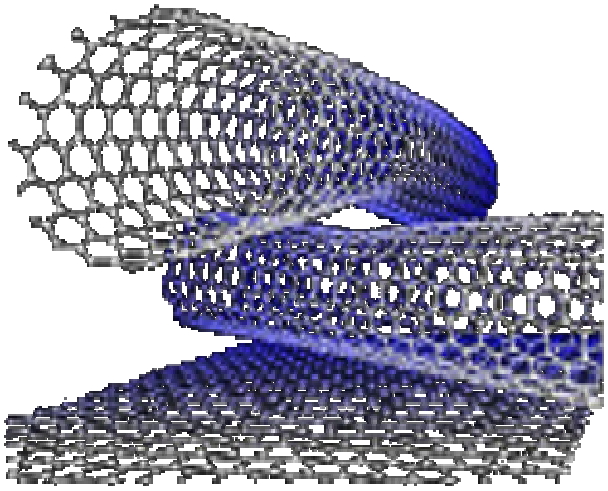
Nanotubes Plant

Final Report



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EXECUTIVE SUMMARY

Nanotubes are a versatile material that have emerging applications in a variety of fields. This report investigates the design and feasibility of a production facility for single-wall nanotubes (SWNT). Cost estimates on the capital investment and operating costs were generated for two scaleable production methods, HiPCO and CoMoCat. As a result of this analysis comparison, HiPCO was chosen as the production method for this facility. An extensive market forecast was created to determine the demand for SWNT and the resulting price. A deterministic model using tax and labor rates for various locations, the forecasted demand and price of nanotubes, and the raw material costs was used to find the optimum plant location and capacity. Output from the deterministic model showed the optimal location of the plant to be Oklahoma. The plant will have a capacity of 241 kg/year of SWNT. The facility will operate under capacity until the tenth year due to the change in the demand. Total capital investment needed for the project will be $2.5 million. The expected net present worth for the project over the ten year span is $16 million. This represents a 46% return on investment.

1.0 INTRODUCTION

Carbon nanotubes are highly versatile materials that are finding applications in a variety of fields. The global market for carbon nanotubes is rapidly growing, making it a promising investment opportunity. Large-scale production methods are being currently developed and implemented in existing nanotubes plant. This project analyzes the technical feasibility and economic potential of building a facility to produce single wall carbon nanotubes.

1.1 History

There are four known forms of pure carbon: diamond, graphite, the buckminster fullerene (buckyball), and carbon nanotubes. For many years, the only two known forms of carbon were graphite and diamond. In 1985, Richard Smalley and a group at Rice University found a new form of carbon consisting of 60 carbon atoms arranged in a sphere. The model spatial arrangement looked similar to the soccer ball. Although buckyballs have some interesting properties, no commercial applications have been found.

In 1991, Sumio Iijima of NEC Corp. discovered carbon nanotubes while trying to synthesize buckyballs.[1] Nanotubes are hollow structures that resemble straws, with the same tendency to bend and spring back. Later research revealed that they can form as concentric tubes (multi-wall) or as single tubes (single-wall). These carbon nanotubes are stronger than steel, lighter than aluminum, more conductive than copper, and good semiconductors. Table 1.1 gives a brief history of the discovery of carbon nanotubes.

Table 1.1[2]: Summary table of the discovery of carbon nanotubes

When	Who	Events
1940s	German Chemist Otto Hahn	When trying to create heavier atoms by arc carbon method of neutron, Hahn reported the existence of carbon chains. Because he was interested in only metal atoms, the research of carbon chains was not continuing.
1970s	England Chemists Harry Kroto and Dave Walton	They were synthesizing long carbon chains to make something like gas cloud in the galaxy.
1985	Kroto and his American colleague, Rick Smalley	They collaborated a project to simulate conditions of red giant stars in the laboratory.
Late 1980s	Scientists around the world	Buckyball was synthesized and confirmed as C_{60}
1991	Japanese Scientist, Sumio Iijima	Discovery of multi wall carbon nanotubes
1993	S, Iijima and T, Ichihashi	Synthesis of single wall carbon nanotubes Begin to use Laser ablation method
1995	A.G. Rinzler	Research of nanotubes as field emitters
1996	Professor Robert F. Curl, Jr., Rice University, Houston, USA, Professor Sir Harold W. Kroto, University of	Awarded 1996 Nobel Prize in Chemistry for the discovery of Buckyball
	Sussex, Brighton, U.K., and Professor Richard E. Smalley, Rice University, Houston, USA,	
1998		Development of HiPCO, CVD methods
1999	Samsung Company	Demonstrated Flat Panel display prototype (4.5", full-color) using nanotube as filed-emission source.
2001	IBM research group	The first computer circuit composed of only one single carbon nanotube was announced
2001	M. Kociak	Intrinsic superconductivity of carbon nanotubes

Diamond

Diamond exists in a cubic and hexagonal form. In the most frequent cubic form each carbon atom is linked with four other carbon atoms by four sp^3 bond in a tetrahedral array with a C-C bond length of 1.544 Å.[3] This is nearly 10% larger than a graphite. However the atomic density is 56% higher than in graphite. The crystal structure is zinc blend type (FCC) with a diatomic basis. The second carbon atom is at position (¼, ¼, ¼) in the unit cell and the lattice constant is a0 = 3.567 Å (Figure 1.1 left).

The physical properties of diamond are given by its structure. Diamond is a wide-gap semiconductor (5.47 eV), the hardest material in nature (Mohs hardness 10) and has the highest atomic density. Diamond, as also graphite (in-plane) have the highest thermal conductivity (~25 W·cm-1·K-1) and the highest melting point (4500 K). The hexagonal diamond (Lonsdaleite) has a wurtzite crystal structure (Figure 1.1 right) and a C–C bond length of 1.52 Å . The gravimetric density of both types of diamond is 3.52 g·cm-3.[4]

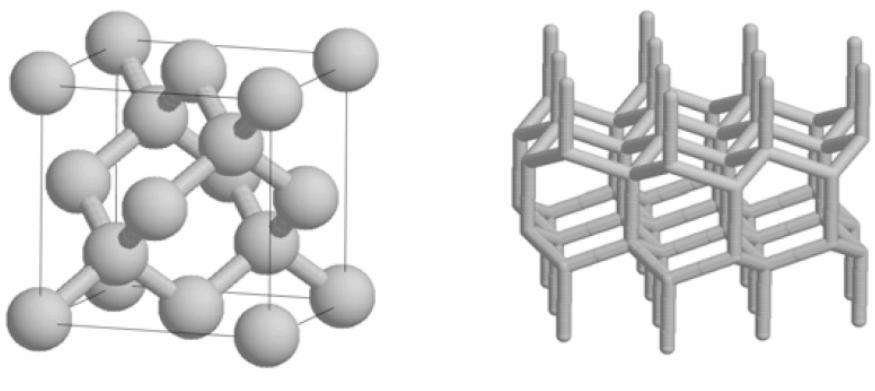


Figure 1.1: Diamond in the cubic form (left) and hexagonal form Lonsdaleite(right)

Graphite

In graphite the atoms are arranged in layers of a honeycomb network in which the carbon atoms are bonded with sp2 σ bonds and a de-localized π bond. In the most common hexagonal crystal form of graphite the layers are stacked in an ABAB… sequence (called Bernal stacking) (Figure 1.2). The in-plane nearest neighbor distance a C-C is 1.421 Å and the lattice constant is a0 = 2.461 Å. The density of graphite is 2.26 g·cm-3.The weak interlayer bonding of graphite originates from the small overlap of the π-orbitals between atoms of adjacent layers and not to Van der Waals bonding.[4]

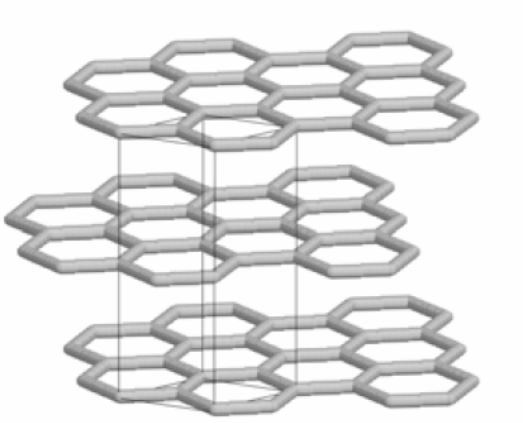


Figure 1.2: Hexagonal Graphite

Fullerenes

Fullerene is either buckyballs or nanotubes.[3] Buckyballs (Figure 1.3) consist of spheres of carbon atoms. The most common buckyballs have 60 atoms, larger buckyballs such as C_{70}, C_{78} and C_{80} can also be found. Buckyballs are chemically quite inert and are quite stable at high temperatures. The bonding of carbon buckyballs is a hybrid between sp^2 and sp^3. Buckyballs behave closer to graphite than diamond.[3]

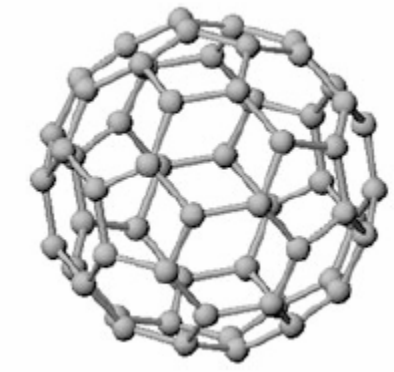


Figure 1.3: **Buckyball, C_{60}**

Amorphous carbon

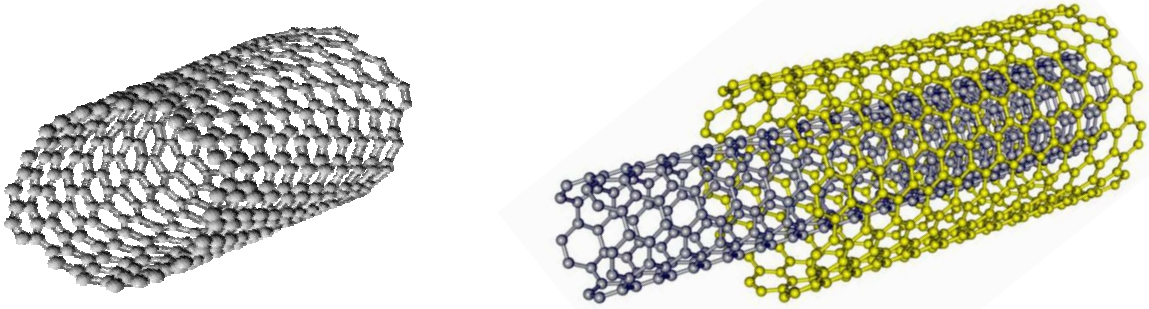
Amorphous carbon (a-C) is a highly disordered network of carbon atoms with predominantly sp^2 bonds, with only approximately 10 % sp^3 bonds and no sp1 bonds. a-C has no long-range order but only some short-range order (~10Å) that depends on the carbon bonding type (sp^2/sp^3) and the hydrogen content.[4]

Nanotubes

Different from buckyballs which have spheres of carbon atoms; nanotubes are cylinders of carbon atoms. A carbon nanotube can be described as a single rolled sheet of graphite. An alternate way to think of a nanotube is that it consists of a C_{60} buckyball that is split down the middle; a cylinder of carbon atoms connects the two halves of the buckyball. Carbon nanotubes can have either closed or open ends. The bonds of these carbon atoms can be described as a strained sp^2 bonds in graphite. The smaller the diameter of the nanotube, the greater the strain of the carbon bond. These cylinders have diameters that range from 0.8 nm to 300 nm, and the lengths range from several micrometers to millimeters. Nanotubes have very high tensile strength and modulus. Carbon nanotubes can also function as either conductors or semiconductors depending on their structure.[3,4]

1.2 Types of Carbon Nanotubes

There are two major types of carbon nanotubes that are currently produced: single walled carbon nanotubes and multiple walled carbon nanotubes.[3] Single walled nanotubes (SWNT's) have one shell of carbon atoms in a hexagonal arrangement. SWNT's are often found in bundles that are formed by a triangular arrangement of individual

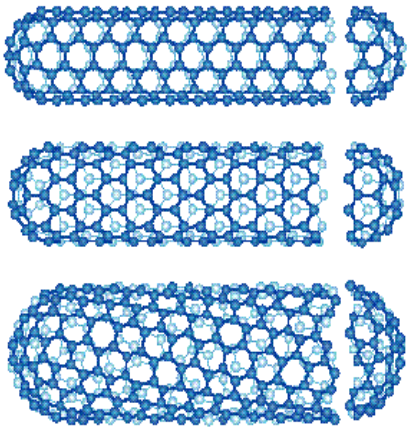


(a) (b)

Figure 1.4: Diagram of (a) single wall and (b) multi-wall carbon nanotubes

SWNT's. The nanotubes are held together in bundles by a weak Van Der Waals forces.[4] Multi-walled nanotubes (MWNT's) consist of multiple concentrically nested carbon tubes. Although there are significant differences between these two types of carbon nanotubes, these differences are relatively minor compared to the differences between nanotubes and other materials.[4] MWNT's have a higher occurrence of structural defects than SWNT's; therefore SWNT's are often more favorable.

Carbon nanotubes have three orientations which determine the properties of the materials whether they conductive tubes or semiconductors. Those orientations are arm chair, zigzag and chiral, shown in Figure 1.5**.** Depending on the applications different characteristics of carbon nanotubes are required. If the desired products are metal carbon nanotubes, then armchair type is desirable. If the desired product is semiconductor, then chiral type is preferable. However, all three orientations are produced in a mixture and are hard to separate. The CVD method which will be discussed later produces more of chiral type CNTs, whereas laser ablation gives metal CNTs.



(a) Chiral

(b) Zigzag

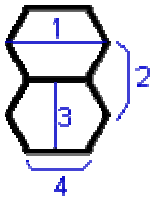
(c) Armchair

Figure 1.5: Arrangements of carbon nanotubes.

1.3 Properties of Nanotubes

The properties of nanotubes are summarized briefly in Table 1.2. Carbon nanotubes have various physical properties and are an important material which can be used for a broad variety of advanced industries such as electronic and information technology. The details of the nanotube applications will be discussed in the next section.

Table 1.2: Nanotubes properties[5]

Equilibrium Structure		
Average Diameter of SWNT's		1.2 -1.4 nm
Distance from opposite Carbon Atoms (Line 1)		2.83 Å
Analogous Carbon Atom Separation (Line 2)		2.456 Å
Parallel Carbon Bond Separation (Line 3)		2.45 Å
Carbon Bond Length (Line 4)		1.42 Å
C - C Tight Bonding Overlap Energy		~ 2.5 eV
Group Symmetry (10, 10)		C_{5V}
Lattice: Bundles of Ropes of Nanotubes		Triangular Lattice (2D)
Lattice Constant		17 Å
Lattice Parameter:		
	(10, 10) Armchair	16.78 Å
	(17, 0) Zigzag	16.52 Å
	(12, 6) Chiral	16.52 Å
Density:		
	(10, 10) Armchair	1.33 g/cm^3
	(17, 0) Zigzag	1.34 g/cm^3

	(12, 6) Chiral	1.40 g/cm^3
Interlayer Spacing:		
	(n, n) Armchair	3.38 Å
	(n, 0) Zigzag	3.41 Å
	(2n, n) Chiral	3.39 Å

Optical Properties

Fundamental Gap:	
For (n, m); n-m is divisible by 3 [Metallic]	0 eV
For (n, m); n-m is not divisible by 3 [Semi-Conducting]	~ 0.5 eV

Electrical Transport

Conductance Quantization	(12.9 k)-1
Resistivity	10^{-4} -cm
Maximum Current Density	10^{13} A/m^2

Thermal Transport

Thermal Conductivity	~ 2000 W/m/K
Phonon Mean Free Path	~ 100 nm
Relaxation Time	~ 10^{-11} s

Elastic Behavior

Young's Modulus (SWNT)	~ 1 TPa
Young's Modulus (MWNT)	1.28 TPa
Maximum Tensile Strength	~ 100 GPa

1.4 Growth Mechanisms of Carbon Nanotubes

This section explains the growth mechanism, as it is applies to all techniques.[6] Specific conditions for the various synthesis methods are discussed later. The growth mechanism of carbon nanotubes is not well understood. Different models exist, but some of them cannot definitely explain the mechanism. The metal or carbide particles seem to be necessary for the growth because they are often found at the tip inside the nanotube or in the middle of the tube. In 1972 Baker made a model of growth of carbon fibers which is shown in Figure 1.6.[7] It is supposed that hydrocarbons like acetylene decompose at

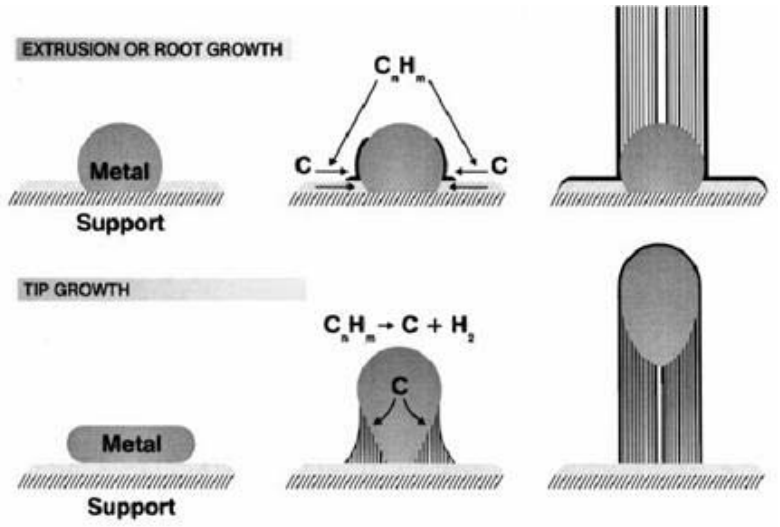


Figure 1.6[7]: Possible carbon nanotube growth mechanism

600°C on the top of a metal cluster on the support. The dissolved carbon diffuses into the cluster, precipitates on the rear side, and forms a fiber. The carbon diffuses through the cluster due to the presence of a thermal gradient formed by the heat release of the exothermic decomposition of the hydrocarbons. The activation energies for filament growth are in agreement to those for diffusion of carbon through the corresponding metal (Fe, CO).[8] Whether the metal cluster moves away from the substrate (tip growth) or whether it stays on the substrate (base growth) is explained by a weaker or stronger metal support interaction.[4]

For the synthesis of nanotubes, the metal clusters must be present in the form of nanoparticles. In addition, it is supposed that the metal cluster can have two roles: 1) as a catalyst for the dissociation of the carbon-bearing gas species; 2) carbon diffuses on the surface of the metal cluster of through the metal to form a nanotube. The most active metals are Fe, Co and Ni, which are good solvents for carbon. The exact chemical

composition of the catalyst particles during the synthesis is known. It was reported that for SWNT's the nano particles have to be smaller than for MWNT's. This is in contradiction to the arc discharge method in which SWNT's grow radially from one larger metal cluster.

1.5 Production Methods

There are three available methods to produce SWNT's: arc discharge, laser ablation, and chemical vapor decomposition.

