible net revenue, given that our assumption of a constant product price is not accurate. This portion of notional analysis illustrates the resulting net revenue, given a notional 2% annual decrease in product price with an initial product price of $1.75 per gram of each product, CNT sheets and CNT yarn. The 25% annual decrease in production costs and 25%

increase in production capacity from the previous section are also incorporated in this analysis. However, in contrast with the previous section in which the constant product price of \$4.18 per gram per product was maintained, this portion of analysis is conducted with the assumption that the price decreases by 2% annually, due to the 25% increase in production capacity of each product.

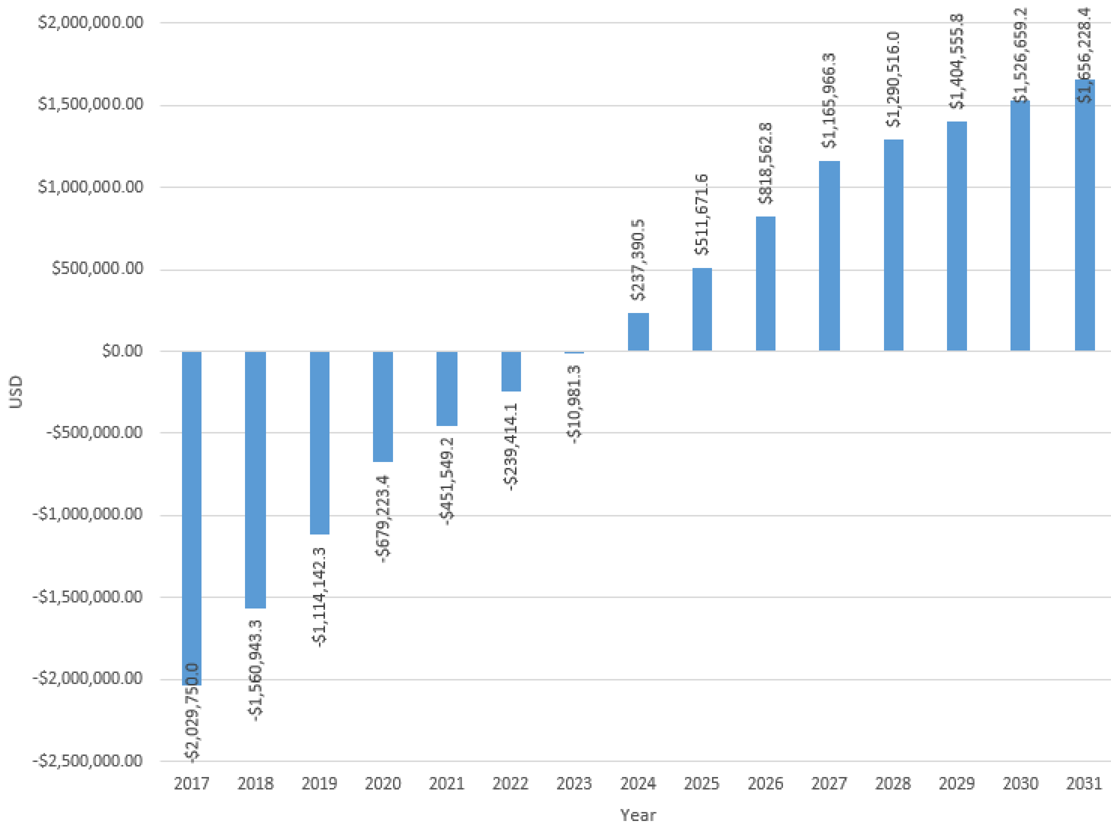

Figure 22. 2% Annual Price Decrease

Figure 22 illustrates the potential net revenue generated, given an annual decrease in product price for both CNT sheets and CNT yarn by 2% from an initial price of \$1.75 per gram per product.

Table 13. 2% Annual Price Decrease: Net Revenue

Year	Price	Net Revenue
2017	$1.75	-$2,029,750.00
2018	$1.72	-$1,560,943.25
2019	$1.68	-$1,114,142.27
2020	$1.65	-$679,223.38
2021	$1.61	-$451,549.23
2022	$1.58	-$239,414.13
2023	$1.55	-$10,981.27
2024	$1.52	$237,390.51
2025	$1.49	$511,671.56
2026	$1.46	$818,562.76
2027	$1.43	$1,165,966.34
2028	$1.40	$1,290,516.04
2029	$1.37	$1,404,555.80
2030	$1.35	$1,526,659.24
2031	$1.32	$1,656,228.43

Table 13 illustrates the potential net revenues generated per the corresponding product price for both CNT sheet and CNT yarn products. This portion of notional analysis suggests that the potential net revenues are impacted, given an alternative product price and also that an annual price decrease may also impact net revenue. Although this portion of notional analysis indicates that the company may not generate positive net revenue until 2024, as opposed to the previous section in which positive net revenue was generated by 2018, this analysis portion may be conducted iteratively with improved confidence in assumed rates of change of price, capacity, and production costs.

4.3 Title III Scenarios

For the purposes of this notional analysis, it is assumed that the company of interest is a Title III investment for the Department of Defense with a total budget of $33,971,374.00. It is assumed that the company has spent $23,715,331.00 and has $10,256,043.00 remaining of the total Title III investment. For the purpose of this notional analysis, it is assumed that the average Title III funds received annually is evenly distributed at $1,185,766.00. Given these assumptions, the company can reasonable expect this annual investment for approximately the next nine years. Although we realize that consistent annual investment will result in a shift in the resulting net revenue by the constant investment amount, the purpose of this section is to illustrate potential analysis which could be conducted given variation of investment distribution.

Figure 23. Title III: Phase I

As illustrated in Table 23, Phase I does not generate substantial net revenue and thus the Title III investment comprises the majority of the net revenue per year if the Title III investment is equally divided among the next nine years of production.

Figure 24. Title III: Phase II and Phase III

Phase II and Phase III results, as illustrated in Table 24, generate identical net revenues in the initial nine years of production and thus the Title III investment does not comprise the majority of the net revenue in Phases II and III. This analysis suggests that Title III investment makes Phase I a viable option for company development while Phases II and III continue to be viable options, as anticipated. Although this portion of analysis is notional due to the fact that the distribution of Title III investment was not known, this portion of analysis demonstrates the potential insight gained regarding the impact of Title III investment on company phases of development.

Title III With Desired Profit Margin

Because the previous notional analysis suggests that Title III investment makes Phase I development viable for the company to achieve commercial viability, given

Phase I assumed parameters, this portion of analysis was conducted to discern the annual Title III investment necessary to result in a desired profit margin for the company. In this case, profit margin is defined as follows, according to Newnan, Lavelle, and Eschenbach [20]:

$$\textit{profit margin} = \frac{\textit{net revenue}}{\textit{cost}} \tag{43}$$

where, profit margin refers to the target profit margin, which in this portion of notional analysis include 3%, 2%, and 1% target profit margins. For the purpose of this portion of analysis, relevant terms are defined as follows:

$$\textit{net revenue} = \textit{net cost} + \textit{net sales} \tag{44}$$

$$\textit{desired profit return} = \textit{absnet cost} \times \textit{target profit margin} \tag{45}$$

$$\textit{investment required} = \textit{desired profit return} - \textit{net revenue} \tag{46}$$

Phase I is analyzed in this initial portion of analysis, given varied desired profit margins. Cash flows have not been discounted.