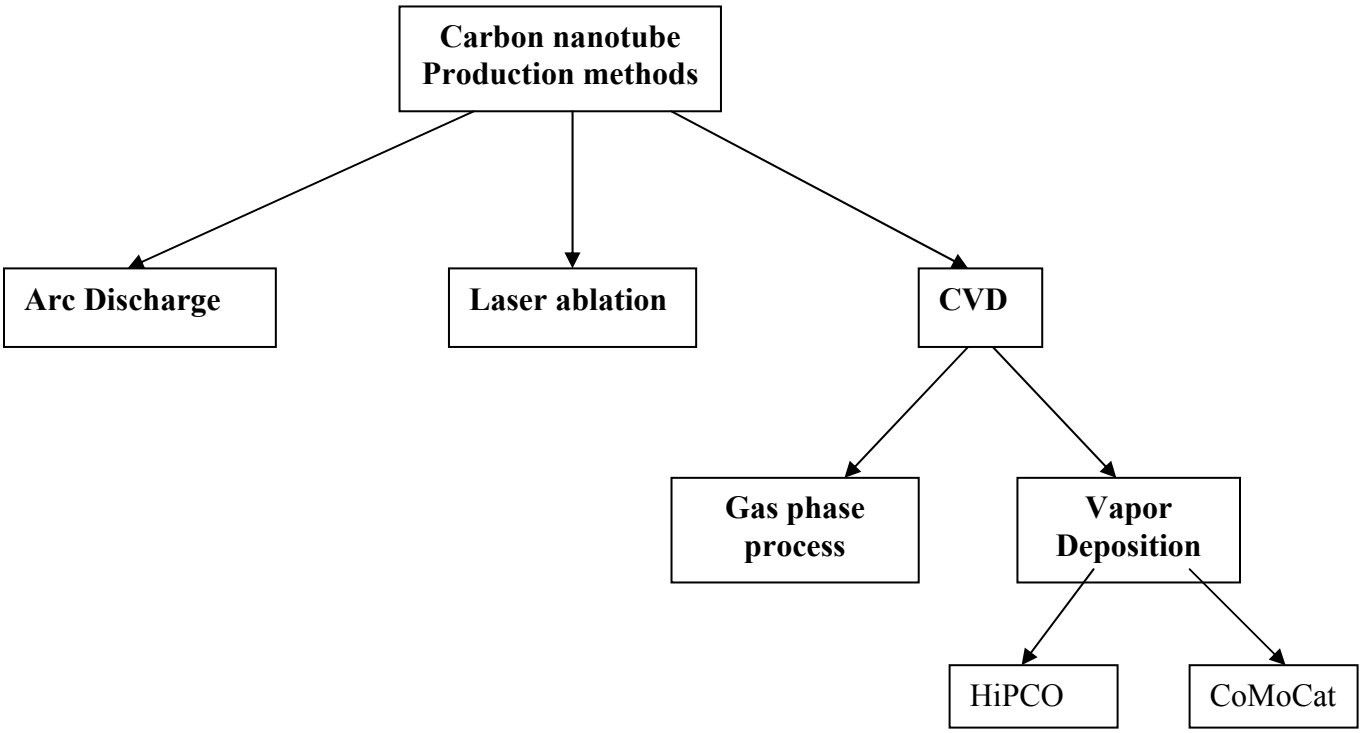


Figure 1.7: Production methods for carbon nanotubes

- Arc discharge produces nanotubes by flowing a precursor gas through a plasma discharge at a very high temperature. This technology produces high quality nanotubes, unfortunately accompanied by a large volume (up to 50%) of

contaminants. Although this process can produce small quantities of nanotubes, it is poorly suited for producing large volumes of nanotubes.

- In the laser ablation technique, a high-power laser beam impinges on a volume of carbon -containing feedstock gas (methane or carbon monoxide). Laser ablation produces a large amount of clean metal nanotubes, whereas arc discharge methods generally produce large quantities of impure material. Laser ablation produces nanotubes by directing a high-energy CO_2 at a carbon target. Pulsed laser vaporization is a specific type of laser ablation. This method employs a high power pulsed graphite. Both of these technologies produce high quality single wall nanotubes with fewer contaminants than arc discharge, but the production rate remains low. Furthermore, this technology is capital intensive and is limited to research quantities. This technology will probably not be used in any commercial applications.
- Chemical vapor deposition produces nanotubes by heating a precursor gas and flowing the gas over a metallic or oxide surface with a prepared catalyst. This technology can produce SWNT's and MWNT's in good yield – over 90% - with few contaminants. Early gas phase processes yields nanotubes with high levels of defects (e.g. missing atoms, out of place bonds). Another type of CVD is the vapor decomposition of CO at high pressure. In this process, the reaction takes place on a catalyst flowing in a reaction stream, rather than bonded to a surface. These processes have been used to produce both single and multi-wall nanotubes, and are probably the most suitable for commercial processes. In general, chemical vapor deposition (CVD) results in MWNT's or poor quality SWNT's.

The SWNT's produced with CVD have a large diameter range, which can be poorly controlled. But on the other hand, this method is very easy to scale up, which favors commercial production.

1.5.1 Arc discharge method

The arc discharge method provides the high temperature needed for the evaporation of carbon atoms into a plasma (>3000°C). With the carbon arc method both multi-wall and single wall nanotubes can be produced. Other carbonaceous products such as carbon whiskers, soot, and fullerenes are also synthesized with this method. The type of product synthesized is determined by the pressure and type of gas used. A diagram of an arc discharge apparatus is shown in Figure 1.8. It consists of two carbon electrodes; the thicker cathode on which the deposit forms is separated from the thinner anode by approximately one millimeter. During the deposition, the graphite anode is consumed. A voltage of 20-25 V is applied between the electrodes and the current is between 50-120 A. The optimal pressure for producing nanotubes is around 500 torr of He. To produce isolated SWNT catalysts such as Co, Ni, Fe, Y and Gd are used. Mixed catalysts such as Fe/Ni, Co/Ni and Co/Pt are used to grow bundles of SWNT. Gram quantities of bundles of SWNT can be produce with the carbon arc method. A hole is drilled in the anode and

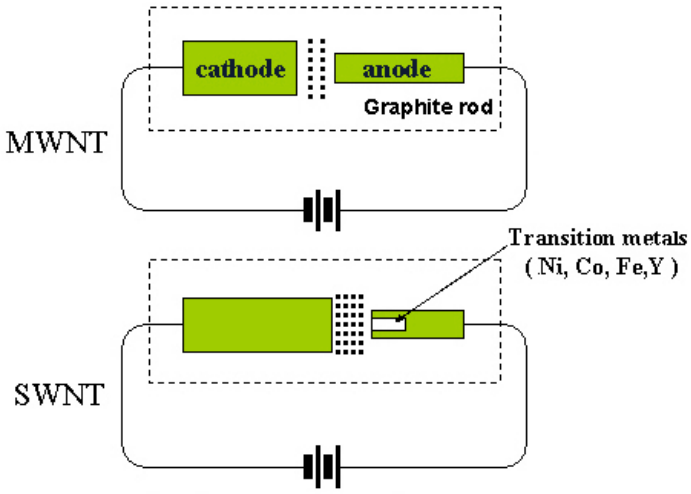


Figure 1.8[9] Arc discharge method

filled with the metal powder. The SWNT's are found in a web-like structure in the chamber and not on the cathode. Nanotubes with a number of impurities can be prepared in high yields with this method. [9]

Although the process of producing nanotubes in an electric discharge sounds relatively simple, there are a number of parameters that are crucial to nanotubes production. These parameters include flow rate, temperature, reactants, voltage, gas ratios, catalysts, contaminants and pressure. Adjusting all these parameters to maximize nanotube production is not an easy task. The primary disadvantage of this technique is that there are a fair amount of contaminants such as graphite, soot, amorphous carbon, and fullerenes. Separating nanotubes from these side products is very difficult and can dramatically increase the cost of the nanotubes.

1.5.2 Laser ablation method

In the laser ablation method, a laser is used to vaporize a graphite target in an electrical furnace heated to 1200°C (see Figure 1.9). Flowing argon gas (~500 Torr) carries the nanotubes from the high temperature zone to the water-cooled copper collector outside the furnace. If a pure graphite target is used MWNT's are also produced. However, if the target is composed of 1.2 atom % Co/Ni with equal amounts of Co and Ni added to the graphite, then SWNT are synthesized.

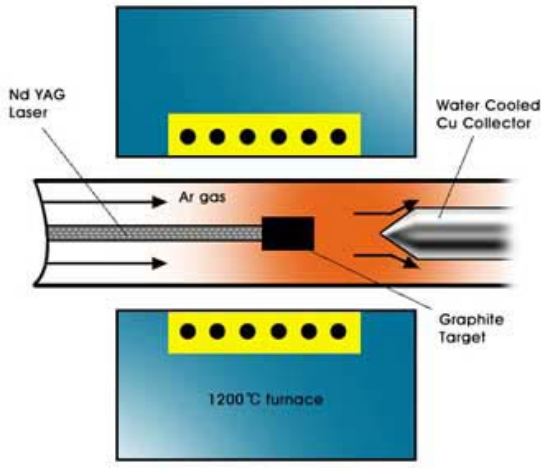


Figure 1.9[9]: Laser ablation

High yields with of 70-90% conversion were reported in the condensing vapor of the heated flow tube. The produced material consists of ropes of SWNT with a diameter ranging from 10 to 20 nm and around 100 μm in length. The average nanotube diameter and the diameter distribution can be adapted by varying the synthesis temperature and the composition of the catalyst. The diameters of the SWNT have strongly peaked distributions.[4]

Compared to the arc discharge method, this method gives fewer side products. However the production rate is much slower.[2] Another disadvantage is the laminar flow requirement through the chamber since the production rate reduces significantly as the flow rate increases.[2] If the goal is to produce research grade carbon nanotubes, this method is a good choice since it produces highly pure materials.

1.5.3 Chemical Vapor Deposition Method

In the CVD method different hydrocarbons like benzene (C_6H_6), pentane (C_5H_{12}) acetylene (C_2H_2), methane (CH_4), and carbon monoxide are decomposed over various metals (Fe, Co, Ni) at temperatures between 500 and 1200°C. This method was used for a long time for the synthesis of carbon fibers before it was discovered that this method could also produce nanotubes. [10] Different modifications of the CVD method exist and are explained in more detail below.

Gas phase processes produce nanotubes with high levels of defects (i.e. missing atoms and out of place bonds), the products mixture contain both MWNTs and SWNTs with

larger portion of MWNTs. Therefore, although the gas phase process technique may give high production rate at lower cost relative to that of vapor deposition, it is not a preferred method. Vapor deposition produces SWNTs with fewer effects. Two offshoots of the vapor deposition method that show high potential for upscale ability are the HiPCO process and the CoMoCat process. In gas phase process, a substrate is not used whereas it in vapor deposition process.

Gas Phase Process

In the gas phase method, no substrate is used. The catalyst is introduced in the flowing gas stream in the form of volatile organometallic molecules. It is also possible to produce carbon nanotubes with this method by the decomposition of hydrocarbons or carbon monoxide in the presence of metallocens or iron pentacarbonyl. SWNTs produced from this method can reach centimeter long strands. A disadvantage of this method is the large amount of encapsulated metal clusters.[11] Figure 1.10 shows the set up of this method. There are two furnaces placed in the chamber. Ferrocene is used as the catalyst. The catalytic metal is vaporized in the first furnace at relatively low temperature and catalytic particles are formed. Then they enter the second furnace where decomposed carbons (i.e, C_2H_2) are diffused to the catalytic metal particles and form carbon nanotubes.[11]

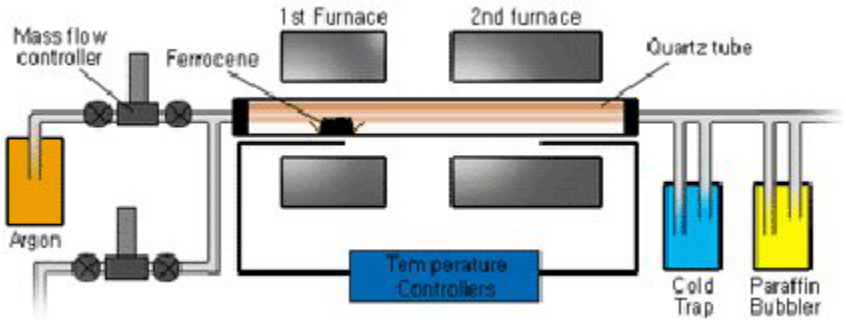


Figure 1.10[12]: Schematic diagram of a vapor phase growth apparatus

Vapor Deposition on Substrates

Vapor deposition techniques that utilize a substrate produce carbon nanotubes at slower production rate compared to gas phase technique.[12] However, the materials produced have fewer defects. Two examples of this method are the HiPCO process and the CoMoCat process.

HiPCO process

The HiPCO process was developed by Richard Smalley at Rice University. In this process, SWNT's are produced through catalytic growth in a continuous-flow gas-phase process by using carbon monoxide (CO) as the carbon feedstock and iron pentacarbonyl ($Fe(CO)_5$) as the iron-containing catalyst precursor.[13] Figure 1.11 shows the laboratory-scale reactor of the HiPCO process. The reactor consists of a thin wall quartz tube, which has an outer diameter of 3 in. The quartz tube is surrounded

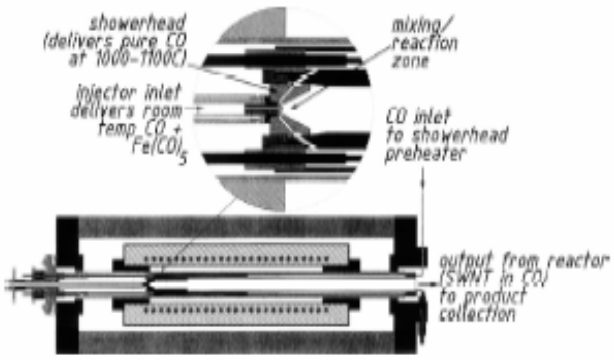


Figure 1.11: **HiPCO reactor**

by an electrical heating element. Both are contained in the aluminum thick cylindrical chamber. A mixture of CO and small amount of $Fe(CO)_5$ flow through a quartz tube, producing iron clusters in the gas phase. These clusters act as nuclei upon which SWNTs nucleate and grow. The reaction is as follows.[13]

$$CO + CO \xrightarrow{Fe(CO)_5} C(s) + CO_2$$

The pressure of the heating element and the space quartz tube and aluminum cylindrical must be kept higher than that of CO. The pressure of CO is controlled at 30 atm and the total flow rate is 215 cm ^{3}/min. The temperature of the reactor is kept at 1050^o C. Both the yield and the size of SWNT's can be controlled over a wide range depending on the conditions and flow-cell geometry. For these particular conditions, SWNTs are produced at the rate of 10.8g/day.[13]

CoMoCat process

The CoMoCat process was developed by Daniel Resasco at the University of Oklahoma. In this process SWNTs are produced by the use of a Cobalt-Molybdenum/SiO_2 catalyst. The apparatus for this process is shown in Figure 1.12.[12] A tubular fluidized bed is maintained within 700 and 950^o C. The catalyst is fed continuously into the reactor, reacting with the pure cold flow of CO at a pressure within 1-5 atm. Optimal selectivity is found when

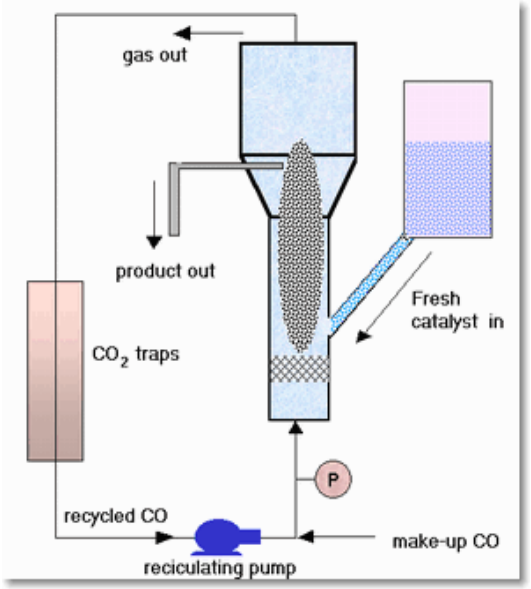


Figure 1.12[12]: Schematic of CoMoCat process

the ratio of Co:Mo is 1:1[5]. The production rate and the quality of the SWNT's depend on the amount of the catalysts used. Generally, the production rate is 0.25g SWNT/gram of catalyst. Table 1.3 summarizes the advantages and disadvantages of each of the methods.

Table 1.3[14]: Comparison of different production methods

Properties	Arc Discharge	Laser Ablation	Gas Phase Process	Vapor Deposition
Nanotube Generator	Requires high voltage arc discharge. Inexpensive.	Requires expensive high energy lasers.	Catalytic particles.	Catalytic particles.
Process	Batch.	Batch.	Continuous.	Continuous or Semi Batch.
Diameter of SWNT Nanotubes	1.2-1.4 nm	1.2-1.4 nm	0.8-1.4 nm	0.8-1.4 nm
Length of Nanotubes	1-10 microns	1-10 microns	Micron or longer	20 cm
Yields	~50%	~70%	50%	~97-99%
Quality of nanotubes	Produces largely defect free nanotubes.	Produces defect free nanotubes. Considered highest quality nanotubes.	Produces MWNT and SWNT; hard to separate. Semi Conductor	Produces tubes with some defects. Number of defects declining. Semi Conductor
Production Quantities	Could exceed 10g/day.	Less than 1g/day.	In full operation, 500-2,000 kg per day.	Theoretically can produce kg or more per day.

Source: BCC, Inc.

1.6 Multi-wall Versus Single Wall

Each type has its advantages and disadvantages. MWNT's are easier and less expensive to produce because current synthesis methods of SWNT's result in major concentrations of impurities that require removal by acid treatment. But MWNT's have a higher occurrence of structural defects, which diminish their useful properties. Many companies prefer SWNT's because they do not have such defects and their properties are consequently stronger.

2.0 MARKET ANALYSIS

2.1 Government Funding

Nanotechnology receives significant government funding across the globe. Much of the current research being performed in nanotechnology is funded by federal grants provided by various government agencies. Global government spending on nanotechnology reached the two billion dollar mark in 2002, and continues to grow. Japan, the United States, and the United Kingdom are at the forefront of this government spending.

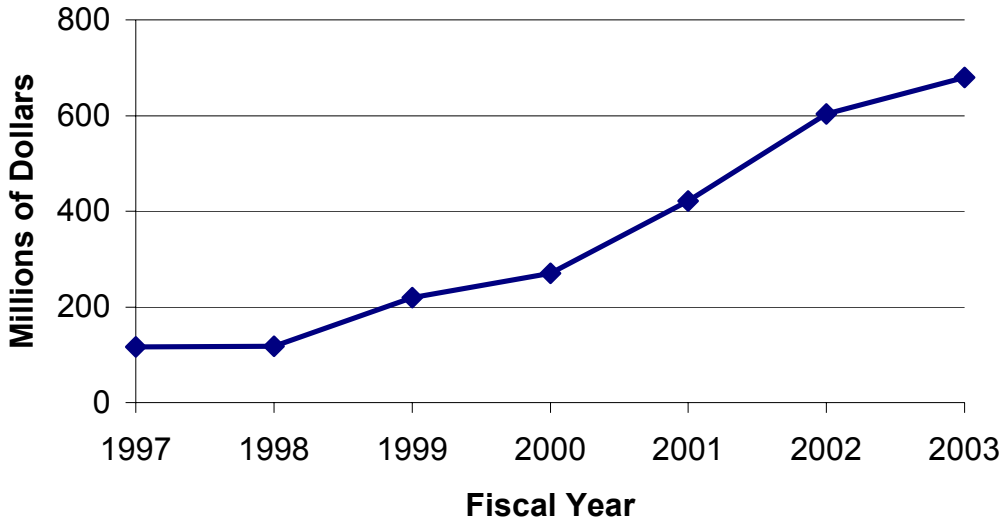


Figure 2.1: **U.S. Government Spending Since 1998**[15]

Government funding for nanotechnology in the United States is on the rise. Figure 2.1 above shows the increase in spending from 1997 to 2003.[16] In February of 2003, President George W. Bush signed into law the Nanotechnology Research and Development Act. The bill authorizes 3.7 billion dollars of government funding for nanotechnology research over four years beginning in fiscal year 2005. The funding is divided among five of the sixteen agencies participating in the National Nanotechnology

Initiative (NNI), a federal program created to coordinate efforts in nanotechnology research. The authorized spending for each of these agencies is shown in Figure 2.2 below.

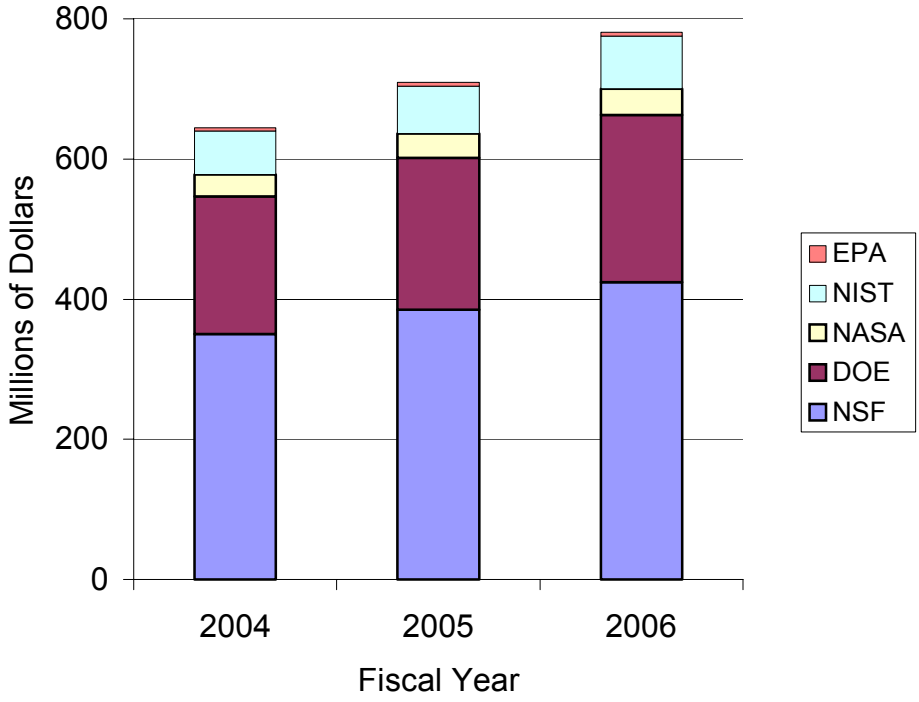


Figure 2.2: Government Spending by Agency [17]

2.2 Current Market for Nanotechnology

The market for nanotechnology is growing at a tremendous rate due to the numerous applications emerging from research. The total global demand for nanoscale materials and devices was $7.6 billion in 2003. The market size is expected to grow at an average annual growth rate of 30.6%, reaching $28 billion by the year 2008.[18] This is an extremely high growth rate. However, new applications are allowing for the creation of new businesses, and nanotechnology is the one of the few sectors in which venture capital is increasing. Venture capital in the nanotechnology sector since 1999 is over

$900 million.[19] This surge in investments into nanotech companies will lead to an even larger market size in the near future. Revenues from nanotechnology are expected to reach over $200 billion by 2006.[20]

2.3 Nanotubes Market

Nanotubes are the fastest growing sector of the nanotechnology market, with a projected average annual growth rate of 173% over the next five years.[21] Market research estimates indicate that the global production of nanotubes in 2003 was between 4 to 10 kg. Prices of high quality nanotubes range from $200 to $1000 per gram. By one estimate, the carbon nanotube market will be valued at approximately $400 million in 2004.[22] The market price of nanotubes is expected to drop due to changes in the market due to several factors: the increases in market size, venture capital, and government spending, as well as several profitable commercial applications on the verge of realization. Add these factors to the advent of new synthesis methods, which will allow for the mass production of nanotubes. Once these methods become available, companies will begin implementing them into their production facilities. These aspects will attract investors looking to get a share of the market by backing new production facilities. The presence of new producers signifies an increase in the output of single wall nanotubes. The supply of single wall nanotubes in the market will surge due to these combined effects. This surge in supply is expected to occur without a significant increase in demand, as most commercial applications are on a longer timeline. This will devalue the nanotubes, lowering their price.

2.4 Competition

There are less than twenty facilities worldwide that currently produce single wall nanotubes. Approximately ten of those companies are located within the United States, while others are located in China, Japan and Western Europe. The figure below shows the geographical location of the U.S. facilities. Several of these companies are already well established in the nanotechnology field. Most of the nanotubes producers offer a range of post-synthesis processing that allows consumers to choose from varying purities and functionalities. With the considerably high projected growth rate of the nanotubes demand, new companies should not face any trouble entering the market.

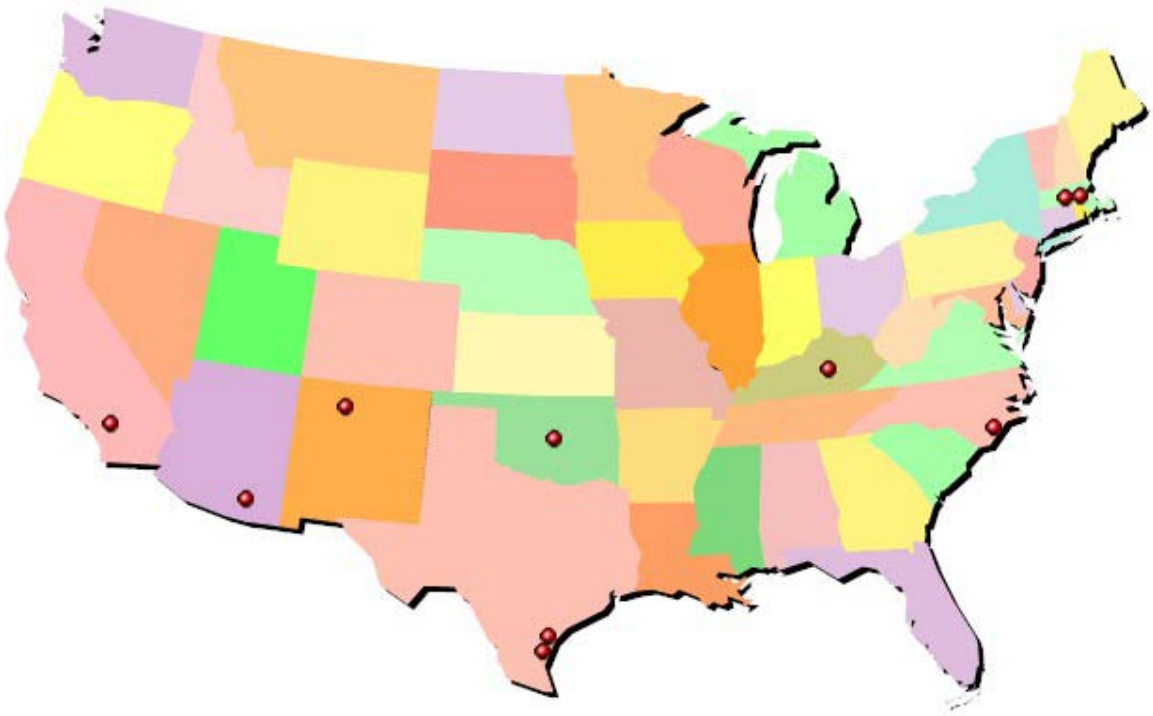


Figure 2.3: Location of Existing Single Wall Nanotube Production Facilities

2.5 Applications for SWNT's

2.5.1 Batteries

Much research is currently being performed on the use of SWNT in rechargeable lithium batteries. Electrodes made from carbon nanotubes can have up to twice the storage capacity of graphite electrodes due to differences in the way the carbon atoms store lithium ions.[23] Battery applications are currently limited to research areas because of the high cost of single wall nanotubes. Some batteries on the market contain graphite electrodes with multi-wall nanotube additives. However, multi-wall nanotubes are much less expensive than single wall nanotubes. A sharp decrease in the price of SWNT's is necessary for their implementation into batteries to be economically practical. Since the market price of nanotubes is expected to go down as new large-scale production methods take over, the utilization of single wall nanotubes in commercial batteries is an imminent prospect.

2.5.2 Flat Panel Displays

The field emission properties of carbon nanotubes have allowed them to be successfully integrated into flat panel displays. Compared to active matrix liquid crystal displays, nanotube displays have a better image quality, consume one-tenth the power to run, and cost one-third as much to manufacture. Nanotube displays can be used for very large screens, such as those used for sporting events or advertising. Plasma, projection, and liquid crystal screens currently dominate the display market, but they have drawbacks. Plasma screens are expensive, ranging from 3,000 to 16,000 dollars, depending on the size and quality. Projection screens are less expensive, but both plasma and projection

have a high rate of power consumption. Plasma screens cannot be used for small displays, such as those in PDA's and cell phones. Nanotube displays are a viable candidate for both large and small sized screens.

Flat panel displays have a twenty billion dollar market, but there are several drawbacks. Motorola has developed the technology to produce nano-emissive displays (NED), which have been licensed by Cetek Technologies for production.[24] Samsung and Dupont also have licenses on carbon nanotube technology to produce flat panel displays.[25] Applied Nanotech Inc. holds over 80 patents on the uses of nanotubes as electron sources in displays.[26] Rights to use this technology would require licenses or payment of royalties. Furthermore, the nanotubes used in flat panel displays must be grown directly onto the surface of a substrate so that they are arranged in highly ordered arrays. A few major companies already have their own labs to produce the quality of nanotubes required for these displays.

2.5.3 Chemical Sensors

Single-walled nanotubes exhibit a significant change in electrical resistance when exposed to certain gases. This property can be exploited for their use in chemical sensors. Research has shown that nanotubes expand in response to certain nerve agents like DMMP because they are strong electron donors that reduce the hole density in the semi-conducting nanotubes.[27] After detection, the sensor can be reversed by heating it to high temperatures.[28] Chemical sensors can detect nerve agents in quantities as low as one part per billion.[29] This is substantially more sensitive than existing solid-state sensors.

Nanosensors could be used in defense applications and in industrial process controls. Researchers at the Naval Research Laboratory are making sensors from nanotubes in the form of randomly arrayed thin film transistors, which can be produced by deposition of suspended SWNT's onto a substrate.[30] This makes chemical sensors a feasible market for the SWNT's produced in our plant.

2.5.4 Hydrogen Storage

The use of hydrogen as a fuel source has always been a popular idea among environmentalists and politicians. The U.S. Department of Energy is starting a program to replace much of the current energy consumption with fuel cells. Researchers have claimed to produce nanotube clusters with hydrogen storage capacities between 4% and 20% of their weight.[31] As with most applications, the use of single-wall nanotubes in hydrogen fuel cells will increase with emerging technology and with the decreasing price of nanotubes.

2.5.5 AFM Probe Tips

Single wall carbon nanotubes have been applied for use as atomic force microscopy probes. Fibers made from single wall nanotubes can be mounted onto silicon tips. Single wall nanotubes can also be directly grown onto a silicon tip by a chemical vapor deposition method. AFM probe tips made from multi-wall nanotubes are currently on the market from several companies, including NanoScience Instruments.[32]

2.5.6 Composites and Fibers

Nanotubes can be incorporated into existing materials to make useful composites. The strength of nanotubes lends itself to the application, producing high-performance materials with improved energy absorption and increased tensile strength. Composites made with carbon nanotubes also have thermal and electrical conducting properties. Researchers have discovered how to spin nanotubes into fibers, which can then be woven into cloth.[33]

2.6 Market Forecast

A detailed analysis of the current market and its expected behavior over the next 10 years was performed. Supply curves were generated based on the number of companies in the market and the average production rate. Demand curves were constructed from market estimates of demand in the research and commercial sectors. The equilibrium points of the supply and demand curves for the next ten years were used to determine the expected equilibrium quantities and prices. Figure 2.4 shows how the equilibrium quantity will

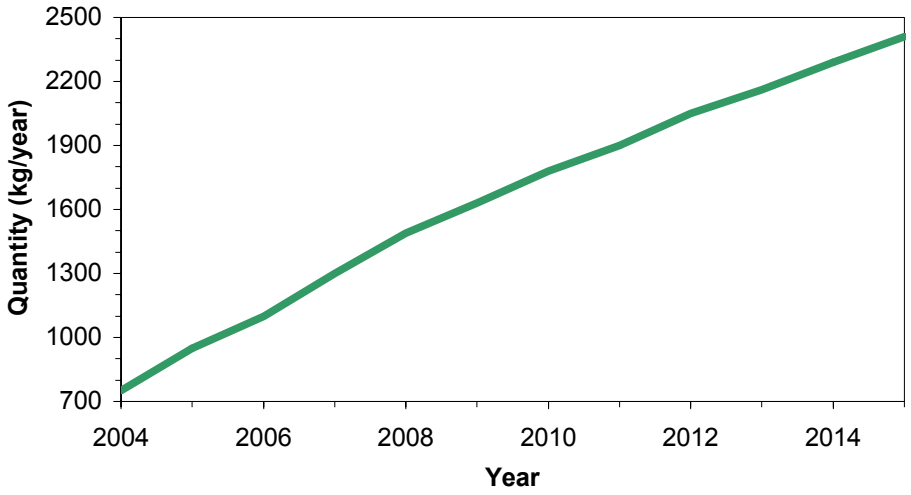


Figure 2.4: Projected Equilibrium Quantities

increase at a nearly linear rate over the next ten years. The equilibrium price is shown as a function of time in Figure 2.5. Additional details about the forecasting process can be found in Appendix A.

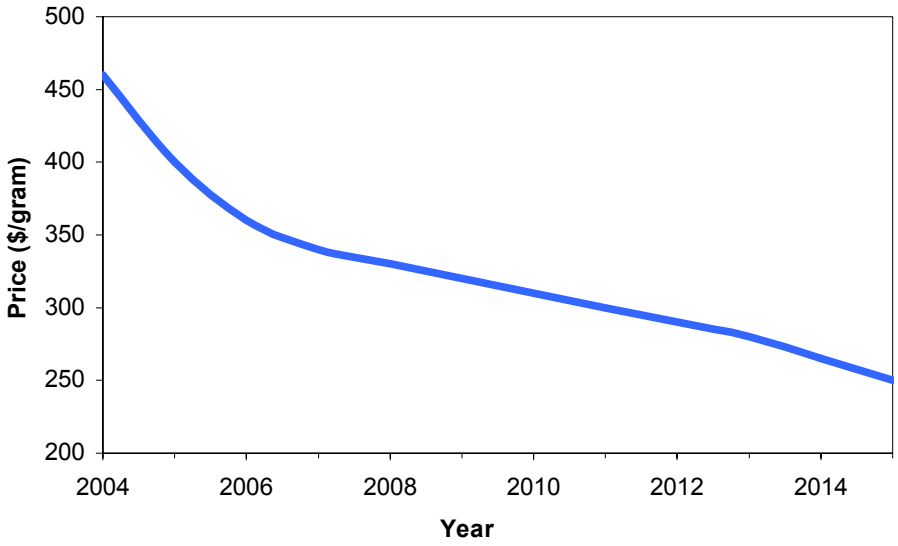


Figure 2.5: Projected Change in Equilibrium Price

2.7 Summary

Most of the applications for single wall nanotubes are currently in development. The markets for several of the applications mentioned above are promising. At present, 90% of the potential market lies in academic and industrial research laboratories. The increase in government funding for nanotechnology research and development should expedite the movement of nanotube applications from the laboratory to the marketplace. Once these applications become commercially viable, the production of nanotubes will increase to meet the growing demand.

3.0 PLANT DESIGN

Two different gas phase processes, HiPCO and CoMoCat, were analyzed in order to determine the best option in terms of operating costs, raw material costs, and equipment costs. Process design layouts were created for both methods. A detailed analysis of the major pieces of equipment was performed with literature research and hand calculations. The equipment costs vary with the production rate, but the values presented are priced for a capacity of 1 kilogram SWNT's per day. This section gives the plant designs for both processes and presents the comparison results.

3.1 HiPCO Process Description

In this process the raw materials include commercial grade carbon monoxide (CO) and iron pentacarbonyl ($Fe(CO)_5$). The commercial grade CO is 98.5% purity. The CO is divided into two different streams. The first stream is sent to a mixer where a mixture of CO with 32 ppm $Fe(CO)_5$ is formed. This mixture is cooled down to 298K with cooling water in a heat exchanger before entering the reactor. The argon stream acts as the carrier gas, and is close enough to room temperature that it does not need cooling. The other CO stream enters the opposite end of the reactor at 30 atm and travels through the channels surrounding the reaction chamber. Upon entering the reaction chambers, the CO has reached 1100^{o} C through heat transfer with the reactor walls. The SWNTs are condensed by the cooling copper rod at the end of the reactor. A filtration system is used to collect the SWNTs product. Carbon dioxide (CO_2) is produced in small quantities as a byproduct of the reaction. After the nanotubes are filtered, they are sent on to the

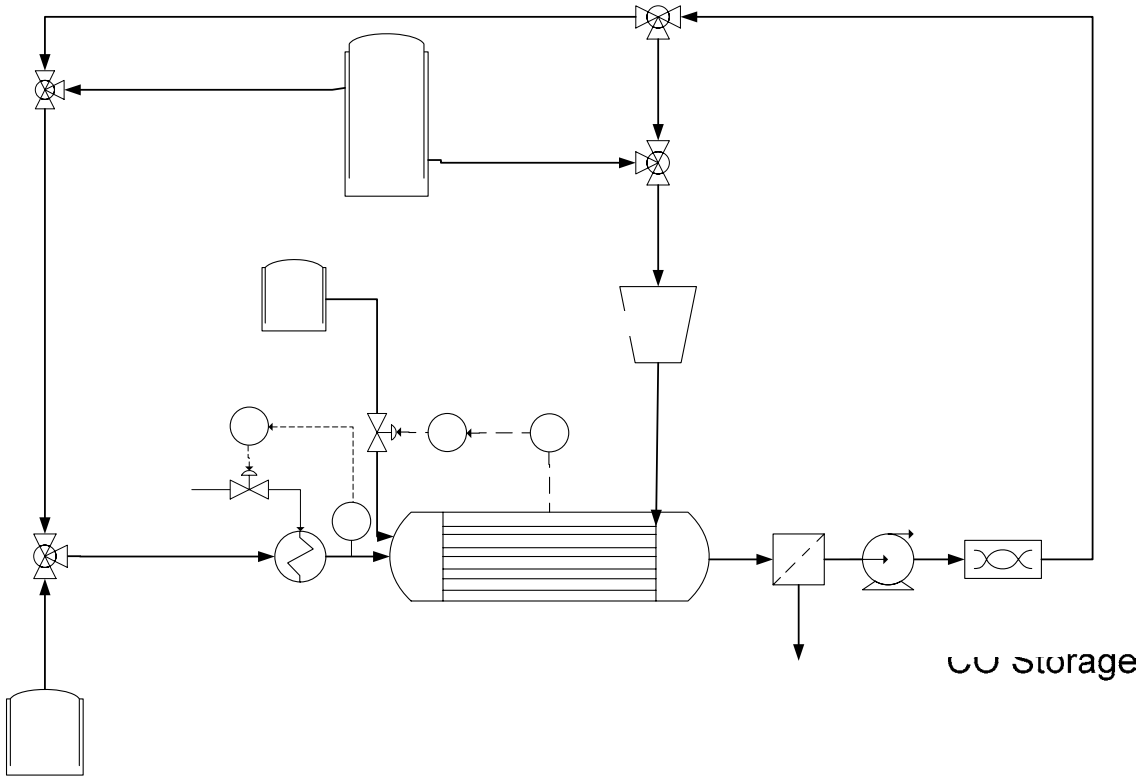


Figure 3.1: HiPCO Process flow diagram

purification process. The mixture of CO and CO_2 gas is flowed through a molecular sieve where the CO_2 is removed. A molecular sieve adsorbent bed is used for the purification of the CO. Molecular sieve zeolites (MSZ) are used as adsorbents because they form very strong bonds with water and CO_2. The molecular sieve is replaced weekly. The purified CO stream is recycled back to the reactor inlet stream by a compressor. The flow sheet of the process is shown in Figure 3.1.