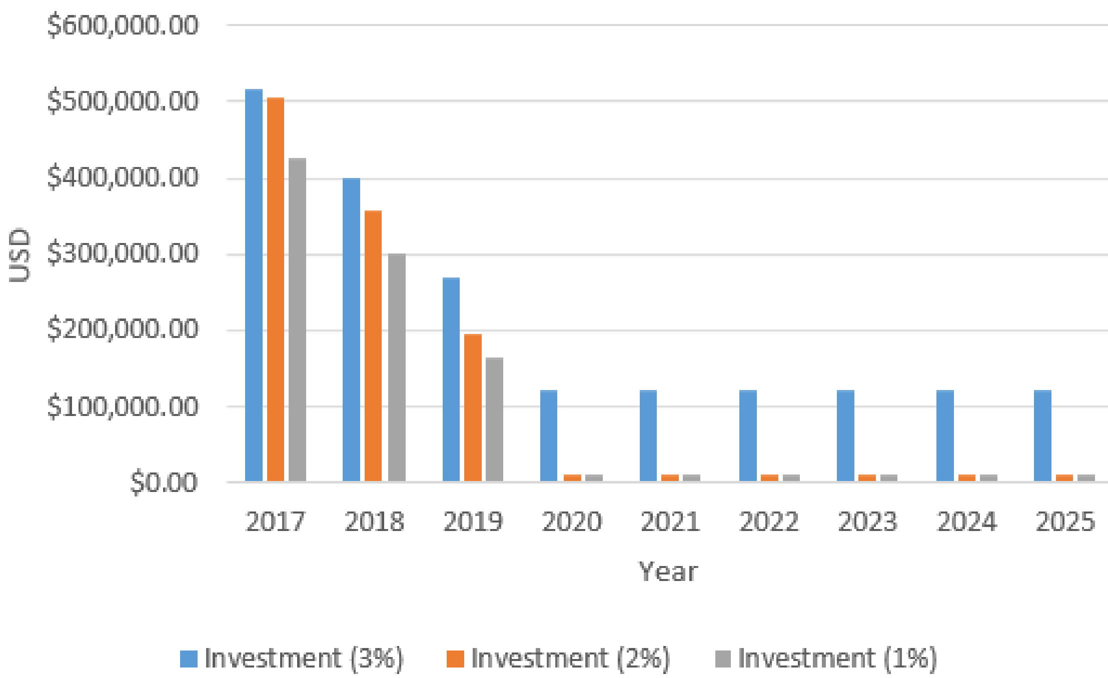

Figure 25. Phase I: Title III Investment Necessary Per Desired Profit Margin

Figure 25 illustrates the comparisons between necessary Title III subsidization required to achieve 1%, 2%, and 3% annual profit margins. Note that as expected, the 1% desired profit margin necessitates the least total Title III investment of $953,159.30 while the 3% profit margin requires a total Title III investment of $1,915,930.00 total.

Table 14. Phase I: Title III Investment Necessary Per Desired Profit Margin

Year	Investment (1%)	Investment (2%)	Investment (3%)
2017	$425,156.70	$504,000.00	$515,670.00
2018	$301,988.30	$357,600.00	$398,830.00
2019	$164,686.50	$194,400.00	$268,650.00
2020	$10,221.30	$10,800.00	$122,130.00
2021	$10,221.30	$10,800.00	$122,130.00
2022	$10,221.30	$10,800.00	$122,130.00
2023	$10,221.30	$10,800.00	$122,130.00
2024	$10,221.30	$10,800.00	$122,130.00
2025	$10,221.30	$10,800.00	$122,130.00
Total	$953,159.30	$1,120,800.00	$1,915,930.00

Because Phases II and III generate identical results in net revenue until 2028 and because the profit margin generated begins at 218%, it is concluded that achievement of these milestones potentially makes Title III investment unnecessary for Phases II and III. This portion of analysis illustrates that achievement of 1%, 2%, and 3% profit margins with Title III subsidization are below the assumed remaining Title III budget remaining at $10,256,043.00. This portion of analysis illustrates which may be conducted, given knowledge of the company's target profit margin and Title III investment requirements.

4.4 CNT Yarn Production Cost Reduction

Because it has been observed that Phase I is not profitable to the company in terms of generating positive annual net revenue, this portion of notional analysis was conducted to determine the percent reduction in production cost of CNT yarn, product A, necessary to generate positive annual net revenue. This portion of analysis explored the possible annual net revenue of the assumed Phase I parameters, given 1% and 5% annual production cost reductions for CNT yarn. This portion of analysis explores production cost reduction in CNT yarn because this product induces a loss of $3.93 per gram of CNT yarn sold. Per assumed Phase I parameters, the cost of production is $18.11 per gram of CNT yarn produced while the price is assumed to be $4.18 per gram of CNT yarn. Thus, each gram of CNT yarn sold results in a $13.93 loss. This analysis illustrates the effect of reducing the cost of production of CNT yarn by 1% and 5% annually from 2018 to 2027.

An annual 1% production cost reduction results in an initial positive net revenue of $44,788.00 in 2021 and a maximum net revenue of $147,620.00 in 2027. An annual 5% production cost reduction results in an initial positive net revenue of $14,966.00 in 2020 and a maximum net revenue of $660,618.00 in 2027. Figure 26 illustrates the resulting annual net revenues given 0%, 1%, and 5% annual production cost reductions for CNT yarn.

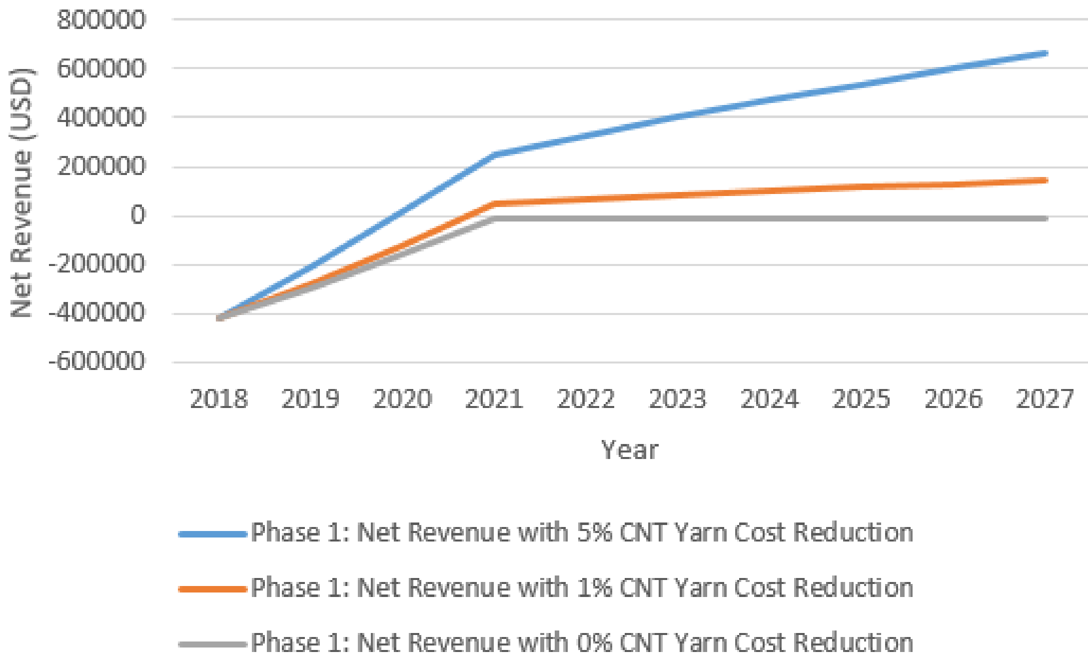

Figure 26. CNT Yarn Production Cost Reduction Comparison

The 0% reduction corresponds to the initial Phase I results in terms of net revenue and is included in this portion of analysis for comparison purposes. This analysis is notional and is made with the assumed parameters of the Phase I scenario. This notional example shows that the highest annual production cost reduction of 5% results in the highest annual net revenues in comparison with the 1% and 0% production cost reduction results. This notional example suggests that a higher annual production cost reduction results in higher net revenue for the company. Given more precise information, this portion of notional analysis may be applicable in determining net revenues given annual production cost reductions.