3.1.2 Reactor

The reactor for the plant was scaled up from the pilot design. The pilot scale reactor is essentially one tube, in which the reaction occurs. Figure 3.3 shows a cutaway of the side of a pilot scale HiPCO reactor. The stream containing the mixture of carbon monoxide

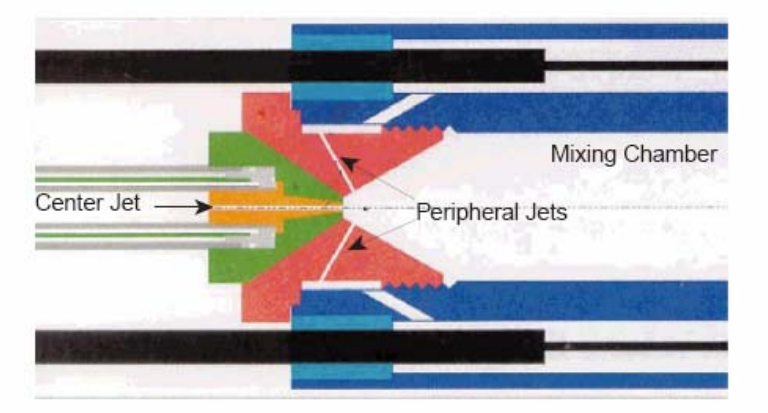


Figure 3.3[34]: Diagram of a pilot scale HiPCO reactor

and $Fe(CO)_5$ is injected at room temperature into the reaction tube through the center nozzle. A thick, larger tube surrounds the reaction tube. Pure, heated CO is injected into the opposite end of the reactor, and flows through six equidistantly spaced channels running the length of this outer tube. The CO enters the inner reaction chamber at an angle of 30°. The SWNTs are condensed by the cooling copper rod at the end of the reactor. The pilot scale reactor can produce up to 10.8 grams/day at the given operating conditions. The scaled-up reactor, shown in Figure 3.4 consists of a bundle of 100 tubes for a production rate of 1 kg/day. All materials are made of stainless steel type 304 due to the corrosive effects of CO and CO_2 at high temperatures and pressures. Heating the

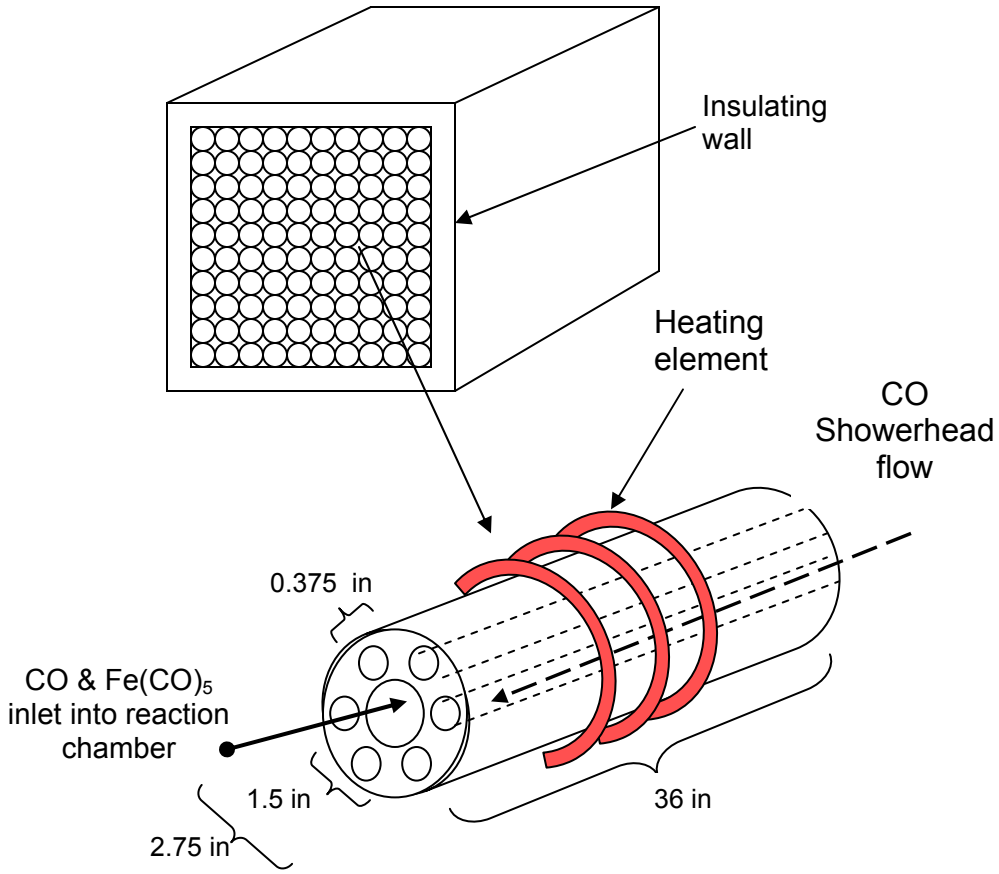


Figure 3.4: Diagram of Scaled HiPCO Reactor

reactor will be accomplished by heating elements surrounding each tube. This will ensure even heating throughout the reactor. The entire reactor will be surrounded by high-temperature insulation. The calculated heat transfer area for the reactor is 189 cm^2. This area was used in determining the utilities needed to run the reactor at the required operating conditions. Additional specifications on the reactor size can be found in Appendix B.

3.1.1 Nanotube Purification

The purification process is based on a process developed specifically for the HiPCO process.[35] A flow diagram of the process is shown in Figure 3.2. Upon leaving the reactor, the nanotubes are compressed onto filter paper of pore size 3 μm. Due to the extremely low density of the nanotubes, a vacuum is used to compress them onto the

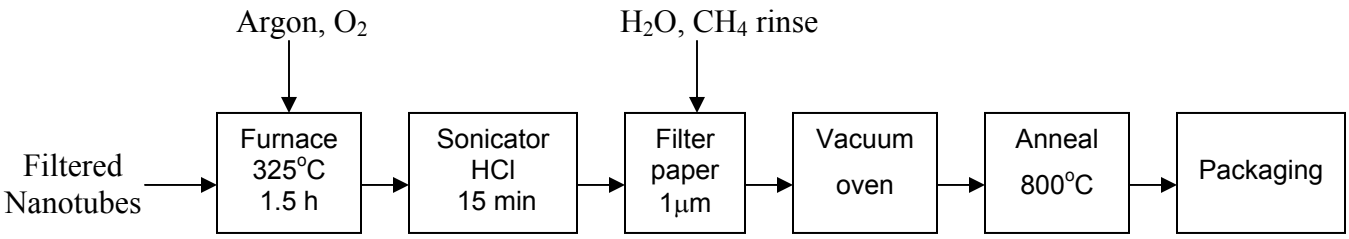


Figure 3.2: HiPCO Purification Flow Diagram

filter paper. This decreases the loss of the product to the air. The nanotubes are then heated in a furnace under a continuous flow of oxygen and argon gas at 325°C for approximately 1.5 hours. Heating oxidizes the iron and causes the carbon shells to break open, thereby exposing the metal. The exposed iron impurities are then removed by 15 minutes of sonication in concentrated HCl solution. The nanotubes are filtered out of solution onto a Teflon membrane of 1 μm pore size, rinsed with deionized water and methanol to absorb the impurities, and dried in a vacuum oven. The nanotubes will then be annealed in air at 800° C for one hour. Annealing produces more ordered ropes of nanotubes. The purification process has been shown to reduce metal impurities in the nanotubes product from 5% to 0.03% by weight.[36] After purification, the nanotubes are

compressed into pellets for easy packaging. Nanotubes are then weighed and placed into plastic containers for sale.

3.1.3 Equipment Cost

Total equipment cost was determined by the sum of the individual equipment costs. Table 3.1 lists the necessary equipment and prices for each.

Table 3.1: HiPCO Equipment Cost

Purchased Equipment	Cost
Reactor	$ 25,050
Compressor	$ 60,000
Molecular Sieve	$ 10,000
Nanotube filter	$ 1,300
Vacuum Oven	$ 2700
Furnace	$ 2000
Ultrasonic Processor	$ 7940
Vacuum pump	$ 500
Total purchased equipment	$ 109,490

3.2 CoMoCat Process Description

In this process the raw materials include commercial grade carbon monoxide (CO), cobalt and molybdenum (Co:Mo) as catalyst and silica (SiO_2) as support. The commercial grade CO is 99.5 % pure[37]. The inert gases used in process are hydrogen (H_2), helium (He) and oxygen/air mixture[38] (Air/O_2). The reaction conditions to which the catalytic particles are exposed are highly controlled at different stages. The ability to regulate temperature and reactive concentrations is important to obtain the high selectivity necessary to produce SWNT's. The yield of nanotubes is affected by the reaction temperature (700°C - 950°C)[39], reactor pressure (10 atm), space velocity for all

gas species (30,000particles/hr)[38] and reaction time (3 min-1 hr)[39] and by pretreatment conditions. The detailed description of how these parameters affect selectivity will be explained later. Additional details on the CoMoCat design can be found in Appendix C.

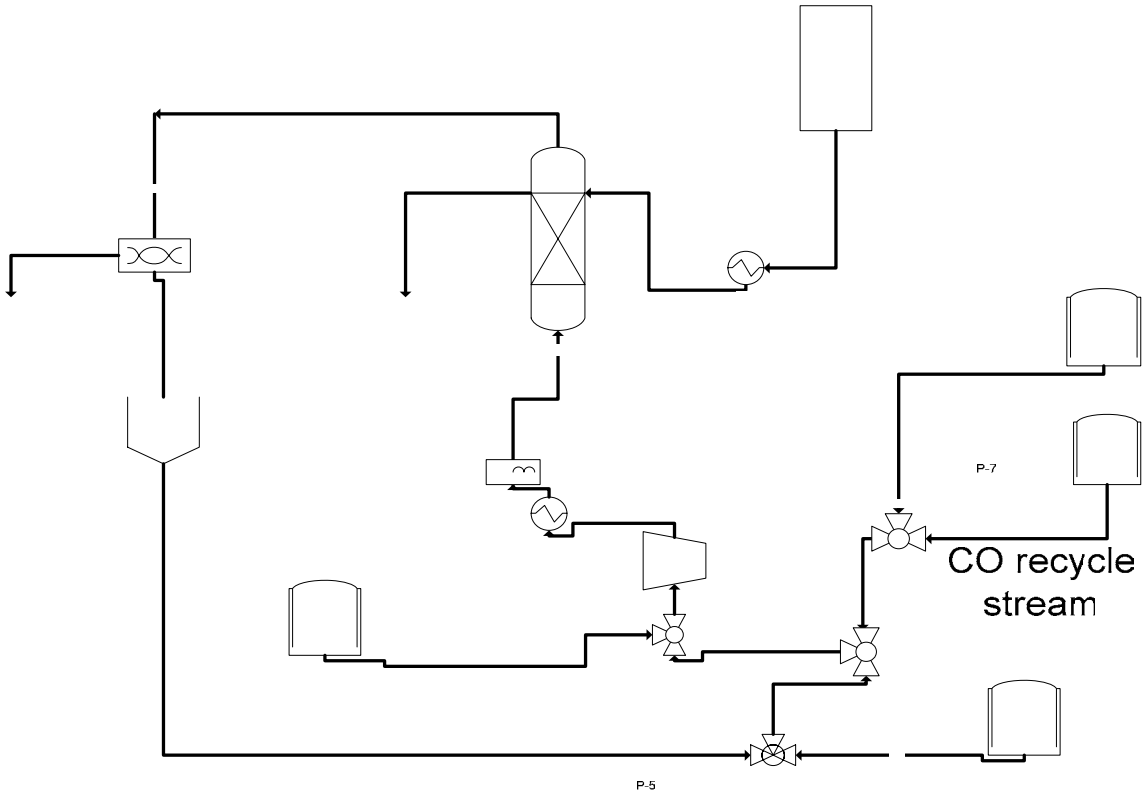


Figure 3.5: CoMoCat Process Flow Diagram

The flow sheet of the process is shown in Figure 3.5. Catalyst particles are first added to the reactor and treated with a heated helium gas, under high pressure. This preheats the catalytic particles to a high temperature and removes air from the catalytic particles. After that catalytic particles are exposed to a reducing gas, H_2, at approximately 500 °C, under high pressure. This prepares the catalyst particles by reducing them. The reducing gas is flushed from the catalytic particles by helium at 750 °C and high pressure to reheat the particles for the next step. The optimum temperature for reaction is 750 °C, because

the carbon deposit increase as temperature decrease but selectivity of carbon nanotubes decrease as temperature decrease. The total batch time is 3.25 hr. The following is the reaction step for one batch in which an effective amount of a carbon monoxide (CO) gas is heated to a reaction temperature approximately 750 °C under high pressure and exposed to the reduced catalytic particles. During this stage carbon nanotubes and amorphous carbon are formed on the catalytic particles. The reaction time can vary from 3 min to 1 hour. Reaction time refers to the time in which the reactor was held at 750 °C and the CO was in contact with the metallic catalytic particles. SWNT yield significantly increase during the first 10 minutes, and growth is less productive beyond that time. The optimum reaction time is 15 minutes. After reaction the reacted particles are exposed to heated (750 °C) post reaction gas He under high pressure. The function of this step is to flush out the remaining CO gas. Afterwards the flushed catalytic particles are cooled with a cooling gas He under high pressure at a lower temperature (300°C). After the reacted particles have been cooled, they are exposed to a stream of a heated oxidative gas O_2 under high pressure at 300 °C[39]. The amorphous carbon particles are burned away from the catalytic particles by heated O_2 leaving only carbon nanotubes in the catalytic particles. The oxidized catalytic particles are then removed from the reactor for purification process.

3.2.1 Nanotube purification

In this process raw materials include commercial grade sodium hydroxide NaOH, oxygen O_2 and hydrochloric acid HCl. The flow sheet of the purification process is shown in Figure 3.6. In this purification method support SiO_2 is dissolved by treatment with a base

(2 M NaOH)[40]. The solid form catalytic particles are further oxidized in air at 200-250°C[39]. Then catalytic particles (CNT's, CoMo, SiO_2 and O_2) are sonicated in acid solution HCl. In this step the metal catalyst particles are dissolved. The total removal of metal is about 95%-99%[40]. Finally the catalytic particles (CNT's, and SiO_2) are sonicated in 2 M NaOH for 5 hr at temperature from 22°C to 70°C. This step eliminates 99 % of the SiO_2[40]. After purification, the nanotubes are further

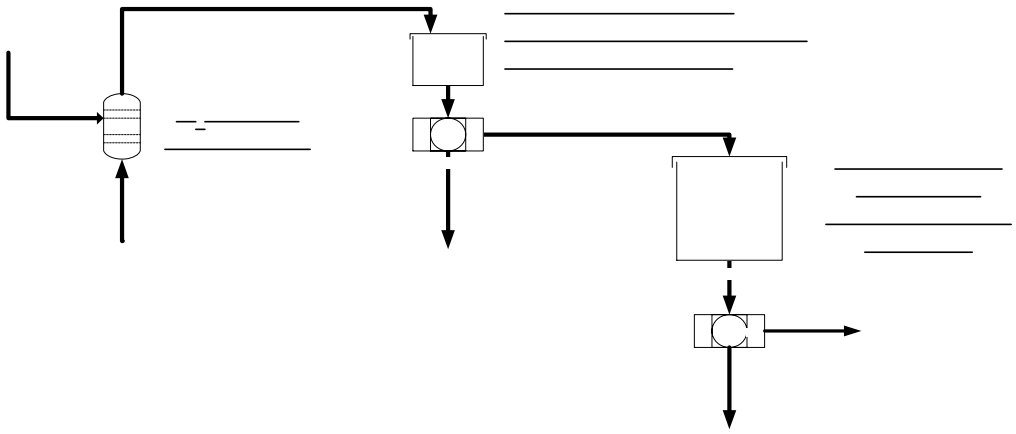


Figure 3.6: CoMoCat Purification Flow Diagram

treated in a handling process. The flowsheet of the handling process is shown in Figure 3.7 The handling process shown on the flow diagram below can produce freeze-dried webs and stable suspensions. The freeze-dried webs are produced by heating SWNT's to the triple point in the gel drying bed. The stable suspension is produced by mixing SWNT's with water (H_2O), surfactant (SDS) and sonicating.

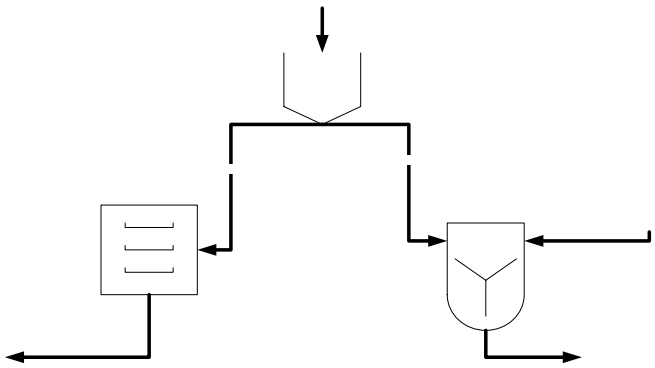


Figure 3.7: Handling Process Flow Diagram

Total equipment cost was calculated $ 144,900.0. Equipment individual prices can be seen in Table 3.2.

Table 3.2: CoMoCat Equipment Cost

Purchased Equipment	Cost
Heater gas	$11,000.00
Heater catalyst	$15,000.00
Filter	1,300.00
Sonicating Beds	11,500.00
Gel drying bed	10,000.00
Insulator wall	$5,000.00
Reactor	$30,800.00
Compressor	$50,300.00
SILIPORITE® Molecular Sieves (remove CO_2)	$10,000.00
Total Equipment cost	**$144,900.00**

3.3 Process Comparison

The HiPCO and CoMoCat production methods were compared in order to choose the design for this production facility. SWNT produced by both methods exhibit a few slight differences. Compared to HiPCO nanotubes, CoMoCat nanotubes are grouped in smaller rope bundles, have a narrower distribution of diameters, and have higher selectivity. In the long run these attributes may make CoMoCat nanotubes a better candidate for some

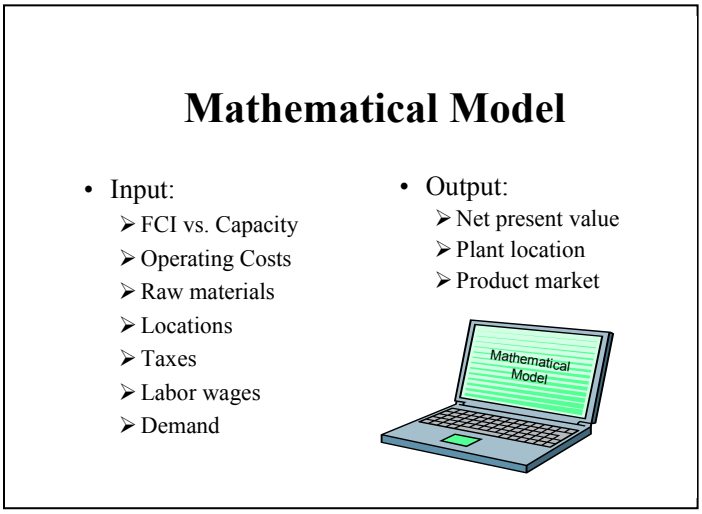
electronics applications. However, with the given market projections, this factor is not expected to have a considerable effect on the selling ability of the product. Therefore, the two processes were compared purely on a cost basis.

Table 3.3: Cost Comparison for HiPCO and CoMoCat

	HiPCO	**CoMoCat**
Annual Operating Cost ($/ year)	2,589,499	2,230,000
Annual Raw Material Cost ($/year)	596,000	2,020,000
Equipment Cost ($)	109,490	144,900

Table 3.3 shows the estimates of operating costs, raw materials costs, and equipment costs for both designs. The annual operating cost for the HiPCO process design is slightly higher than that for the CoMoCat design, but the raw materials cost for CoMoCat is considerably higher than HiPCO. The raw material cost for CoMoCat is lot higher due to high cost of the catalysts. Based on this, the HiPCO process proves to be a more cost effective design. It is therefore recommended that the single wall nanotubes production facility use the HiPCO process design.

4.0 MATHEMATICAL MODEL



Two mathematical models will be generated, the deterministic model and the stochastic model. The deterministic model is used to determine the profitability of the enterprise. This optimization program will supply initial business plan, will predict changes that will be made in the future and has to be adapted to fit changing input.

The second model is the stochastic model that will estimate the risk associated in investing in this business. This is performed based on the uncertainty in demands, product prices and raw material costs.

4.1 Model Input

To determine the net present worth, input that will affect this value will be analyzed. The parameters below will be considered as part of an optimization model.

- Equipment costs as a function of plant production
- Fixed Capital Investment (FCI)
- Operating Costs as a function of plant production
- Cost of raw materials
- States property taxes for plant locations
- Demand at different product markets over the next 10 years

- Forecasted product prices over the next ten years.
- Salvage value and working capital as a percentage of FCI
- Depreciation and lifetime of project

4.1.1 FCI versus capacity and operating costs versus production

All of the equipment costs were totaled for several different capacities. Then, we determined the total direct costs, total indirect costs and working capital costs based on a excel calculations. This can be accomplished, because calculations were based on equipment cost. Figure 4.1 relates the fixed capital investment to various capacities of the plant.

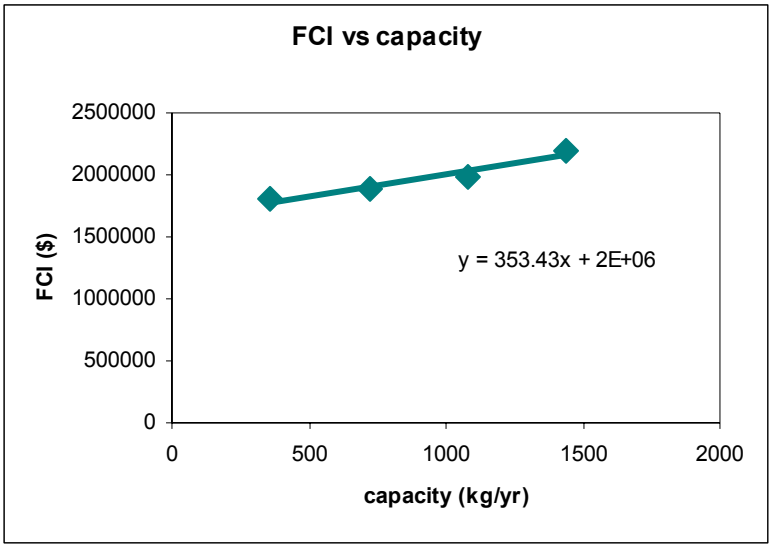


Figure 4.1: Fixed capital investment versus SWNT capacity

Operating costs based on production rate is calculated by summing the separate costs associated with the process.

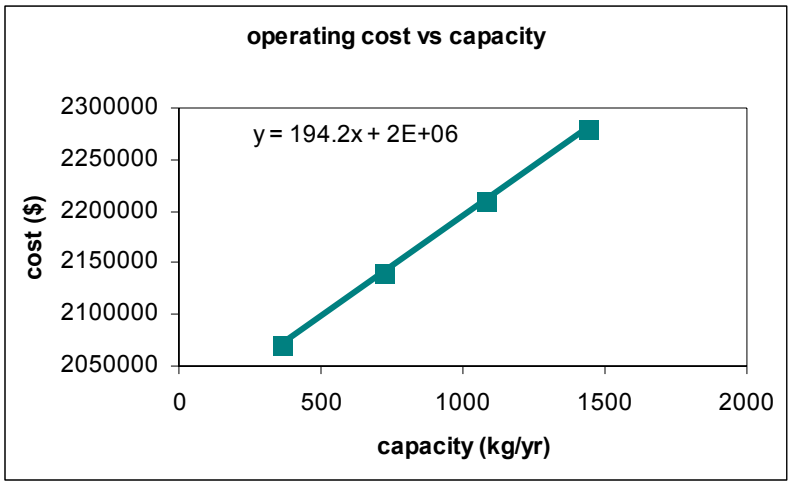


Figure 4.2: Operating costs versus SWNT capacity

4.1.2 Raw Materials

The selection for the best raw material relates the purity, quantity of the raw material being available and the local taxes associated with the raw materials. The raw materials used for HiPCO design are carbon monoxide (CO), iron pentacarbonyl, ($Fe(CO)_5$) and Argon (Ar). The materials used for purification process includes sodium hydroxide (NaOH) and hydrochloric acid (HCl). The raw materials are available at different purities and quantities from a number of chemical supply companies. The plant location will affect the sales tax on raw materials. However, this will not have a significant effect on the total product cost. The figures below give the cost of raw materials versus the capacity of the plant.

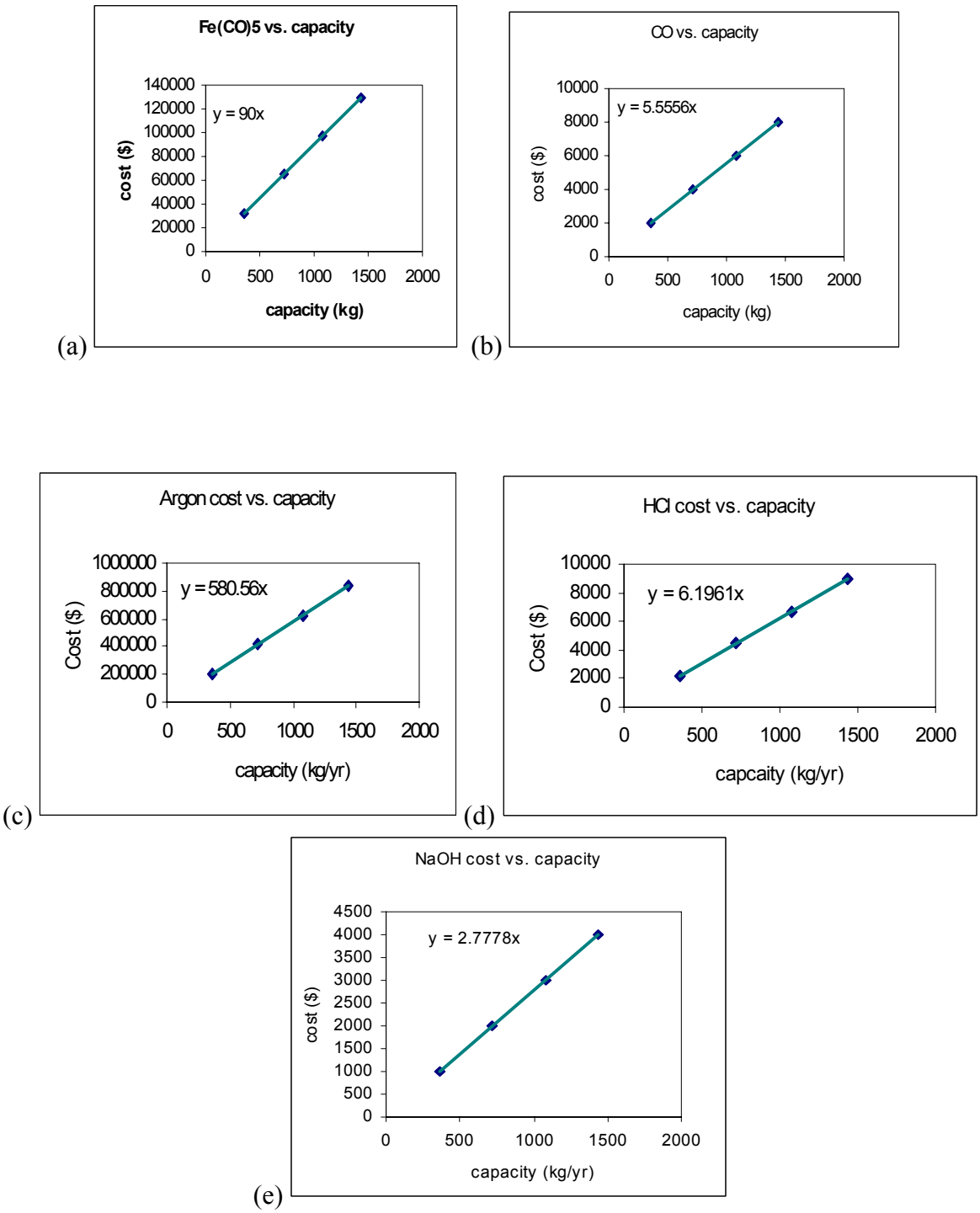


Figure 4.3: Costs of raw materials versus the capacity of the plant.

For the calculations, refer to APPENDIX D.

4.1.3 Locations

The location of the plant is an important choice in the plant design, but should not have enough of a significant cost effect to make it a consideration in the mathematical model. Variables with location include taxes associated with land and plant holdings, cost of living, relative labor rate index and utility prices. The information regarding labor cost employment was provided by the National Commission on Entrepreneurship (NCOE). Bankrate provided information related to land and plant holdings for prospective locations.

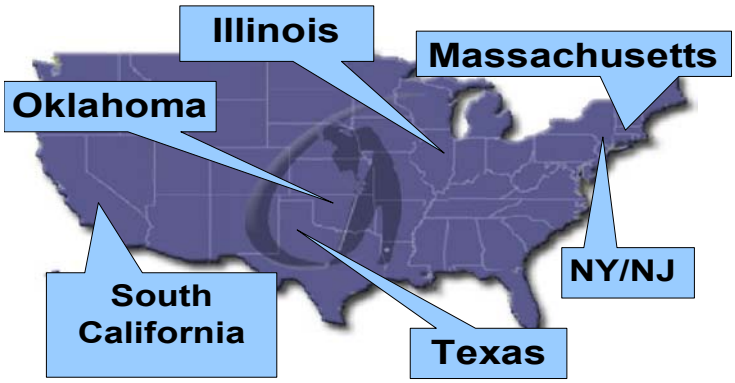


Figure 4.4: Areas of high-growth companies.

The potential wholesale markets vary according to location and possible SWNT demand. These locations were determined by locating companies or research centers that would purchase SWNT's, for their products or research. In particular, companies specializing in electronics, chemistry, pharmaceuticals, chemical plants, aerospace materials, and nanotechnology tools will consider purchasing nanotubes. Being close to these research locations and companies would be beneficial to public relations, but not to cost. This would facilitate dealings with patrons and keep our staff apprised of new SWNT

developments and applications. However, this would not have a significant effect on the cost of building or operating our plant. The plant distance from customers would also not be a concern in regards to transportation costs. Six areas within the United States will be considered for the final plant location.

Table 4.1: Strengths and weakness associated with each plant location

Location	Strength	Weakness
Illinois	-2 of 6 NSF Nano research centers at Northwestern and UIUC (including RPI's center, due to NSEC grant partnership) -Strong nano research base -Significant additional talent and infrastructure nearly at Purdue, Notre Dame, and Wisconsin	Investment capital believed to be more conservative than elsewhere
Massachusetts	- 1 of 6 NSF nano research centers at Harvard - Track record of establishing new industries - Abundant entrepreneurship	- State has little money to fund initiatives - High cost of living
NY/NJ	- 3 of 6 NSF Nano research centers at Columbia, RPI and Cornell - Great access to NYC-based venture capital - NJ very supportive of industry-academic partnerships. Lucent recently donated its facility to serve as a NJ Nanotech Park - Over $ 150M in state and IBM support for Center for Excellence in Nano (NY University at Albany)	- No coordinated effort yet - High cost of living

Texas	- 1 of 6 NSF Nano research centers at Rice - Experience in attracting tech companies - Texas Nanotechnology initiative fostering collaboration between industry, academia, government	- Austin- Huston – Dallas cluster is geographically dispersed - No concrete state funding or initiative yet
South California	- $ 100 M in state funding pledged over 4 years - VC firms view funding of So. Cal start- ups favorably - Cal. NanoSystems Institute fostering academic-industry collaboration	- Competitive entrepreneurial environment can make funding difficult - High cost of living
Oklahoma	-University of Oklahoma research -SouthWest NanoTechnology Inc. one of the most attractive companies -CoMoCAT technology	-Taxes

Another consideration for plant location involves local and state taxes. Table 4.2 provides taxes associated with each prospective plant location. For our model, an average tax rate and utility price from these six locations was assumed.

Table 4.2: Taxes associated with each prospective plant location

State	State Income Tax	State Sales Tax	Property Tax
California	1% - 9.3%	6%	30
Texas	0%	6.25%	25
NY/NJ	1.4% - 6.37%	6%	34
Massachusetts	5.30%	5%	30
Illinois	3%	6.25%	33.33
Oklahoma	0.5% - 7%	4.50%	15

4.1.4 Additional Input Specifications

The mathematical model will be designed by assuming it is straight- line depreciation over 10 years for fixed capital investment. The project will be given a lifespan of ten years beginning in 2006. Salvage value was set at 10 % of FCI. Average raw material costs, taxes, utilities, and property taxes will be included in the model to give the most accurate estimate.

4.2 Model Equations and Constraints

4.2.1 Equations

This section includes the equations that will be included in mathematical model to determine the best location and maximum NPW for SWNT production plan. The following are the equations used in mathematical model.

Estimation of Capital Investment

Fixed capital investment will be estimated by the percentage of delivered-equipment cost for solid-fluid processing plant (APPENDIX D). The other items included in the total direct plant cost are then estimated based on percentage of delivered-equipment cost. The additional components of the capital investment are based on average percentages of the total direct plant cost, total direct and indirect plant costs, or total capital investment. This is summarized in the following cost equation:

$$C_n = \sum (E + f_1 E + f_2 E + f_3 E + ... + f_n E) = E \sum (1 + f_2 + f_3 + ... + f_n) \quad (4.1)$$

$$FCI_i = A * bi_i + B * bc_i + C * Capacity_i \quad (4.2)$$

where: FCI = fixed capital investment

A = fixed cost for piping, pumps, compressors, molecular sieves

B = cost to expand capacity for number of tubes in the reactor

C = Linear cost for size reactor sized for maximum production

bi_i = binary variable, will be mentioned later

bc_i = binary variable, will be mentioned later

FCI is assumed to be 85% of total capital investment, and working capital is assumed to be 15% of total capital investment. Therefore, the equation for TCI is given as the following:

$$TCI = FCI + Iw$$
$$TCI = FCI / 0.85 \quad (4.3)$$

Estimation of Revenue

Revenue comes from sale of the product or products produced by plant. The total annual revenue from product sales is the sum of the unit price of each product multiplied by its rate of sales:

Revenue

$$\text{Re}venue_{i,tp}(\$/yr) = \sum (sales\_of\_product, kg/yr)(product\_sales\_price, \$/kg) \quad (4.4)$$

Estimation of total product cost

The total product cost includes the total of all costs of operating the plant, selling the products, recovering the capital investment, and contributing to corporate functions such as management and research and development. The total product cost is divided into two categories: operating cost/manufacturing cost and general expense. Total product costs are calculated based on annual basis. Factors that need to be included in order to estimate the total product cost are listed as the following:

- Manufacturing costs
- Variable production costs
    - Raw material costs: costs of carbon monoxide and argon gas
    - Operating labor
    - Operating supervision and clerical assistance
    - Utilities: electricity, process cooling water, natural gas, and waste disposal
    - Maintenance and repairs: annual costs of these are assumed to be 10% of total equipment cost
    - Operating supplies
    - Patents and Royalties: is paid to the inventor, and is assumed to be 10% of total product sale.
    - Catalyst(s): Iron pentacarbonyl ($Fe(CO)_5$)

- Fixed charges
- Depreciation: straight line depreciation
- Financing: Since the required funds need to be borrowed from the external source(s), the interest in this case is considered as a cost. The annual interest rate is assumed to be 10% of the total value of the borrowed capital.
- Local taxes
- Property Insurance

- Plant overhead costs: is assumed to be 60% of the total expense for operating labor, supervision, and maintenance.

- General expenses

  - Administrative costs: these expenses are related to executive and administrative activities. These expenses can be different at various locations. For a preliminary estimate, it is assumed to be 20% of operating labor.
  - Distribution and marketing costs: The plant produces single walled carbon nanotube, which is a new product, and the amount to be sold will be in small quantities. Therefore, it is reasonable to assume that these costs are 10% of total product cost.
  - Research and development costs: New methods and products are constantly being developed in nanotechnology field. To remain in a competitive industrial position requires research and development costs. This is assumed to be 10% of total product cost.

In short, the total product cost is illustrated in the following equation. The result can be seen in APPENDIX D.

$$Total\,\mathrm{Pr}oductCost = ManufacturingCosts + Variable\,\mathrm{Pr}oductionCosts + \\ + PlantOverheadCosts + GenerealExpenese \tag{4.5}$$

Estimation of annual cash flow

$$CF_{i,tp} = \mathrm{Re}venue_{i,tp} - (\mathrm{Re}venue_{i,tp} - Dep \times FCI_i) \times propertytax \tag{4.6}$$

Estimation of net present worth

The probability measures include time value of money, with continuous cash flow and discounting. The economic evaluation is based on

Net present worth factor:

$$PWF_{cf,j} = \left(\frac{e^{r} - 1}{r} \right) \cdot e^{-rj} \tag{4.7}$$

where P^*_j: net present worth factor,

r = r_{ma} = minimum acceptable rate of return = continuous-compounding discount rate, fraction/y

Present worth of annual cash flow:

$$P_j = CF_j \times P_j^* \tag{4.8}$$

where CF_j: cash flow at year j

Net present worth:

$$NPW = \sum_{j=1}^{N} PWF_{cf,j}[(s_j - c_{oj} - d_j)(1-\phi) + rec_j + d_j] - \sum_{j=-b}^{N} PWF_{v,j} F_j \tag{4.9}$$

where NPW: net present worth; $PWF_{cf,j}$: present worth factor; $PWF_{v,j}$: appropriate present worth factor for investments occurring in year j, F_j: total investment in year j; the other parameters are as defined before.

For net present worth positive, the discounted cash flow rate of return, or DCFR, is the return obtained from the investment in which all investments and cash flow are discounted, which is the case in our model. It is determined by setting the NPW equal to zero and solving for the discount rate that satisfies the resulting relation. This is performed by using the solver in Excel.

$$0 = \sum_{j=1}^{N} PWF_{cf,j}[(s_j - c_{oj} - d_j)(1-\phi) + rec_j + d_j] - \sum_{j=-b}^{N} PWF_{v,j} F_j \tag{4.10}$$

4.2.2 Constraints

The purpose of constraints is to make the model realistic. It limits the supply by the demand. The first year production was set at zero for construction.

$$Plants = \sum_i bi_i \tag{4.11}$$

where: bi_i = binary variable. It equals to 1 if the plant is constructed, else 0

$$Capacity_i \times bi_i \geq \sum_j x_{i,j,tp} \tag{4.12}$$

where: $Capacity_i$ is the capacity for the plant; x is the amount sold to the market

$$Demand_i \times (P) \geq \sum_j x_{i,j,tp} \tag{4.13}$$

where: Demand is total market demands in the US and Canada; P is the percentage of the market targeted

$$MaxCap_i \geq \sum_j x_{i,j,tp} \tag{4.13}$$

where: MaxCap is the maximum capacity of plant

$$x_{i,j,tp=1} = 0 \tag{4.14}$$

no production at year 1 due to construction.

4.3 Model Output

4.3.1 Deterministic model results

The deterministic model is used to determine the number of plants should be built, the plant's location, capacity, and year of expansion. From GAMS, the location of the plant should be in Oklahoma. The net present value over ten years of project lifespan is eighteen million dollars.

The figure below shows the maximum capacity and the production rate of the plant. The rate of return on investment is 46%. The maximum capacity of the plant is 400kg. However, based on the demand from the targeted market, the capacity of the plant should not exceed 241kg.