4.5 Technology Learning

In addition to the relevance of investment, it is also potentially useful to gain insight regarding the impact of technology learning and experience on the company. Because it is assumed that Phase I parameters have been achieved by the company, this portion of analysis is conducted with Phase I parameters and aimed to achieve insight regarding the relationship between technology learning and cost. Although we lack knowledge regarding the company's current production experience, we assume that the technology learning model is applicable.

Settings

According to Sterman [26], companies are typically able to produce products at lower costs as experience in production of the product accumulates. In learning or experience curve models, cumulative experience is replaced by cumulative production, according to Sterman [26]. The following settings apply to both CNT sheet and CNT yarn technology learning sub-models. The initial production experience, Q_i, is set at 500,000 due to the assumption that the initial production experience consisted of 1,000,000 tons of CNT product in 2016 and that each product was produced in equal amounts. Thus, the initial production experience for each Technology-Learning sub-model is set at 500,000. The progress ratios, E_c, analyzed include 0.95, 0.8, and 0.6. To illustrate the meaning of each of these progress ratios, consider Ahmandian's [1] example in which a progress ratio, E_c, is set at 0.8. This indicates a learning curve in which, for each doubling of experience, there is a 20% reduction in cost [1]. Therefore, a progress ratio of 0.95 indicates a 5% reduction in cost and a progress ratio of 0.6 indicates a 40% reduction in cost for each doubling of experience.

Results

Ahmadian[1] indicates that the learning index, L_c, is anticipated to decrease over time. The purpose of this analysis is to illustrate the influence of various progress rations, E_c, on the technology learning curve. Because the progress ratio is a measure of learning strength in terms of decreasing production cost, different progress ratios result in varied rates of change in the learning curve. Figure 27 illustrates the anticipated result for CNT Sheets in which the highest progress ratio of 0.95 results in a relatively slower decline in learning index than progress ratios of 0.8 or 0.6.

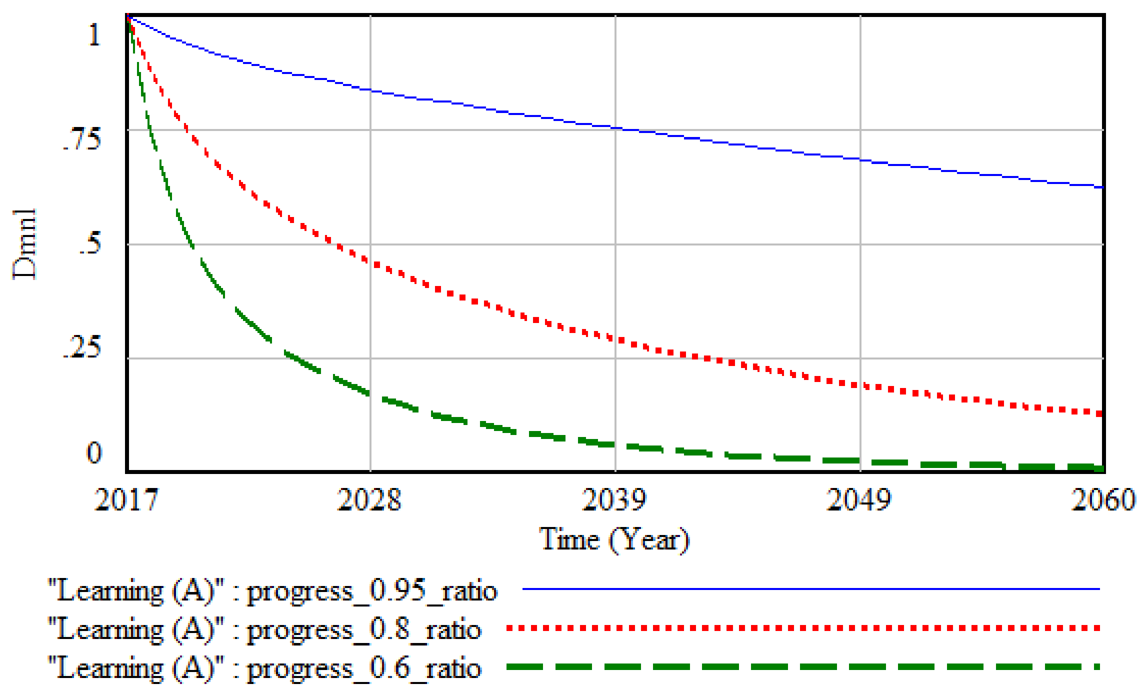

Figure 27. Technology Learning Results: CNT Sheets

Figure 27 illustrates the technology learning sub-model notional results for CNT sheets, given varied progress ratios. Figure 28 illustrates the technology learning sub-model results for CNT yarn, given varied progress ratios. The results are identical due to the fact that Phase I is assumed to differ in price of CNT product alone and price does not influence production rate or technology learning.

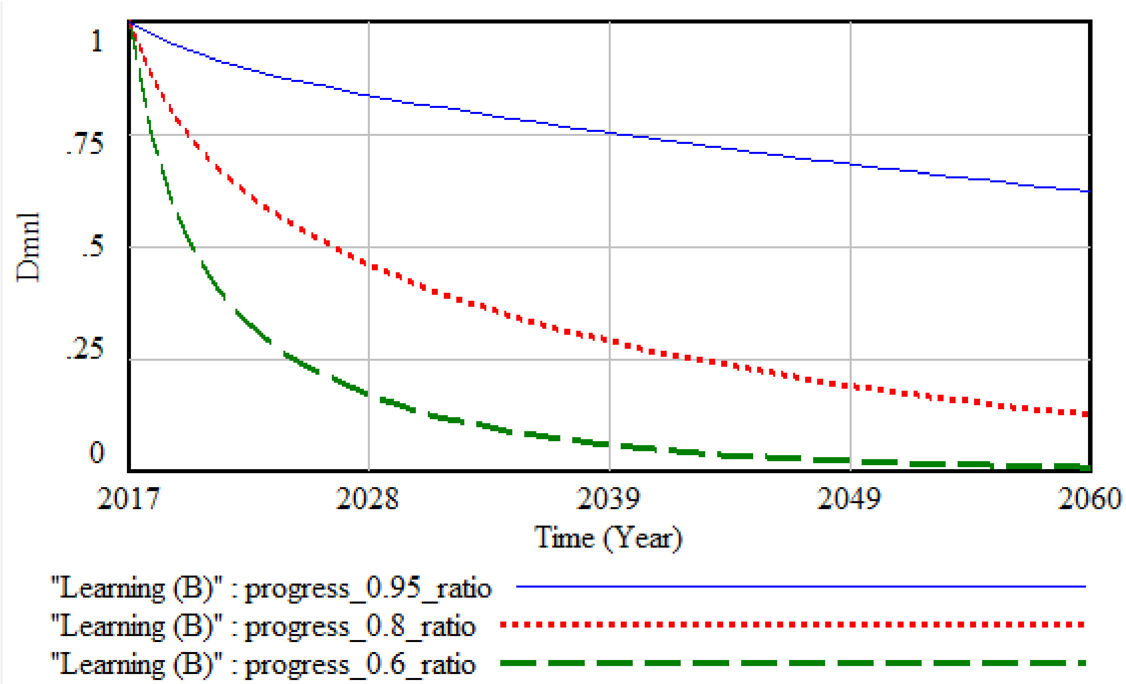

Figure 28. Technology Learning Results: CNT Yarn

The technology learning sub-model results are consistent with what would be expected. The will enable subsequent analysis of the relationship between unit cost as production experience increases. This portion of notional analysis also enables subsequent analysis of unit cost since the learning index, L_C, is a shadow variable in the technology cost sub-model.