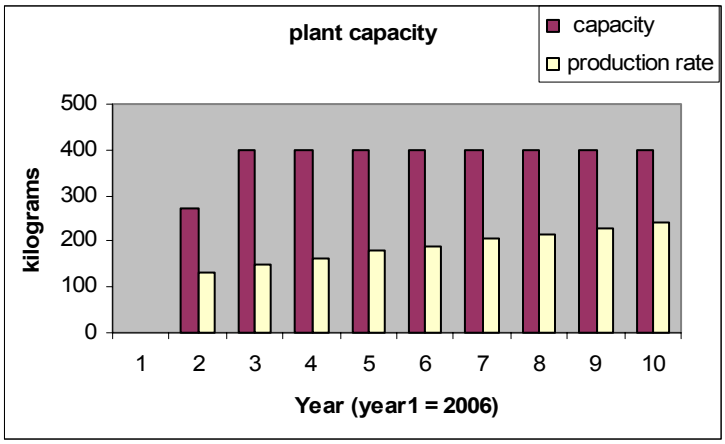


Figure 4.5: Production rate of the plant

The deterministic model also estimates the revenues, operating costs, the capital investment, and other costs. These are summarized in the figure below.

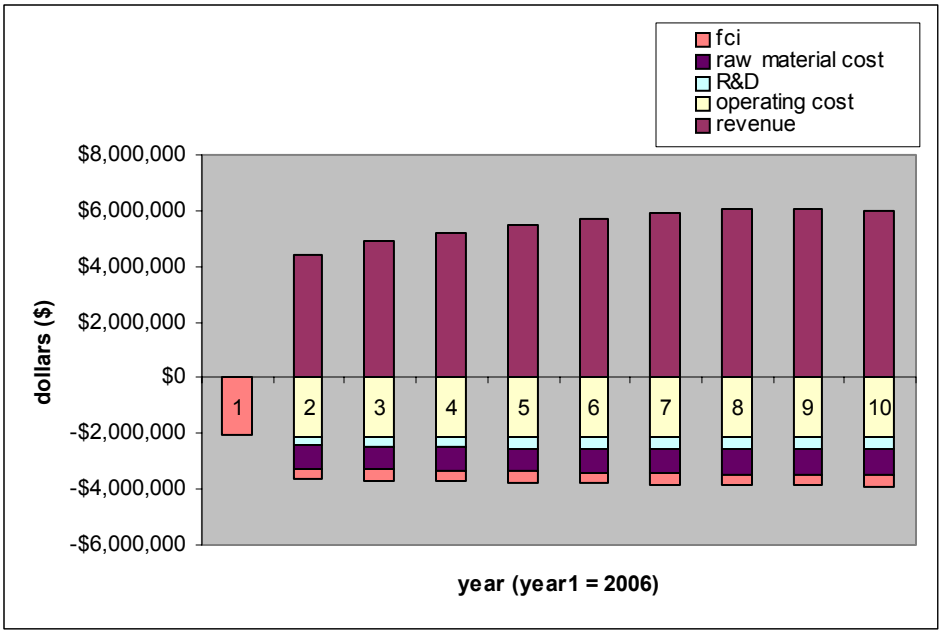


Figure 4.6: Estimation of expenses and revenues

The figure below gives the projected annual cash flows, assuming that we succeed in targeting 10% of the market.

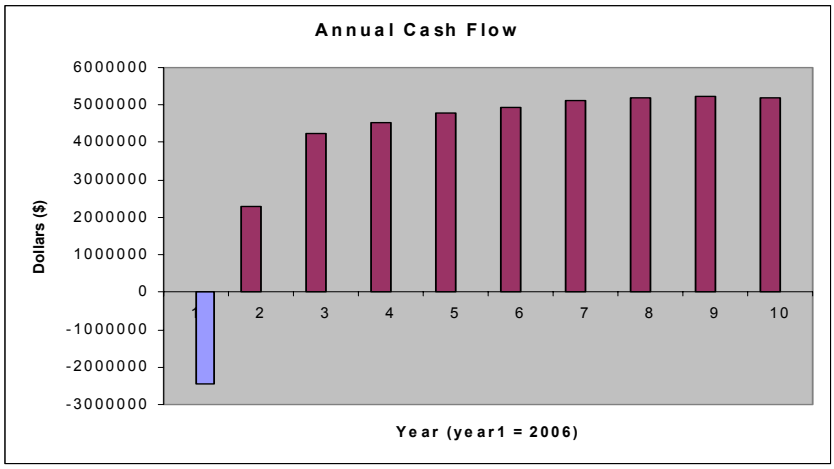


Figure 4.7: Estimation of annual cash flow

4.3.2 Sensitivity Analysis

Next, the mathematical model is used to perform the sensitivity analysis based on the uncertainty in product prices, catalyst costs and demands. The plant location is fixed at Oklahoma. Only one uncertainty in one parameter is changed each time while keeping the remaining parameters fixed. The results from the sensitivity analysis are summarized in the table below:

Table 4.3: Sensitivity results

	Uncertainty	NPW	Max plant capacity (kg/yr)
Demand	44%	$717,829.00	29
selling price	45%	$322,287.00	241
catalyst price	50%	$1,651,600.00	241
CO			
Argon			
HCl			
NaOH			

4.3.3 Risk analysis

The figure below shows the result obtained from the stochastic model. The stochastic model estimates the risk associated with the business. In the stochastic model, all the parameters mentioned above, which are prices, demands, and raw material costs were varied with 40% of standard deviation. The location was fixed in Oklahoma. The risk curve shows that this is a highly profitable process with low risk.

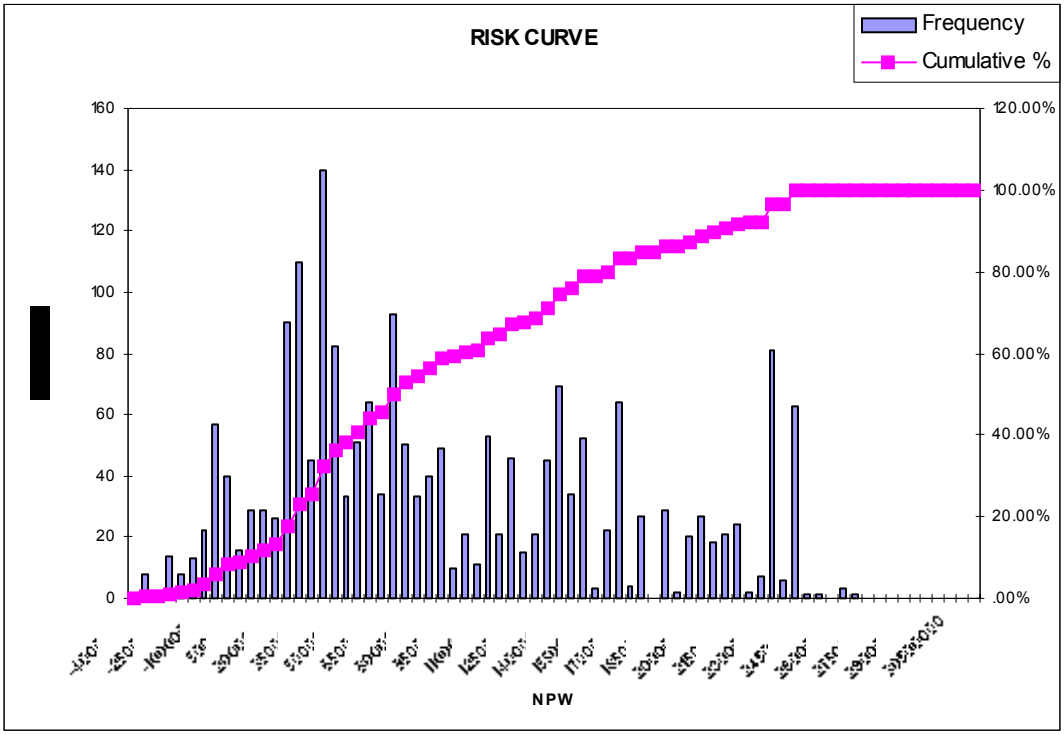
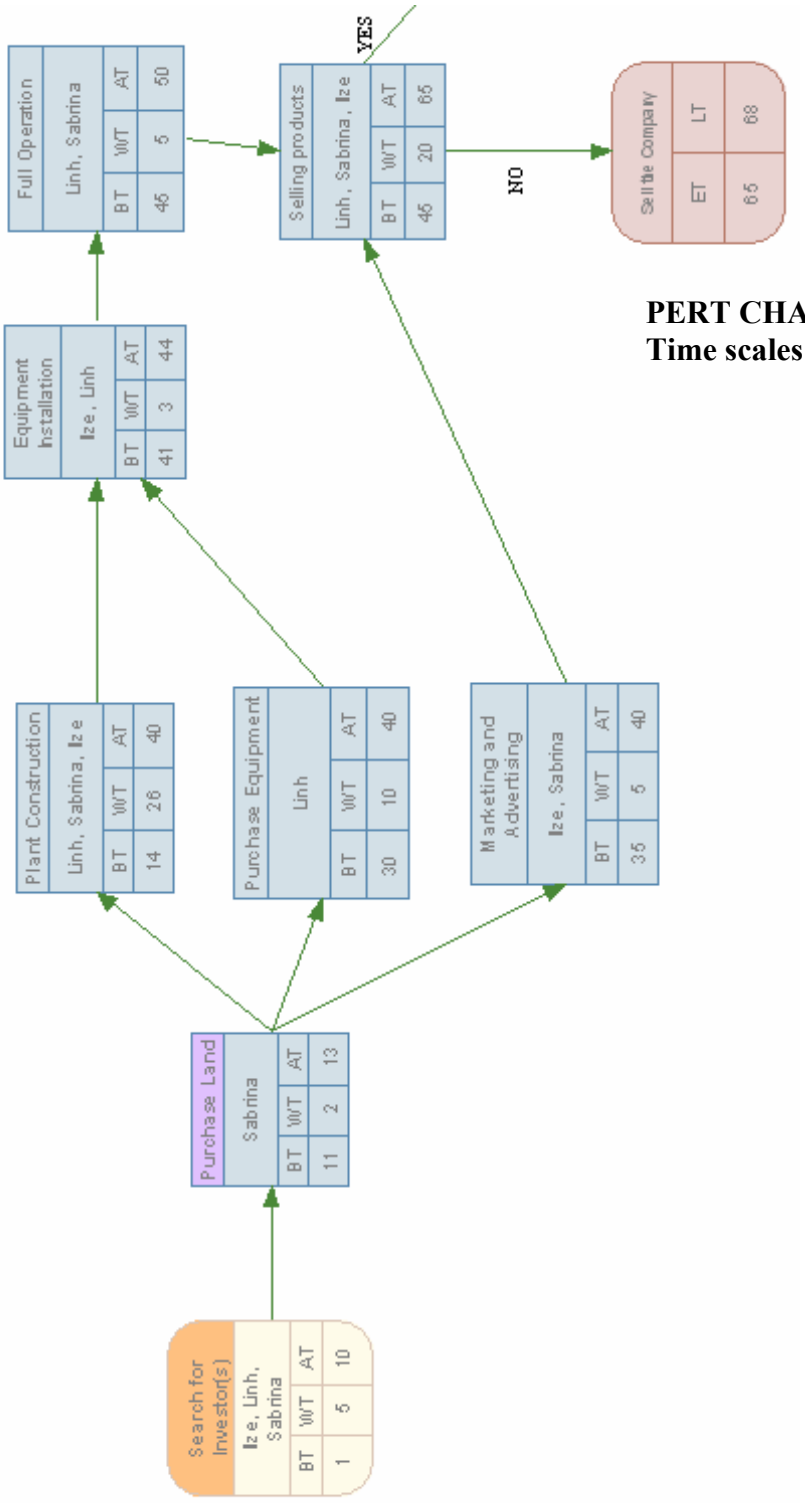
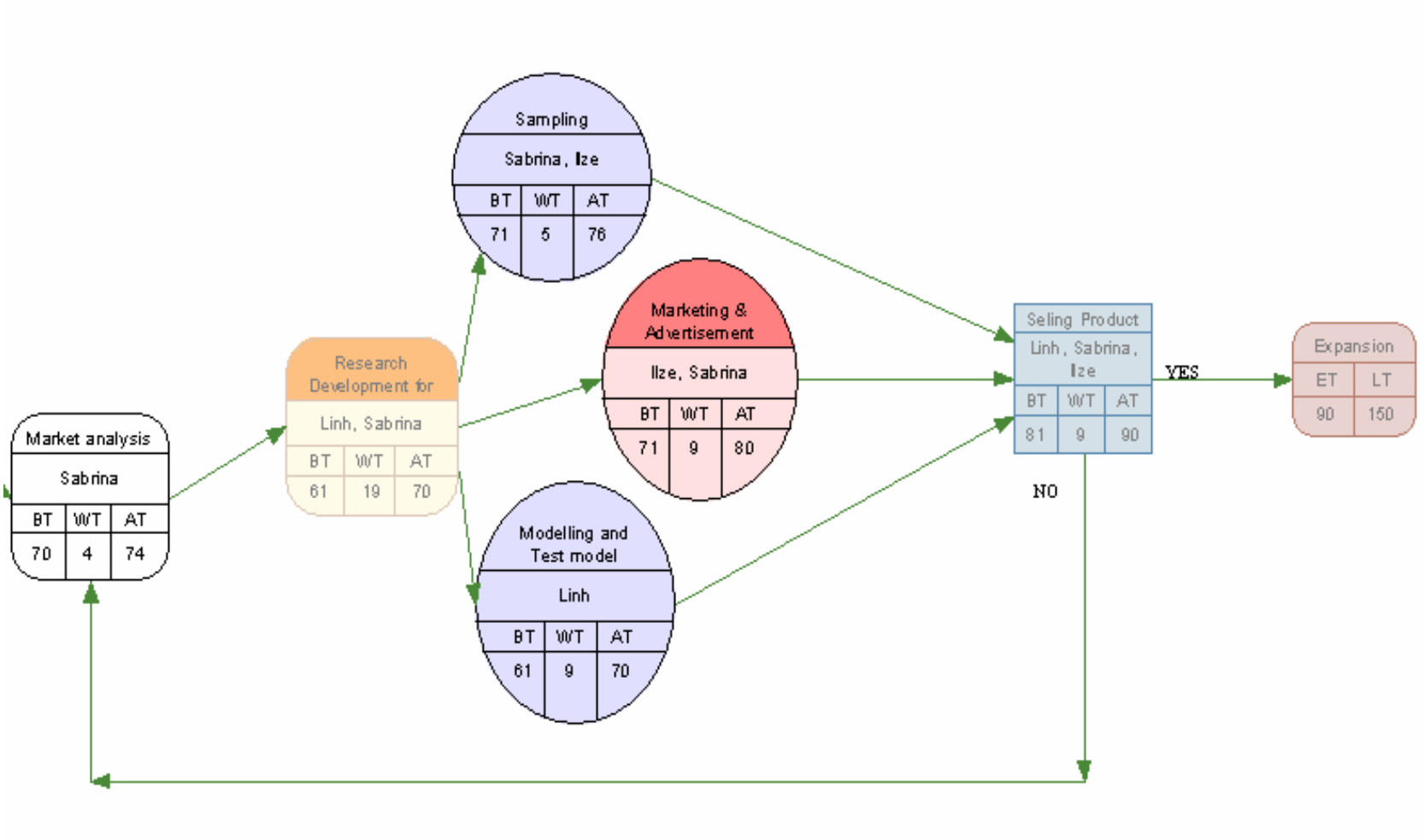


Figure 4.8: Risk Curve

5.0 BUSINESS PLAN



PERT CHART:
Time scales are in weeks


Market analysis
Sabrina
BT WT AT
70 4 74
Research Development for
Linh, Sabrina
BT WT AT
61 19 70
Sampling
Sabrina, Ilze
BT WT AT
71 5 76
Marketing & Advertisement
Ilze, Sabrina
BT WT AT
71 9 80
Modelling and Test model
Linh
BT WT AT
61 9 70
Seling Product
Linh, Sabrina, Ilze
BT WT AT
81 9 90
YES
NO
Expansion
ET LT
90 150

5.1.0 THE COMPANY

OUNano, Inc. was formed in January, 2004 with a plan to develop, manufacture and market single-walled carbon nanotubes. The company is a young enterprise, currently in the beginning stages of development. Preliminary analysis projects the company to be highly profitable and to meet the demands of an ever-increasing market. The organization will be composed of highly qualified personnel at all levels. Employees will possess a strong commitment to the field of nanotechnology and the researchers who continue to expand it. The company is confident in its ability to produce high quality single wall carbon nanotubes, and to establish itself as a leader in the nanotubes sector.

5.1.1 Objectives

Long-term objectives for our company are to establish a strong client base and to become a recognized leader in the manufacture of carbon nanotubes. Short-term goals include securing funding for the construction of our facility, and completing a preliminary marketing and advertising campaign

5.1.2 History

The company is the idea of three chemical engineering graduates from the University of Oklahoma. The company is currently seeking an investor to back the enterprise. The high demand for single-wall carbon nanotubes is the basis for the plant. Utilizing a gas phase process similar to the HiPCO process developed by Richard Smalley at Rice University, the facility will be able to produce nanotubes on a large scale. The enterprise is expected to be highly profitable, capturing a considerable share of the market.

5.1.3 Organization

The proposed manufacturing facility will employ approximately twenty people, including equipment technicians, operators, supervisors, management, marketing, and customer service representatives. When funding is secured and construction on the new facility is underway, the hiring process for a majority of these positions will begin. Employees will receive two weeks of vacation each year, as well as ten holidays. In addition, all employees will be provided with medical and dental insurance and a retirement plan with stock options. Because of our small size, the company will be able to be highly selective in our choice of personnel. This will allow the company to maintain a high standard of competence. The organization chart below summarizes the key personnel of the company:

Key Personnel

Dr. Miguel Bagajewicz, a professor at the University of Oklahoma, has two positions as Samuel Roberts Noble Foundation Presidential Professor and as Director of the Center for Engineering Optimization. He will be the president of the company. His extensive experience in design, operation, and optimization of process plants make him an excellent choice for the company president.

Sabrina Pepper is a recent graduate of the University of Oklahoma. She possesses a bachelor's degree in chemical engineering. Her past work experience includes working at the Oklahoma Medical Research Foundation in the crystallography department, where she conducted research on the crystallization of antibodies. As one of the founders of the company, Ms. Pepper will act as the chief executive officer for the company.

Linh Do also received a bachelor's degree in chemical engineering from the University of Oklahoma. Ms. Do is a member of the Applied Surfactant Research Center. She has three years of experience in the surfactant field. Ms. Do will hold the position of Chief Development Engineer, and will be responsible for improvements and alterations to the synthesis process used in the facility.

Ilze Veideman, also a chemical, engineering graduate from the University of Oklahoma, is the third founder of the company. She has done undergraduate research on the electrical properties of carbon nanotubes. Ms. Veideman will serve as Vice President of Marketing.

PERSONNEL COUNT

Engineering/Development	
Management	2
Non-management	4
Production/Service Delivery	
Management	2
Non-management	4
Marketing	
Management	1
Non-management	2
Sales/ Customer Support	
Management	1
Non-management	3
General & Administrative	
Management	1
Non-management	2
Total Personnel	**22**

5.1.4 Operations

At the present time, our company is seeking to secure funding for a new facility. Construction and engineering for the new building will be sub-contracted. Preliminary cost estimates for the plant have been performed, and will be presented in the finance section.

Once completed, the facility will produce purified single-walled carbon nanotube through a gas phase process. The process is a commercial-scale version of the patented HiPCO process. Licensing and royalties will be paid to Richard Smalley for the use of the technology. While the prototype has yet to be built, the design and specifications of the product are substantially complete.

5.1.5 Future

The future of the company largely depends on the state of the market and the development of new nanotube-related technologies. As more large-scale production methods are developed for carbon nanotubes, our facility may consider adjusting its production rate and pricing. In addition, as new applications for nanotubes become commercially promising, the increased demand for nanotubes may prompt the expansion of our plant.