4.6 Technology Cost

This portion of notional analysis is possible due to the fact that the learning index, L_c, variable is a shadow variable in the technology cost sub-model, which provides a means by which insight may be gained regarding product unit cost.

Settings

The following settings apply to both CNT sheet and CNT yarn technology cost sub-models and are designed with the notional parameters of Phase I. Per the analysis conducted by Ahmadian [1], the fixed to variable cost ratio, γ, is set to 3 in this portion of demonstrative analysis. As more information becomes available, this ratio may be altered for future research. The initial price, P_i, is set to \$4.18, in the previous notional scenarios as it is the assumed current price per gram of both CNT sheets and CNT yarn. The desired profit margin, μ_d, is set to 10% due to the assumption that this is a desirable profit margin for the company. This variable may be altered for future research in the event of additional information, regarding desired profit margin. The progress ratios, E_c, in the technology-learning sub-models for both CNT sheets and CNT yarn are set at 0.95 for this portion of analysis. This is relevant because the learning variable, L_c, is a shadow variable in the technology cost sub-model. As more precise information from the company is made available, this portion of notional analysis may be refined to produce more accurate results.

Results

As the unit cost of a capacity utilization increases, unit cost of a product decreases, according to Ahmadian [1]. The following analysis and discussion is made with the assumption that the company is primarily interested in reducing the unit cost of CNT products in order to maximize net revenue. Figure 29 illustrates this anticipated result due to the fact that the highest capacity utilization, 90%, results in the lowest unit cost for both CNT sheets and CNT yarn, relative to the lower 80% and 70% capacity utilizations analyzed. CNT sheet and CNT yarn results are identical in this demonstrative portion of analysis.

Table 15. CNT Capacity Utilization: Unit Costs

Capacity Utilization	Minimum Unit Cost	Maximum Unit Cost
90%	$2.45	$4.11
80%	$2.69	$4.51
70%	$2.99	$5.02

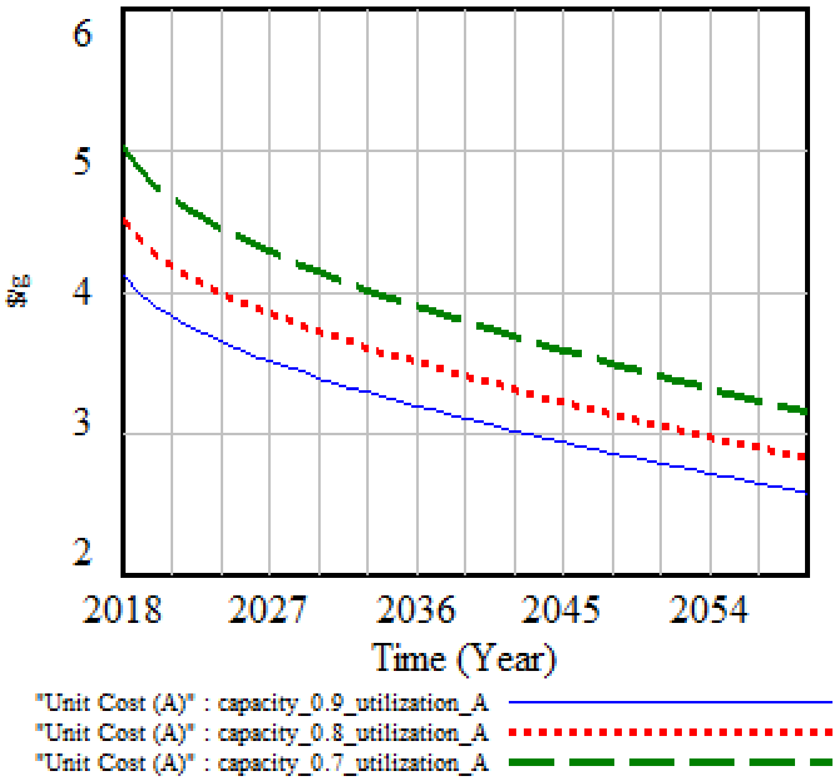

Figure 29. Technology Unit Cost

Table 15 illustrates that the 90% capacity utilization for CNT product results in a maximum unit cost of $4.11 and a minimum unit cost of $2.45. Because the 90% capacity utilization results in the lowest maximum unit cost, relative to the 80% and 70% capacity utilizations, 90% is the most desirable capacity utilization. Although these results are not surprising per the analysis conducted by Ahmadian [1], this portion of analysis illustrates potential analysis which may be conducted given clarifying information from the company regarding model parameters.

4.7 Model Validation

Although the previous notional analysis indicated elements of anticipated model behavior, it is also imperative that we demonstrate our confidence in the accurate behavior of our model per the compiled literature review in Chapter II. The purpose of this section is to illustrate the impact of varying different parameters of the model in order to refute or confirm expected model behavior. Because it is assumed that the company has successfully achieved an annual output of one ton CNT products, and Phase I annual output is the closest approximation of output at 0.9 tons, Phase I parameters are applied for the following parametric sensitivity analysis.

Parameter-Verification Test

According to Forrester and Senge [10], an interrelated test with the structure-verification test is the parameter-verification test, which entails the determination of the plausibility of model parameters conceptually and numerically corresponding to real life parameter values. Because the CNT innovation diffusion model, technology-learning, and technology-cost sub-models are developed with parameter values and ranges based on previously conducted model development by Ahmadian [1], the three sub-models initially pass the parameter-verification test. However, extended assurance of passing the parameter-verification test may be gained given the review of personnel from the company of interest and verification that the parameter values and ranges selected are realistic. The following analysis regarding varying adoption fraction and contact rate parameters also illustrate the CNT innovation diffusion model potentially passing the parameter-verification test.

Adoption Fraction

CNT yarn and CNT sheets result in identical results in this section of the analysis and thus the results of CNT sheets are solely presented. The purpose of this section is to illustrate the effect of altering the adoption fraction. According to the Bass diffusion model, the annual amount of adoptions per year gradually increases to a peak and finally gradually decreases, forming a bell-shaped curve. The term “adoption fraction” refers to the percentage of practitioner with non-practitioner contacts which result in a successful adoption, or in this case purchase, of the technology. As the adoption fraction increases, it is expected that the rate of adoption will also increase because the rate of adoption, which in this model is denoted as “adoptions,” is the product of the “adoption fraction” and the “practitioner with non-practitioner contacts.”