5.2.0 THE MARKET

Most of the applications for single wall nanotubes are currently in development. At present, 90% of the potential market lies in academic and industrial research laboratories. Our plant will produce un-functionalized single wall nanotubes, which we will sell to clients that wish to use the product as is or to perform their own chemical processing.

5.2.1 Objectives

The current prospective for our product are mainly research and development laboratories in the academic and industrial sectors. Their objectives are mainly to improve the viability of various applications of carbon nanotubes and to discover new applications. Prospective buyers for our product will want unprocessed carbon nanotubes that they can modify in their own laboratories. Prospects will want to purchase our product because of our ability to sell in large quantities. As new applications become ready for commercial implementation, the market for our product will expand significantly.

5.2.2 Segmentation

We expect the market for nanotubes to be quite diverse, as it is beneficial to a wide number of applications. Most of the smaller segments of the market are not yet fully developed. We plan to focus on more specific market segments for the first one to two years while applications in other segments develop. Due to the unprocessed nature of our product, the majority of our prospects will be academic and industrial research laboratories.

5.2.3 Size

Nanotubes are the fastest growing sector of the nanotechnology market, with a projected average annual growth rate of 173% over the next five years.[41] Market research estimates indicate that the global production of nanotubes in 2003 was between 4 to 10 kg. Prices of high quality nanotubes range from $200 to $1000 per gram. By one estimate, the carbon nanotube market was valued at approximately $12 million in 2002.

5.2.4 Environment

The trend towards increased government spending on nanotechnology research and development should speed up the development of commercial applications. As the number of applications increases, the demand for nanotubes will also increase in those segments

5.3.0 THE OFFERINGS

The pricing for our products will initially be about $500/gram. This price is the average price of our competitors. Our product will have a medium to high level of purity, allowing it to compete easily with that of our competitors. The large demand for nanotubes should provide easy entry into the market and allow us to secure a stronghold in the market.

5.3.1 Description

Our company plans to offer single wall carbon nanotubes produced from a commercial scale gas phase synthesis process. The technology will be licensed from Richard Smalley of Rice University, who developed the HiPCO process that our synthesis is based upon. In this process, a mixture of carbon monoxide gas and iron pentacarbonyl will be injected into the reactor along with a stream of pure carbon monoxide. The reactor will be kept at high temperature and pressure, around 1050^{o} C and 30 atm. A detailed description of the process and reaction can be found in the technical document that accompanies this business plan.

5.3.2 Status

The production facility is in the planning stage of development. Preliminary design and planning has been completed for the process. Necessary funding for the venture is expected to be secured by the beginning of next year. Construction of the facility will begin soon after, and should last around six months. This does not include the installation of the equipment, piping, and instrumentation, which will take additional time. The projected date for beginning production is set for June of 2006.

5.3.3 Value

The single wall nanotubes produced in our facility will appeal mainly to industrial and academic laboratory researchers. Since the nanotubes will be sold in an essentially unprocessed form, customers will be able to perform their own processing methods to mold the nanotubes to their own specifications. Since the cost to produce the nanotubes is considerably less than the current market price, the venture should be highly profitable.

5.3.4 Cost to Produce

Component	Basis for Estimate	Cost ($/yr)
I. Manufacturing cost		
A. Direct production costs		
1. Raw materials		
$Fe(CO)_5$		$ 209
CO	Commercial Grade	$ 177
Argon	liquid (230 psi)	$ 393,300
Filter Paper	Millipore (Grade 102) 3μm pore	$ 500
Filter Paper	Cole-Parmer 1μm pore	$ 1,500
	Subtotal:	***$ 395,686***
2. Operating labor		$ 2,000,000
3. Direct supervisory and clerical	15% of operating labor	$ 300,000
4. Utilities		$ 2,589,499
5. Maintenance and repair	6% of FCI	108256.5609
6. Operating supplies	15% of maintenance and repair	$ 5,611
7. Laboratory charges	15% of operating labor	$ 52,560
8. Patents and royalties	15% of total product cost	$ 860,758
	Variable cost	***$ 5,916,685***
B. Fixed charges		
1. Capital costs		
Property taxes	2% of FCI	$ 36,086
Insurance	1% of FCI	$ 18,043
sub-total		***$ 54,128***
C. Overhead costs	60% of labor & supervision	***$ 1,380,000***
II. General expenses		
A. Administration costs	20% of labor & supervision	$ 88,074
B. Distribution and selling costs	5% of total product cost	$ 286,919
C. Research and development	10% of total product cost	$ 573,839
sub-total		***$ 948,832***
Total annual product cost		$ 8,695,331
	Unit cost ($/gram)	**$ 23.82**

5.3.5 Support

Customer support is not expected to be a significant requirement for our product. All customer relations issues will be directed to the sales staff. Sales representatives will be highly knowledgeable in regards to the product properties and synthesis process, and will therefore be able to answer questions or troubleshoot problems that customers may have.

5.4.0 MARKETING STRATEGY

The goal of our company is to secure a strong share of the nanotubes market. The intent is to use a moderately aggressive market penetration pricing strategy combined with a pull promotion strategy. We will price our product slightly below the average of competitive nanotube prices during the first several years to achieve a significant market portion.

5.4.1 Targets

The main targets for our product will initially be academic and industrial research labs. Due to the increase in government funding for nanotechnology research and development, researchers will have the ability to purchase more nanotubes for experiments. Our product will also be marketed to composites manufacturers that can utilize the unprocessed form of single wall nanotubes. As more applications emerge, the market for our product will expand.

5.4.2 Corporate Image

The objective of our company is to establish a reputation as a leader in the nanotubes industry. In order to achieve this image, we will maintain a commitment to high quality products and service.

5.4.3 Promotion

A "PULL" strategy will be employed to promote our product. A major commitment will be made to advertising our product in the chosen sectors. Publicity from selected nanotechnology business conferences and media events will accompany the advertising campaign.

Product Image

We want our products to be perceived at two levels: by researchers and by industrial companies that will use our components. We want companies to base their perception on the relationship we will establish with them through our sales and delivery organizations. It is also influenced by how their customers accept the products made with our nanotubes. The researchers will base their opinion on the price and quality of our nanotubes. At both levels, our product image goal is one of "top of the line" in both quality and price.

We expect quite a bit of publicity for our company. We plan to speak at a number of nanotechnology and business conferences. Press releases will also be sent to major news agencies and a number of nanotechnology publications.

Advertising
Advertising for our new company will help our company compete in the nanotubes market. Advertisements will be purchased in nanotechnology publications such as *Small Times.* Our focus will center on the academic research sector. Information about our product may also be sent out by mail to research institutions.

5.4.4 Pricing
We intend to price our nanotubes around the average pricing of the competition in order to capture as much market share as possible. Pricing our product at $500/gram will make us a considerable profit since the product cost is just under $16/gram. Because competitors have so much marketing strength, we may switch to a more aggressive pricing strategy and lower the selling price to gain a stronger hold on the market.

5.4.5 Sales
Sales representatives employed by our company will be highly trained and knowledgeable about our product. They will be able to answer any questions regarding the properties of our nanotubes. Our product will be available for order by phone or through our website.

5.4.7 Logistics
The nanotubes product will be packaged and shipped directly from our manufacturing facility. Since most orders will be in small quantities, perhaps several grams, transportation costs will not be an important factor. Purified nanotubes will be compressed into small pellets, weighed, and placed in plastic jars. Orders will be shipped by mail in small boxes, and should arrive within 3-5 business days. We plan to use UPS delivery service to deliver our product to the customers. This way, customers may choose the option of rush delivery at an additional charge. This arrangement will place the cost of shipping onto the customer.

5.4.8 Support
Our nanotubes product will come with a property specification guarantee. Any orders that do not meet these specifications may be returned for a full refund or exchange. All returns will be handled by our shipping department. Sales representatives will be in charge of customer support.

5.5.0 COMPETITIVE ANALYSIS

Currently, there are sixteen nanotube producers worldwide, half are in the U.S.

Company	Synthesis Method	Purity (%)	Price ($/g)
Carbolex	Arc Discharge	70 - 90	60 -100
Carbon Solutions Inc.	Arc Discharge	60-80 70 - 90	250 400
CNI	HiPCO	>90 Fluorinated	500 900
IIJIN	CVD & Arc Discharge	SWNT	60-200
MER	Arc Discharge	10 - 40	80
Nanocarblab	Arc Discharge	40-90	100
Nanolab	CVD	90	200 - 400
Nanostructured & Amorphous Matereials	CVD	>90	200
SweNT Inc.	CoMoCat	>90	500

5.6.0 OPERATIONS / PRODUCTION

The manufacturing operation is the "backbone" of our company. The process of synthesizing carbon nanotubes is continuous. The operation will be managed by very experienced individuals, using state of the art equipment and employing intelligent, and also highly experienced, personnel. Because some aspects of the operation are unique, the only way the personnel can get the necessary experience is for us to train them. Our hiring policies and education techniques will continue to grow as the company expands and changes. Our planned facilities and equipment will be operated at full capacity for the first few years. Projected growth will be continuously analyzed as the market continues to grow.

5.6.1 Organization

We currently plan to hire around 6 employees for the production and delivery sections of our company. Most of the necessary workers will be hired from the local area. Personnel will be required to possess a high level of experience and training. Equipment operators will need to be familiar with the reactor and the synthesis process. The manufacturing process requires that two of these operators be available at all times.

5.6.2 Suppliers

We have not yet selected the definitive suppliers for our process. However, the raw materials needed are all common chemicals and could be purchased from a number of different supply companies. We expect to have all suppliers selected before construction on the plant is complete.

5.6.3 Technology

The manufacturing technology that will be used in our plant is the patented HiPCO process. Licensing rights will be secured before production begins.

5.6.4 Quality

The quality and composition of our product will be analyzed before selling. The nanotubes are all guaranteed to a specified purity, so we will take considerable precautions to ensure that those tolerances are met. Approximately 10% to 15% of each day's batch will be checked to specifications. If more than 5% of those are rejected, the whole batch will be checked.

5.7.0 FUNDING REQUIREMENT

Our company is currently seeking an equity investment of $2,500,000 for the start-up of the enterprise. The investment will be used to fund the preliminary stages of the company's development.

5.7.1 Use of funds

An estimated $2.5 million will be used for the construction of the new facility. This will include the purchase of land and the construction of the facility, as well as the equipment and installation costs. The table below shows the breakdown of direct and indirect costs projected for the new facility. A portion of the investment will be used for preliminary advertising and promotion of the company's product. Additional funds will be used for the executive's salaries.

5.7.2 Investor Involvement

We are proposing that this be an equity investment for which the investors will receive 15% ownership in the company. Management will provide a seat on the company's board of directors. Ongoing reports of key ratios, profit-loss statements, balance sheets, and annual audits would be provided to the investor. It is management's intent that the investor will enjoy returns on investment in excess of that of alternative investments, as a privately held company, while providing investor liquidity of his investment by taking the company public at its earliest opportunity.

Table 5.1 Estimated Total Capital Investment

Component	Basis for Estimate	$
Direct Cost		
Onsite		
Purchased Equipment:		
Reactor		$25,050.00
Compressor		$60,000.00
Molecular Sieve		$10,000.00
Nanotube filter		$1,300.00
Vacuum Oven	Cole-Parmer: electronic control, 0.67 ft^3	$2,700.00
Furnace	Cole Parmer 800W	$2,000.00
Vacuum Pump		$500.00
Ultrasonic processor	Cole-Parmer: 1500 W, 10 L cap. (100L/h)	$7,940.00
Total purchased equipment		*$109,490.00*
delivered equipment	10% of purchased cost	$23,923.50
pruchased equiment installation	*Subtotal: delivered equipment*	$63,796.00
instrumentation$Controls(installed)	47% of delivered equipment	$95,694.00
Piping(isntalled)	36% of delivered equipment	$49,441.90
Electrical systems(installed)	68% of delivered equipment	$39,872.50
Buildings(land and constructions)	11% of delivered equipment	$639,593.50
Yard improvements	18% of delivered equipment	$39,872.50
Service facilities	10% of delivered equipment	$87,719.50
Total Direct Cost		$1,207,343.40
Engineering and supervision		$25,000.00
Construction expenses		$250,000.00
Legal expenses		$9,170.68
Contractor's fee		$150,000.00
Contingency		$80,701.94
Advertising		$10,000.00
Marketing		$5,000.00
Total Indirect Cost		**$529,872.62**
Fixed Capital Investment		**$1,737,216.02**
Working Capital	15% of TCI	**$306,567.53**
Total Capital Investment		**$2,043,783.55**

APPENDIX A

MARKET FORECAST

A.1 Economic Forecasting

Economic forecasting is a useful tool for investors and business planners. Nearly all forecasting involves looking at the past behavior of a particular industry or product. However, since nanotubes are a relatively new discovery, and their applications are even more recent, no past exists on which to base a future model. Forecasting is not an exact science, and there are many models, both simple and complex, on which forecasts can be based. The economic forecast in this section is a highly simplified model derived from information and news sources about nanotubes applications and market behavior[42] combined with basic economic principles of supply and demand equilibrium.

A.2 Supply

The current global production of SWNT was determined by analyzing the production rates of existing companies. Table A.1 shows a list of SWNT manufacturers and their reported daily output. The total and average global production was then determined from these values.

Table A.1: Production Rates of SWNT Manufacturers

Company	Production (g/day)
Carbolex	35
Carbon Solutions Inc.	50
CNI	500
IIJIN	200
MER	10
Nanocarblab	3
Nanocyl	20
Nanolab	50
NanoLedge	120
Nanostructured & Amorphous Materials	50
Shenzhen Nanotech	200
SouthWest NanoTechnologies Inc.	500
AVERAGE	145
TOTAL	1738

The increase in the number of SWNT production facilities since the year 2000 was used as a basis for determining the number of companies entering the market over the next ten years. The number of companies is expected to continue to increase at the current rate for the next several years and then gradually slow down. Figure A.1 shows a time series of the expected entry of companies into the market.

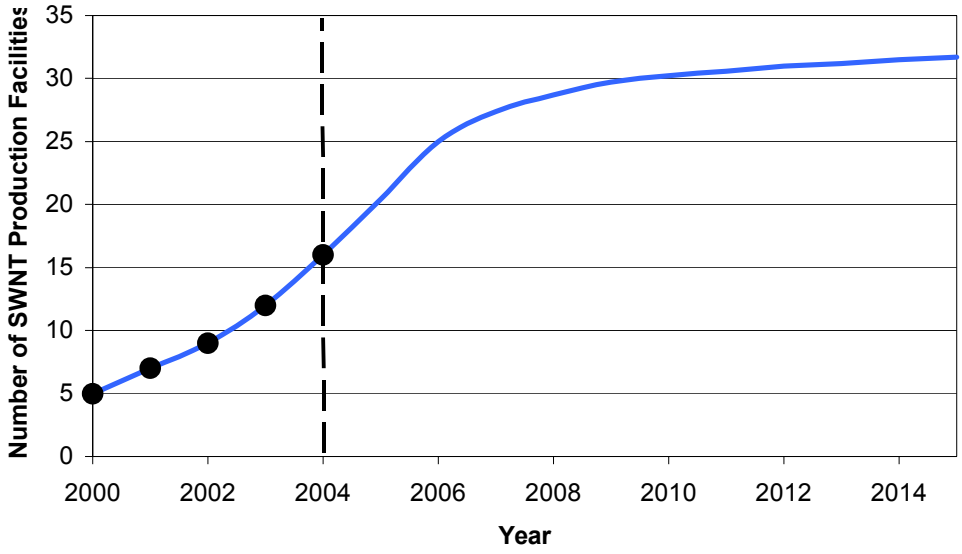


Figure A.1: Projected Entry of Companies into the Market

The projected number of companies was then used in combination with the previously determined average production rate to determine the market supply lines for each of the next ten years. With emerging technologies and improved synthesis methods, the average production rate of SWNT facilities was assumed to be able to increase by 10% annually. Supply was assumed to behave linearly, with no nanotubes produced at a market price of $0 per gram, and with plants producing the maximum output for a market price of $500 per gram. A supply line was then constructed for each year up through 2015. Figure A.2 shows the supply curves for the next 10 years.

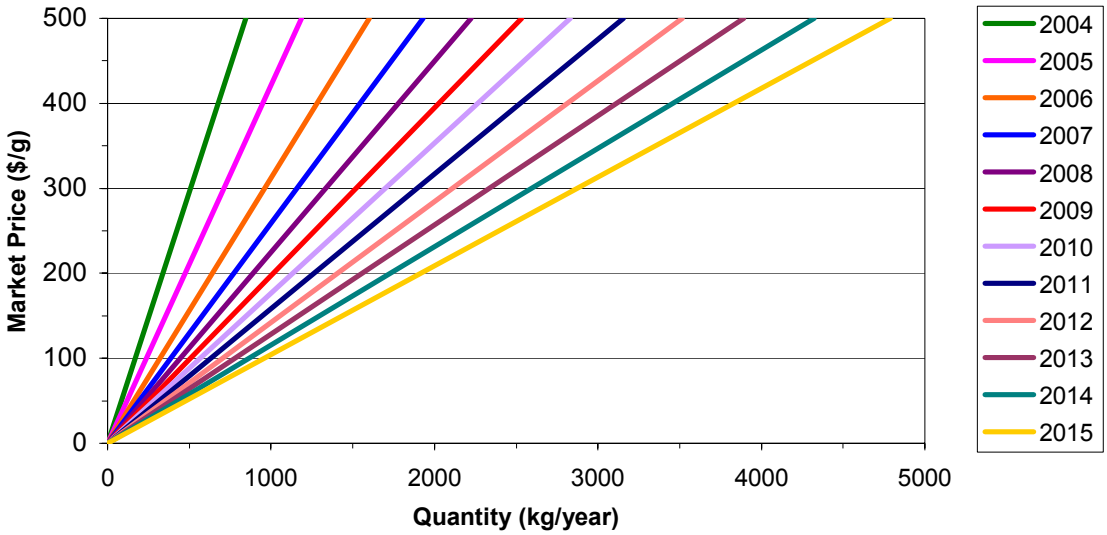


Figure A.2: Forecasted Supply Curves

A.3 Demand

Demand for SWNT is divided into two main sectors: research and commercial use. The demand for research grade nanotubes was assumed to increase at the same rate as government spending on nanotechnology research and development. Previous government spending was plotted on a time series graph[43], and the future spending was expected to increase according to an "s"-shaped curve. Government spending for various countries is shown in Figure A.3.

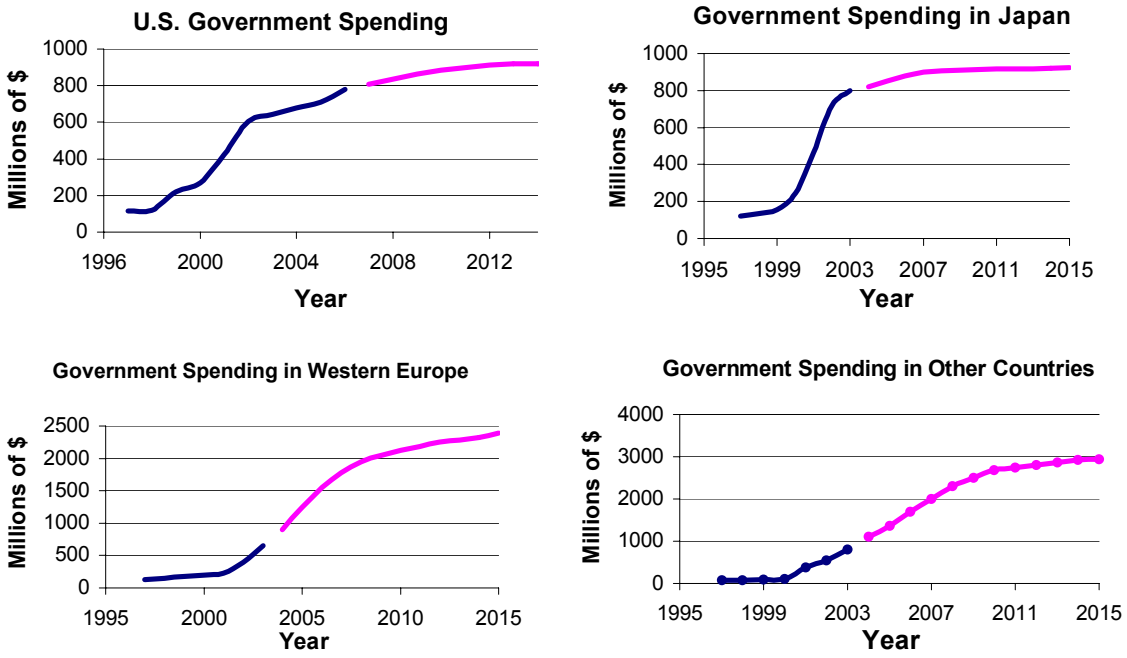


Figure A.3: Projected Government Spending by Country

The global government spending was found by summing the spending for each country. Figure A.4 shows the projected global spending over the next 10 years.