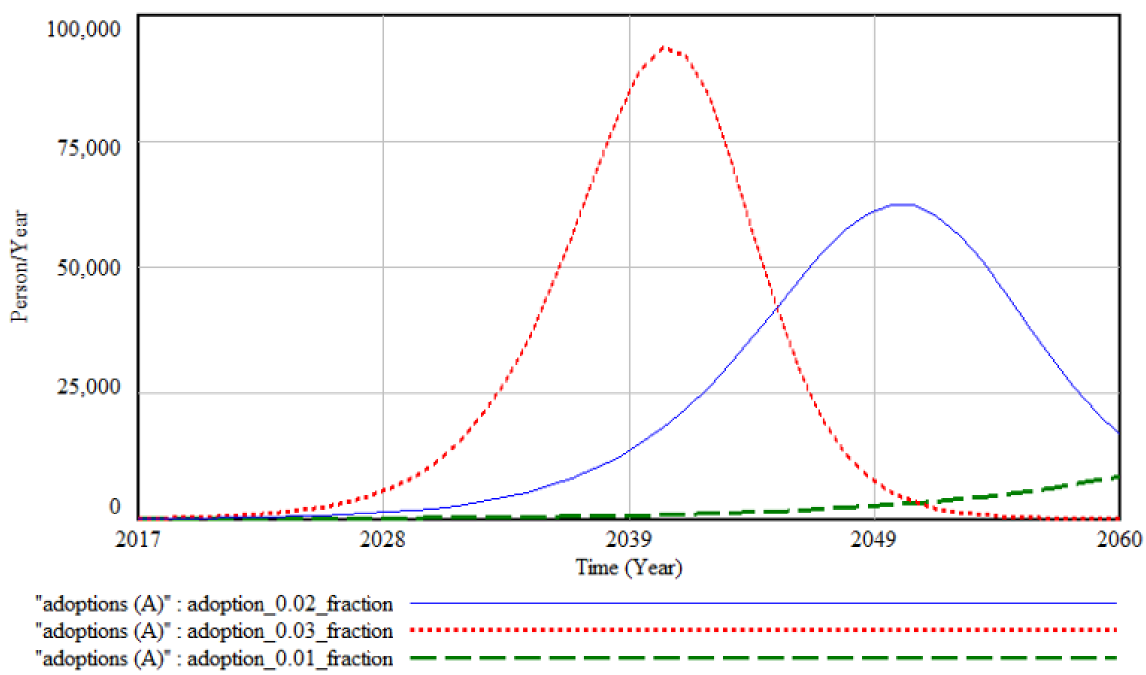

Figure 30. Adoption Fraction: Impact on Adoptions

As the adoption fraction increases, the amount of new adoptions also increases and is depicted in Figure 30. For example, the adoption fraction of 3% results in the maximum number of adoptions in 2040 at 93,590 new practitioners in this scenario. However, at the lower adoption fraction of 2%, the maximum number of adoptions occurs at a lower rate in 2050 at 62,360 new practitioners. Because it is assumed that the company of interest is motivated to gain as many new customers as possible, in this notional example, at the fastest rate possible, a higher adoption rate is desirable.

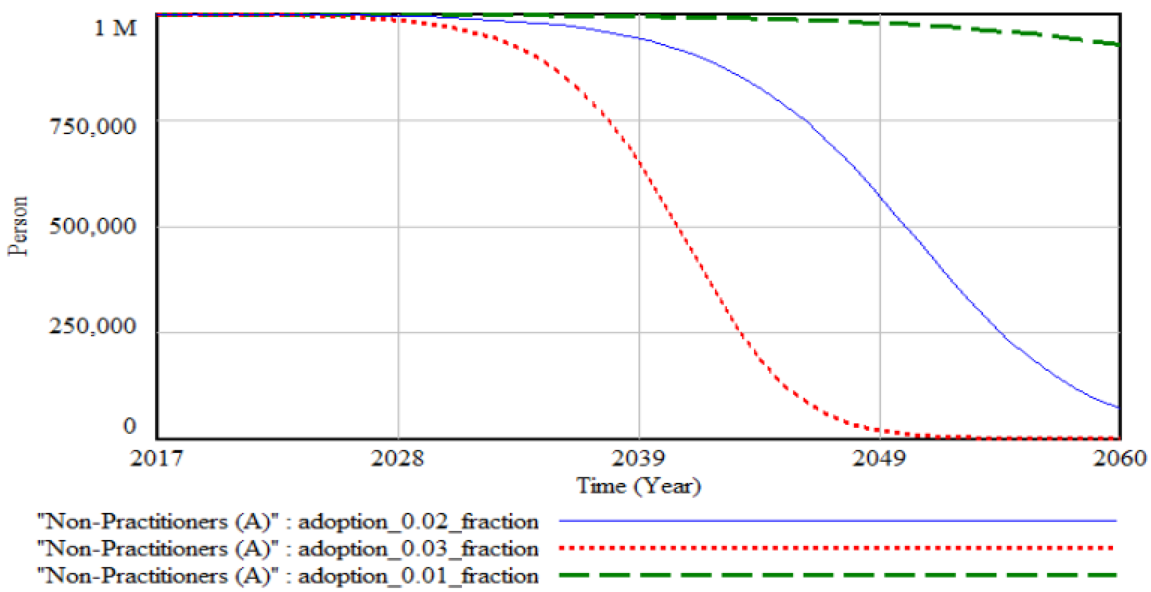

Figure 31. Adoption Fraction: Impact on Non-Practitioners

The varied adoption rate also influences the number of non-practitioners, as illustrated in Figure 31, and practitioners, as illustrated in Figure 32, each year, according to both the Bass diffusion model [3] and Ahmadian [1]. Because the 3% adoption rates influences the rate at which non-practitioners become practitioners, it is expected that a higher adoption fraction will result in fewer non-practitioners each year than the number of non-practitioners among lower adoption fractions.

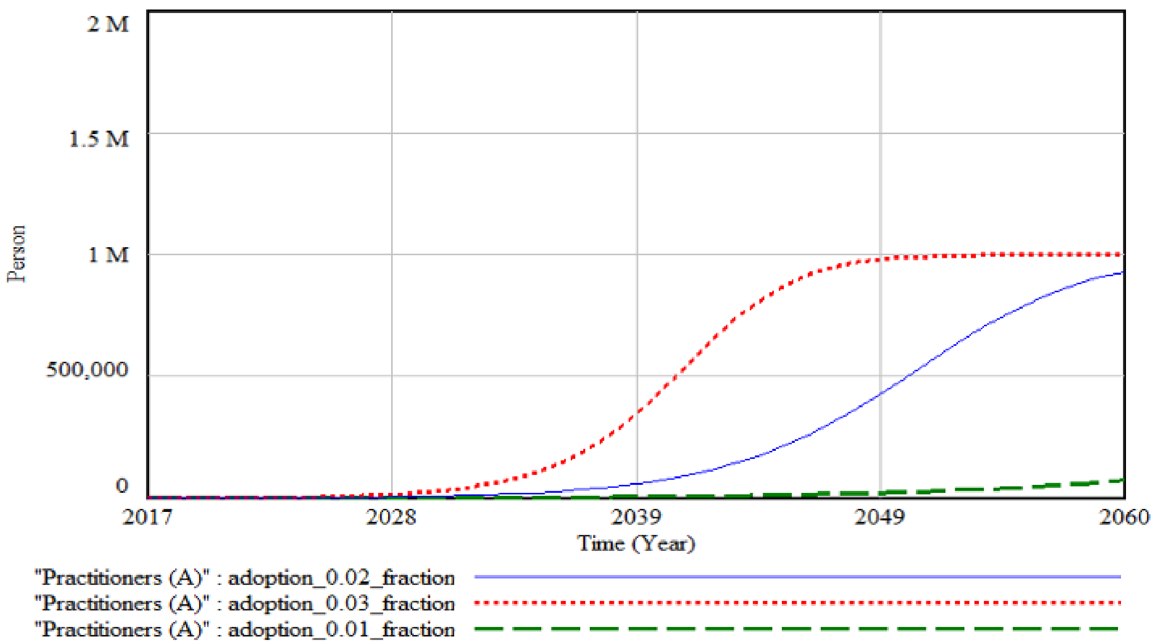

Figure 32. Adoption Fraction: Impact on Practitioners

As the number of non-practitioners increase, the number of practitioners also proportionally increase. These relationships is confirmed by the practitioner and non-practitioner graphs.

Table 16. Adoption Fraction Net Revenues

Adoption Fraction	Minimum Net Revenue	Maximum Net Revenue
0.01	-$419,900.00	-$9,000.00
0.02	-$311,900.00	-$9,000.00
0.03	-$203,800.00	-$9,000.00

Table 16 illustrates the net revenues generated, given varied adoption fractions. Note that the highest adoption fraction of 3% results in the lowest minimum net revenue of -$203,800.00, which suggests that a higher adoption rate is desirable, given the assumption that the company desires to minimize cost.

Contact Rate

In addition to the adoption rate, the contact rate is also varied in the CNT innovation diffusion model to refute or to confirm anticipated model behavior. CNT yarn and CNT sheets result in identical results in terms of impact on the number of adoptions, in this section of notional analysis, and thus the results of CNT sheets are solely presented. The results for both products are identical in terms of the number of annual adoptions in this portion of analysis because the contact rates for each product are varied at equivalent rates. The purpose of this section is to illustrate the effect of altering the contact rate. The term “contact rate” refers to the number of contacts each non-practitioner experiences annually. As the number of contacts per non-practitioner increases, the practitioner with non-practitioner contacts also increases due to the fact that practitioner with non-practitioner contacts is the product of practitioner prevalence and non-practitioner contacts [26].

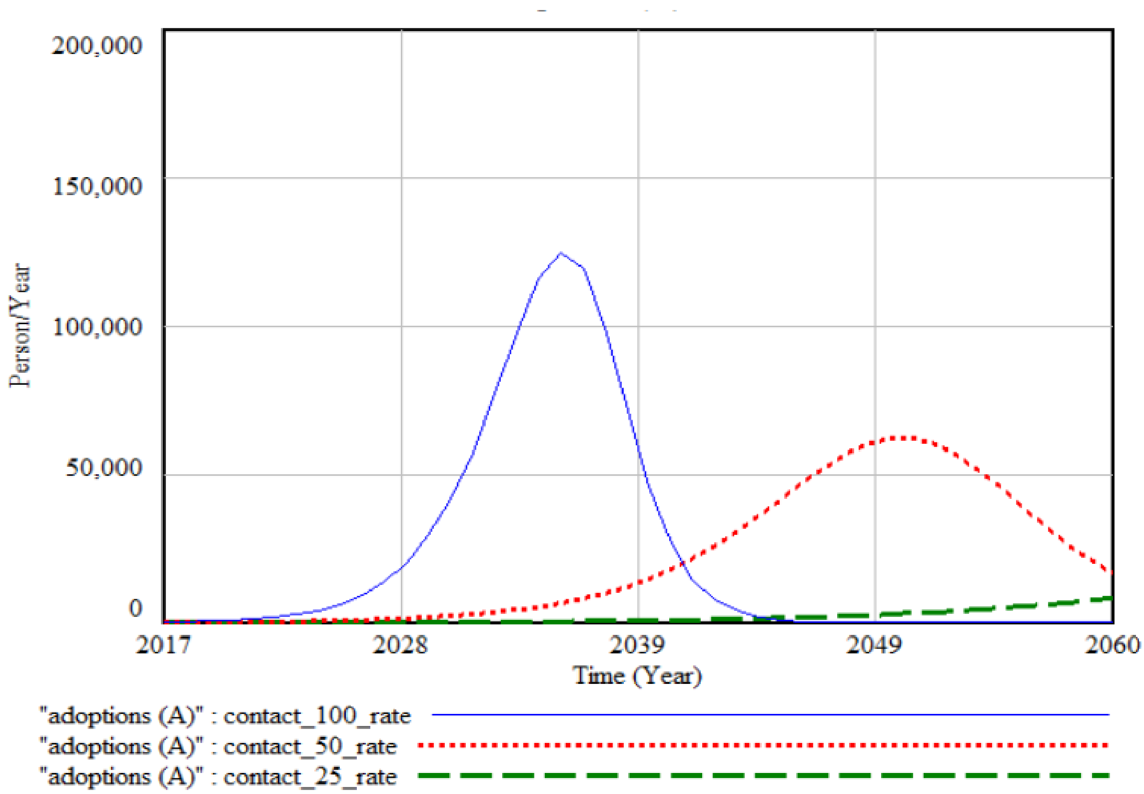

Figure 33. Contact Rate: Impact on Adoptions

Ahmadian [1] notes that an increased contact rate is anticipated to increase the rate of adoptions of a new technology. Per Figure 17, it is evident that the highest contact rate analyzed, at 100 contacts per year, results in the relatively fastest rate of adoption of the technology. For the increased contact rate of 100 per year, the maximum number of adoptions reaches 124,900 new practitioners in 2035. Conversely, the lower contact rate of 50 per year results in a lower maximum number of adoptions of 62,360 new practitioners in 2050. Because it is assumed that the goal of this company is to acquire as many new customers as possible as soon as possible, a higher contact rate is desirable.

Table 17. Contact Rate Net Revenues

Contact Rate	Minimum Net Revenue	Maximum Net Revenue
25	-$419,900.00	-$9,000.00
50	-$311,900.00	-$9,000.00
100	-$95,720.00	-$9,000.00

Table 17 illustrates the net revenues generated, given varied contact rates.

This portion of notional analysis indicates that the highest adoption fraction of 3% and highest contact rate of 100 per year result in the least net revenue lost and are thus confirmed to be the more desirable parameter settings for Phase I in this model. As more accurate information regarding parameter values is made available, this portion of analysis may be conducted with more accuracy.

Structure-Verification Test

According to Forrester and Senge [10], "verifying structure means comparing structure of a model directly with structure of the real system that the model represents." Because the CNT innovation diffusion model structure follows closely that of previous model development conducted by Ahmadian [1] and the primary goal of this model is to illustrate the potential outputs of a system dynamics model in terms of net revenue, sales revenue, cost of production, and adoption rates of CNT sheets and CNT yarn products, this model appears to initially pass the structure-verification test. In addition, because the technology-learning sub-models are designed to determine the potential learning indexes of both CNT sheets and CNT yarn products and follows closely that of previous model development conducted by Ahmadian [1], the technology-learning sub-models initially pass the structure-verification test. It is also noted, because none of the sub-models developed directly contradict knowledge of the company of interest, the sub-models initially pass the structure-verification test. However, extended assurance of passing the structure-verification test may be gained given a review of the models by personnel from the company of interest when available.

Dimensional-Consistency Test

The dimensional-consistency test encompasses "dimensional analysis of a model's rate equations," according to Forrester and Senge [10]. Because Vensim [30] is the software used to develop the CNT innovation diffusion model, technology-learning, and technology-cost sub-models, the dimensional-consistency test is made possible through testing unit consistency within Vensim prior to conducting analysis. Throughout the development and analysis in this study, units and dimensions are verified to ensure that the model simulates appropriately. Because of the unit and dimensional check within Vensim prior to any simulation throughout the analysis of this study, the CNT innovation diffusion model, technology-learning, and technology-cost sub-models initially pass the dimensional-consistency test. However, a more extended confirmation of the dimensional-verification test may be possible given review by the company of interest to ensure that the units and dimensions applied are consistent with reality.

4.8 Chapter Summary

This chapter provides further explanation for model assumptions and scenario design. Phases I, II, and III assumptions and results indicate that Phase III is the most desirable achievement for the company due to the fact that this phase results in the highest potential net revenue of $262.5 million in 2060, per the assumptions made for these notional analyses. However, if Phase III is not achievable and assuming that Phase I parameters are achieved, the cost of production per gram of CNT yarn must be reduced by 1% annually to achieve positive net revenue of $147,620.00 in 2027, using the notional parameters in this study. Greater annual decrease of CNT yarn cost of production per gram will further increase the potential net revenue of the company, such as a 5% decrease which results in a potential net revenue of $660,618,32.00 in 2027. It is therefore concluded that the company should make reduction of CNT yarn production cost per gram a priority to ensure positive net revenue in the next ten years. Given the anticipated results of the technology-learning sub-model analysis for both CNT sheets and CNT yarn, such that higher progress ratios result in relatively slower decline in learning index per the study conducted by Ahmadian [1], this portion of the model is determined to behave appropriately and as expected. In addition, given the anticipated results of the technology-cost sub-model analysis for both CNT sheets and CNT yarn, such that increased capacity utilization results in a reduced unit product cost per the study conducted by Ahmadian [1], this portion of the model is determined to behave appropriately and as expected. Due to initially passing the structure-verification, parameter-verification, and dimensional-consistency tests, the CNT innovation diffusion model, technology-learning, and technology-cost sub-models are determined to be useful with relative confidence. While the results summarized here should not be used for direct decision making, due to the estimation of key parameters for these illustrative analyses, they do provide an initial step forward in adding to the overall question of continued support. The model is adaptable and can be re-run with current data when it becomes available.

V. Conclusions

5.1 Chapter Overview

The purpose of this section is to illustrate the conclusions drawn from analysis conducted in chapter IV and to provide future research potential, given insight gained throughout this study. The conclusions of this study are developed based solely on the contents of this study, compiled literature review, model assumptions, model design, and notional analysis conducted. This study is demonstrative in nature insomuch as illustrating potential analysis that may be conducted iteratively with more information provided by the company. The illustrative results of this study should not be used as the basis for decision making.

5.2 Conclusion

This research effort is illustrative due to the lack of information availability and thus should not be used as a source of decision making. However, the value of this effort is in the development of system dynamics models which may be analyzed to gain insight into the potential commercial viability of the company. Given the assumed parameters of the proposed Phase I of company development, Phase I is not viable as a step or not viable at all based on the notional analysis results, if the motivation of the company is to minimize net cost and maximize net revenue. Phases II and III indicate the potential to generate positive net revenue annually and are thus recommended as development goals for the company. In this notional illustrative investigation, Phase I potentially generates a maximum annual net revenue of -$9,000 beginning in 2020, while Phase II and Phase III potentially generate $5.092 million in 2020. This difference in net revenue is predominantly due to the notional difference in production price for CNT products. In Phase I, CNT sheet cost is assumed to be $2.45 per gram and CNT yarn cost is assumed to be $18.11 per gram produced. In Phases II and III, both CNT sheets and CNT yarn cost $1.00 per gram produced, per the company's proposed cost per gram per product. The market price per gram of CNT product is assumed to be $4.18 per gram of CNT product in each phase in this illustration. It is recommended that the company continue to focus on production cost reduction to generate positive net revenue and thus commercial viability. Clarification regarding model assumptions and design would improve the accuracy of these results and is recommended in subsequent analysis efforts. Title III investment is observed to be a substantial necessity to the company, particularly if Phase I development is achieved, due to the notional results that annual Title III investment generates a maximum positive annual net revenue of $1,176,768.00 from 2020 to 2025.

The purpose of this study is to gain insight regarding the potential commercial viability of the company in terms of predicted net revenue of CNT sheet and CNT yarn products with limited information and various assumptions, upon which the CNT innovation diffusion, technology learning, and technology cost sub-models are based. Because this study indicates notional analysis which may be conducted iteratively, with improved information from the company and clarification of assumptions, this study successfully achieves the primary focus of this analysis in terms of insight gained regarding the company of interest.

5.3 Future Research

Future research should include dialogue with the company to clarify appropriate model structure and parameter values. Because validation is an iterative process, review of the models may also allow for clarification regarding the validity of the models in accurately representing the system of interest. We also suggest review of the models developed but excluded from analysis in this study. Dialogue with the company should also include clarification regarding the assumptions made in the development of the system dynamics models. It is also suggested that the company clarify which phases of development, if any, have been achieved and what subsequent milestones the company intends to achieve. Additional clarification with the company may improve the ability of the models developed to more accurately provide insight into the future commercial viability of the company. It is further suggested that any other products produced by the company, beyond the primary products of interest in this study which included CNT sheets and CNT yarn, are considered in future analysis. The development of customer profiles in terms of typical product amounts, product types, and recurring purchases will aid future analysis and may help focus sponsor efforts. This information may be incorporated in the system dynamics models to gain understanding regarding the impact of different customer profiles on commercial viability. Future research may also include the exploration of feedback loops within the model, such as the relationships between price, adoption fraction, and the number of practitioners. The inclusion of a global market analysis to determine global CNT market evolution is also an area of future research. It may be beneficial to consider the position of the company in terms of the global CNT market and how this company is expected to perform in the foreseeable future. As more data is available, additional studies may be conducted to gain a more accurate vision of this company's future as a commercial manufacturer of CNT products. This will also aid in clarifying the necessary development funds.

Appendix A.

Table 18, Table 19, and Table 20 indicate the elements of models implemented in the analysis of this study and include the variable names, variable types, units, and equations as they appear in the Vensim system dynamics models. Note that "person" is synonymous with a "customer" and "unit" is synonymous with "gram." Also note that "dmnl" indicates a dimensionless variable.

Table 18. CNT Innovation Diffusion Model Equations

Variable (A = CNT sheets; B = CNT yarn)	Type	Units	Equation
practitioner with non-practitioner contacts (A)	auxiliary	person/year	non-practitioner contacts (A) * practitioner prevalence (A)
non-practitioner contacts (A)	auxiliary	person/year	Non-Practitioners (A) * "contact rate (A)"
contact rate (A)	auxiliary	1/year	25
adoption fraction (A)	auxiliary	dmnl	0.01
practitioner prevalence (A)	auxiliary	dmnl	Practitioners (A)/total population
product per adoption (A)	auxiliary	unit/person	1000
product per practitioner (A)	auxiliary	unit/(year*person)	1000
production capacity (A)	auxiliary	unit/year	800000
product price (A)	auxiliary	dollar/unit	4.18
cost to produce one unit (A)	auxiliary	dollar/unit	2.45
Net Revenue (A)	auxiliary	dollar/year	sales revenue (A)-"cost (A)"
total population	auxiliary	person	Non-Practitioners (A) + "Practitioners (A)"+"Non-Practitioners (B)"+"Practitioners (B)"
cumulative amount (A)	level	unit	500*"product per practitioner (A)"+integ(production rate (A))
cumulative revenue (A)	level	unit	500*"product price (A)"+integ(sales revenue (A))
cumulative production cost (A)	level	dollar	500*"cost to produce one unit (A)"+integ(cost(A))
Non-Practitioners (A)	level	person	1000000+integ(-"adoptions (A)")
Practitioners (A)	level	person	500+integ("adoptions (A)")
production rate (A)	auxiliary/flow	unit/year	IF THEN ELSE("adoptions (A)"*"product per adoption (A)"+"Practitioners (A)"*"product per practitioner (A)">="production capacity (A)","production capacity (A)","adoptions (A)"*"product per adoption (A)"+"Practitioners (A)"*"product per practitioner (A)")
adoptions (A)	auxiliary/flow	person/year	("practitioner with non-practitioner contacts (A)" * "adoption fraction (A)")
sales revenue (A)	auxiliary/flow	dollar/year	production rate(A)*"product price (A)"
cost (A)	auxiliary/flow	dollar/year	cost to produce one unit (A)*"production rate(A)"
practitioner with non-practitioner contacts (B)	auxiliary	person/year	non-practitioner contacts (B) * practitioner prevalence (B)
non-practitioner contacts (B)	auxiliary	person/year	Non-Practitioners (B) * "contact rate (B)"
contact rate (B)	auxiliary	1/year	25
adoption fraction (B)	auxiliary	dmnl	0.01
practitioner prevalence (B)	auxiliary	dmnl	Practitioners (B)/total population
product per adoption (B)	auxiliary	unit/person	1000
product per practitioner (B)	auxiliary	unit/(year*person)	1000
production capacity (B)	auxiliary	unit/year	100000
product price (B)	auxiliary	dollar/unit	4.18
cost to produce one unit (B)	auxiliary	dollar/unit	18.11
Net Revenue (B)	auxiliary	dollar/year	sales revenue (B)-"cost (B)"
cumulative amount (B)	level	unit	500*"product per practitioner (B)"+integ(production rate (B))
cumulative revenue (B)	level	unit	500*"product price (B)"+integ(sales revenue (B))
cumulative production cost (B)	level	dollar	500*"cost to produce one unit (B)"+integ(cost (B))
Non-Practitioners (B)	level	person	1000000+integ(-"adoptions (B)")
Practitioners (B)	level	person	500+integ("adoptions (B)")
production rate (B)	auxiliary/flow	unit/year	IF THEN ELSE("adoptions (B)"*"product per adoption (B)"+"Practitioners (B)"*"product per practitioner (B)">="production capacity (B)","production capacity (B)","adoptions (B)"*"product per adoption (B)"+"Practitioners (B)"*"product per practitioner (B)")
adoptions (B)	auxiliary/flow	person/year	("practitioner with non-practitioner contacts (B))" * "adoption fraction (B)")
sales revenue (B)	auxiliary/flow	dollar/year	production rate (B)*"product price (B)"
cost (B)	auxiliary/flow	dollar/year	cost to produce one unit (B)*"production rate (B)"

Table 19. Technology-Learning Sub-Models: CNT Sheets and CNT Yarn

Variable (A = CNT sheets; B = CNT yarn)	Type	Units	Equation
Learning (A)	auxiliary	dmnl	("Cumulative Production (A)"/"Initial Production Experience (A)")^"Learning Curve Exponent (A)"
Learning Curve Exponent (A)	auxiliary	dmnl	Ln("Progres Ratio (A)")/Ln(2)
Progress Ratio (A)	constant	dmnl	0.95
Initial Production Experience (A)	auxiliary	unit	500,000
Cumulative Production (A)	level	unit	"Initial Production Experience (A)"+INTEG("Production (A)")
Production (A)	auxiliary	unit/year	("adoption fraction (A)"*"product per adoption (A)")+("Practitioners (A)"*"product per practitioner (A)")
Learning (B)	auxiliary	dmnl	("Cumulative Production (B)"/"Initial Production Experience (B)")^"Learning Curve Exponent (B)"
Learning Curve Exponent (B)	auxiliary	dmnl	Ln("Progres Ratio (B)")/Ln(2)
Progress Ratio (B)	constant	dmnl	0.95
Initial Production Experience (B)	auxiliary	unit	500,000
Cumulative Production (B)	level	unit	"Initial Production Experience (B)"+INTEG("Production (B)")
Production (B)	auxiliary	unit/year	("adoption fraction (B)"*"product per adoption (B)")+("Practitioners (B)"*"product per practitioner (B)")

Table 20. Technology-Cost Sub-Models: CNT Sheets and CNT Yarn

Variable (A = CNT sheets; B = CNT yarn)	Type	Units	Equation
Fixed to Variables Cost (A)	constant	dmnl	3
Initial Price (A)	constant	$/gram	4.18
Desired proft Margin (A)	constant	dmnl	0.1
Capacity Unitilxation (A)	constant	dmnl	0.9
Unit Cost (A)	auxiliary	$/gram	Unit Variable Cost (A)+("Unit Fixed Cost (A)"/"Capacity Utilization (A)")
Initial Unit Fixed Cost (A)	auxiliary	$/gram	("Initial Price (A)"/(1+"Desired Profit Margin (A)"))*("Fixed to Variable Cost (A)"/(1+"Fixed to Variable Cost (A)"))
Unit Fixed Cost (A)	auxiliary	$/gram	Initial Unit Fixed Cost (A)*"Learning (A)"
Initial Unit Variable Cost (A)	auxiliary	$/gram	Initial Price (A)/(1+"Desired Profit Margin (A)")*(1/(1+"Fixed to Variable Cost (A)"))
Unit Variable Cost (A)	auxiliary	$/gram	Learning (A)*"Initial Unit Variable Cost (A)"
Fixed to Variables Cost (B)	constant	dmnl	3
Initial Price (B)	constant	$/gram	4.18
Desired proft Margin (B)	constant	dmnl	0.1
Capacity Unitilxation (B)	constant	dmnl	0.9
Unit Cost (B)	auxiliary	$/gram	Unit Variable Cost (B)+("Unit Fixed Cost (B)"/"Capacity Utilization (B)")
Initial Unit Fixed Cost (B)	auxiliary	$/gram	("Initial Price (B)"/(1+"Desired Profit Margin (B)"))*("Fixed to Variable Cost (B)"/(1+"Fixed to Variable Cost (B)"))
Unit Fixed Cost (B)	auxiliary	$/gram	Initial Unit Fixed Cost (B)*"Learning (B)"
Initial Unit Variable Cost (B)	auxiliary	$/gram	Initial Price (B)/(1+"Desired Profit Margin (B)")*(1/(1+"Fixed to Variable Cost (B)"))
Unit Variable Cost (B)	auxiliary	$/gram	Learning (B)*"Initial Unit Variable Cost (B)"

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REPORT DOCUMENTATION PAGE			*Form Approved* *OMB No. 0704-0188*

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
22-03-2018	Master's Thesis	May 2016 - March 2018

4. TITLE AND SUBTITLE A System Dynamics Innovation Diffusion Model Applied to Carbon Nanotube Manufacturing	**5a. CONTRACT NUMBER**
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S) MacKinnon, Frances G, 1Lt	**5d. PROJECT NUMBER**
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Institute of Technology Graduate School of Engineering and Management (AFIT/EN) 2950 Hobson Way Wright-Patterson AFB OH 45433-7765	**8. PERFORMING ORGANIZATION REPORT NUMBER** AFIT-ENS-18-M-139
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Intentionally Left Blank	**10. SPONSOR/MONITOR'S ACRONYM(S)**
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT

Distribution Statement A. Approved for Public Release

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The transition of advanced technologies from their nascent state to viable commercial entities is a critical step in assuring the United States' national technological superiority and support is often required to incubate such technological developments. This study investigates the necessary adoption fractions, contact rates, production capacities, production costs, product prices, monetary support, and time necessary for the company of interest to be considered a commercially viable producer of CNT products. The subsidization required to generate varied profit margins is also explored. The application of system dynamics models determined to approximately represent the real diffusion and production of both CNT sheet and CNT yarn products generates insight regarding policy improvement for the company to achieve competitive commercial CNT production and provide an assessment of when CNT production may be profitable. This study should not be used as the basis for decision making due to the fact that the analysis is based on notional data and scenarios.

15. SUBJECT TERMS

carbon nanotube; technology diffusion; system dynamics

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
U	U	U	UU	128	Dr. Richard F. Deckro, AFIT/ENS
					19b. TELEPHONE NUMBER *(Include area code)* (937) 255-3636 x4325 richard.deckro@afit.edu