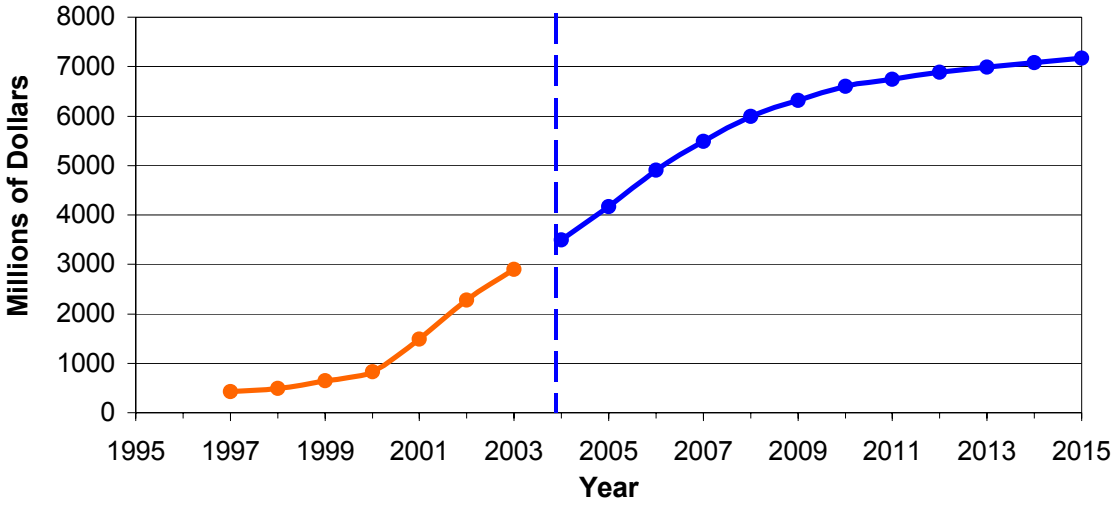


Figure A.4: Projected Global Spending on Nanotechnology R&D

Table A.2 shows the annual percent increase in global government spending, and the corresponding increase in the demand within the research sector.

Table A.2: Research Demand for SWNT

Year	Global Spending (10^6)	% Increase	Research Demand (kg/year)
2003	2895	27.3	635
2004	3499	20.9	767
2005	4170	19.2	915
2006	4911	17.8	1077
2007	5486	11.7	1203
2008	5992	9.2	1314
2009	6323	5.5	1387
2010	6599	4.4	1447
2011	6746	2.2	1480
2012	6889	2.1	1511
2013	6987	1.4	1532
2014	7081	1.3	1553
2015	7168	1.2	1572

For the commercial sector, the demand was determined for six major applications of SWNT: batteries, flat panel displays, hydrogen storage, AFM probe tips, chemical sensors, and fibers and composites. Both the price of the nanotubes and the point in time will have a significant effect on the demand for these applications. To take into account both of these two variables, the demand was estimated for a range of market prices over the next ten years. (This does not indicate that the price will stay constant over that period of time, it is just a predictor of the behavior of the demand when two factors are varied.)

Flat Panel Displays

According to Applied Nanotech Inc., a company that holds over 80 patents on the use of nanotubes in electronic devices, nanotube displays will be able to capture one-half of one percent of the flat screen market in the next five years.[44] Approximately 10 million flat panel screens were sold last year.[45] Assuming an average display size of 900cm^2, the mass of nanotubes in each display was calculated with the length of the nanotubes in the arrays to be 1 micron [46] and the density to be 1.35 g/cm^3. These figures, coupled with the emerging technologies and lowering prices formed the basis for the estimates of the increasing demand for nanotubes in flat panel displays. A similar approach was used for each for each of the remaining applications. The projected demands are shown in the figures below.

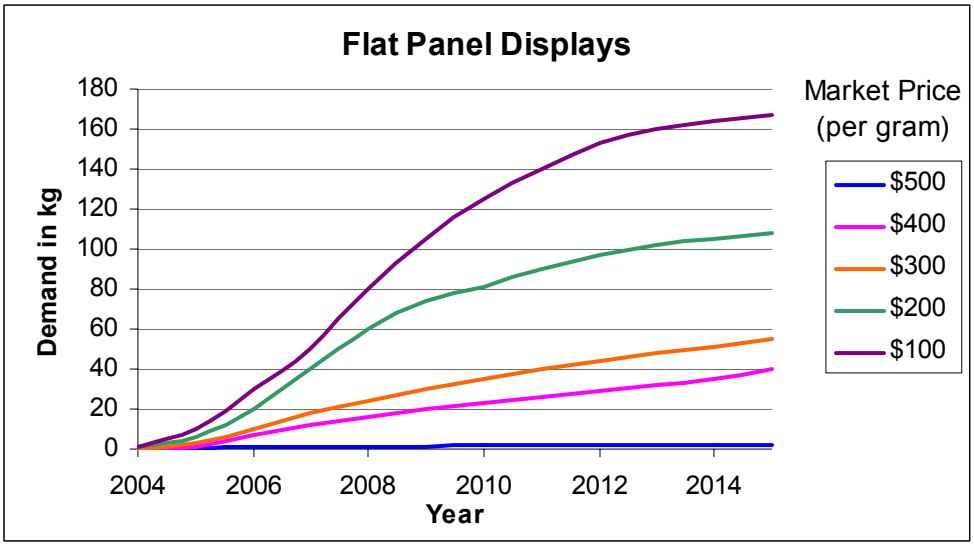


Figure A.5: Projected Demand for Nanotubes in Flat Panel Displays

Batteries

Batteries made with nanotube anodes will be able to store twice as much power as traditional lithium batteries. The demand projections for nanotubes batteries are based on a $2 million demand for lithium batteries.[47] The nanotubes batteries will be slow to take over a share of the market due to the still developing technology involved with the application as well as the higher price of the raw materials and end product. Figures A.6 and A.7 show the projected demand.

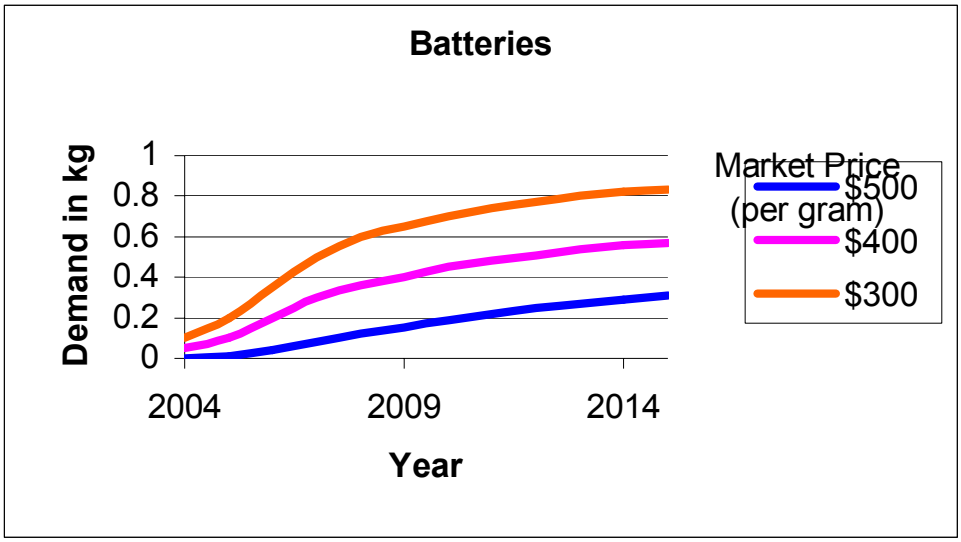


Figure A.6: Projected Demand for High Priced Nanotubes in Batteries

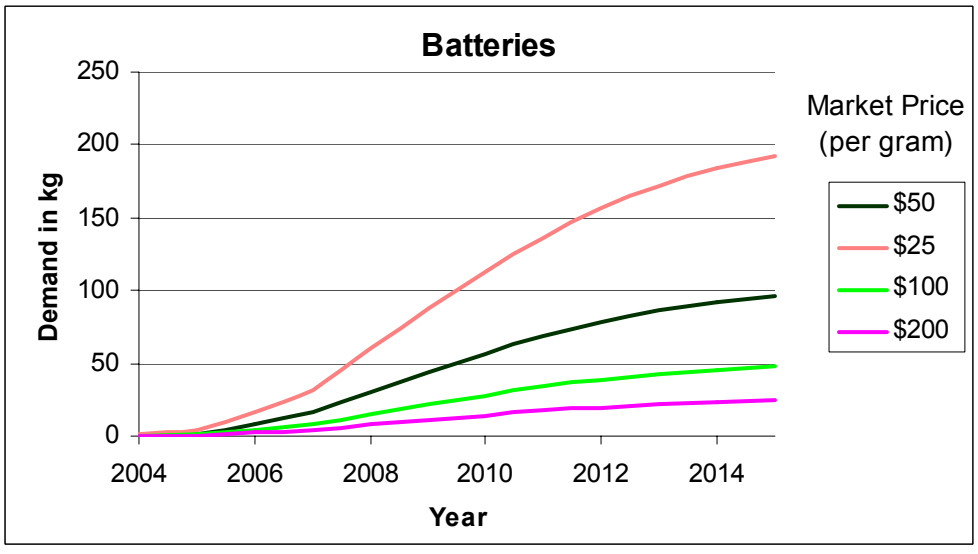


Figure A.7: Projected Demand for Low Priced Nanotubes in Batteries

Chemical Sensors

The market for chemical sensors in 2001 was valued at $5 billion dollars.[48] The function of nanotubes sensors make them highly adaptable in both industry and military applications. As with other applications, nanotube sensors will be slow to capture a portion of the total market, but will increase with technological improvements over time and with lower prices of raw nanotubes. The projected demand for nanotubes in chemical sensors is shown in Figure A.8 below.

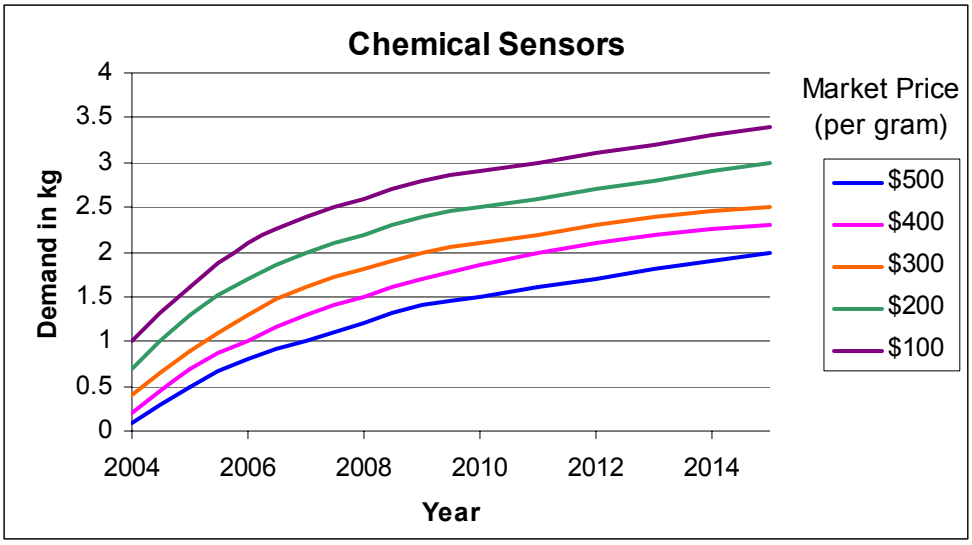


Figure A.8: Projected Demand for Nanotubes in Chemical Sensors

Hydrogen Storage

The current market for hydrogen storage devices is $700 million.[49] Although the size of the market for this application is smaller than those of other applications, the demand is expected to be slightly higher due to the larger required amounts of nanotubes in each fuel cell device. The projected demand for nanotubes in hydrogen storage applications is shown in Figure A.9.

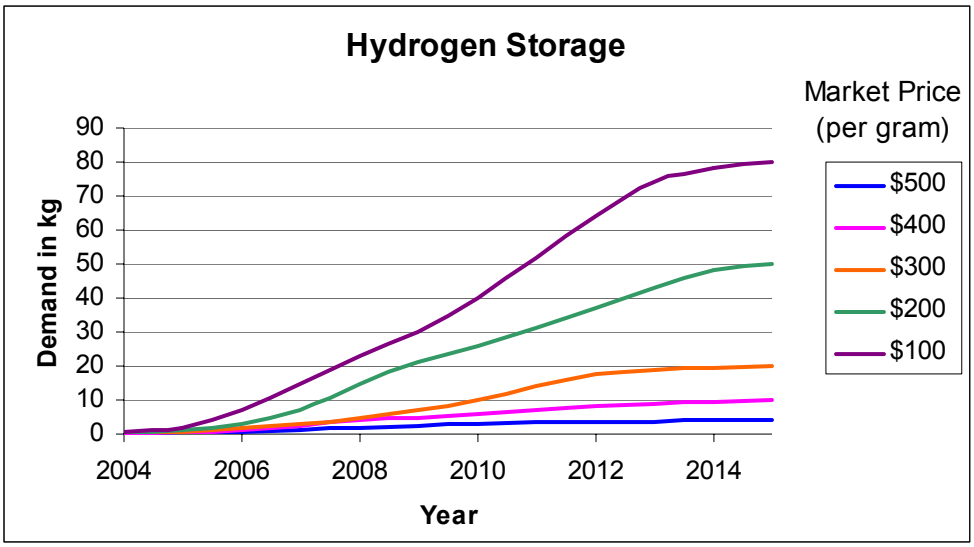


Figure A.9: Projected Demand for Nanotubes in Hydrogen Storage Devices

AFM Probe Tips

AFM probe tips made from nanotubes are already being produced and sold. The demand for this type of application is obviously limited. However, with superior performance of the nanotube tips over those made from other types of materials, the nanotube tips should eventually capture the entire market. Demand projections for AFM probe tips are shown in Figure A.10.

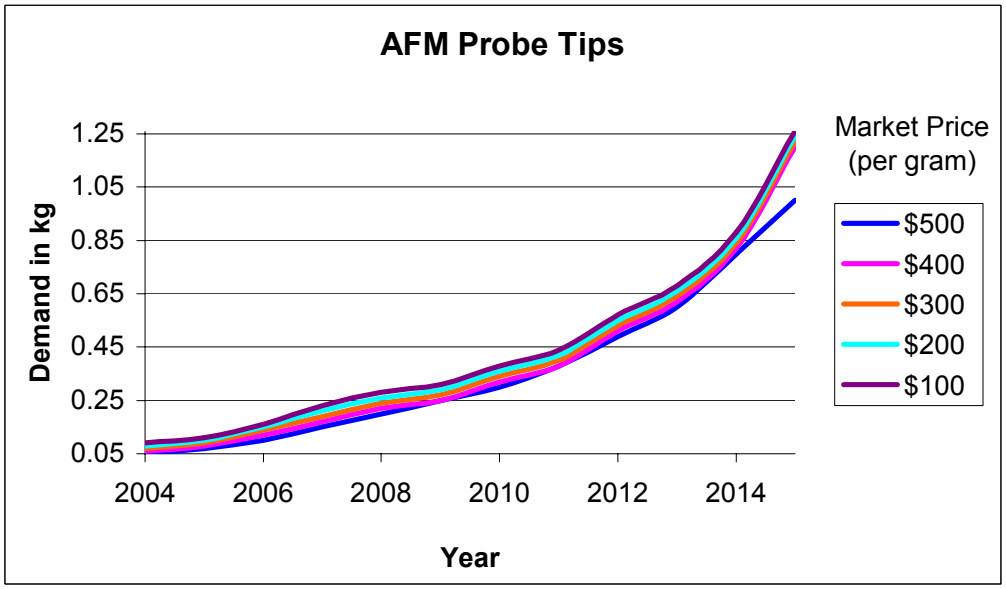


Figure A.10: Projected Demand for Nanotubes in AFM Probe Tips

Fibers and Composites

The strength and semiconducting properties of nanotubes make them a strong candidate for additives in certain materials. Extra-strong fibers of SWNT are already being made, and MWNT are currently being used in a wide range of composites, including automotive and aerospace parts. The demand for fibers and composites made from SWNT will increase as new applications are discovered and as the price of raw nanotubes decreases. The demand for nanotubes in fibers and composites is shown in Figure A.11.

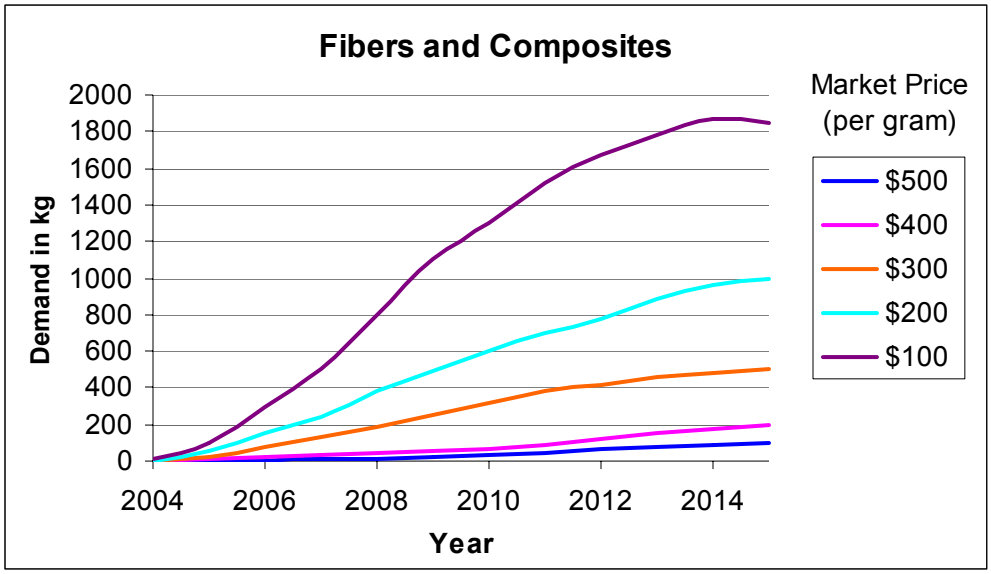


Figure A.11: Projected Demand for Nanotubes in Fibers and Composites

The sum of the demands for nanotubes in applications and research was used to determine the total demand for each of the next ten years. The demand curves will shift to the right as time progresses as a result of newly developed and improved commercial applications. The current demand for nanotubes is fairly inelastic, meaning that the demand changes very little in response to large changes in selling price. Figure A.12 shows how the demand becomes less inelastic over time, and at lower selling prices. This is due to the growing number of commercial applications, and the increased purchasing ability of the commercial sector at lower prices.

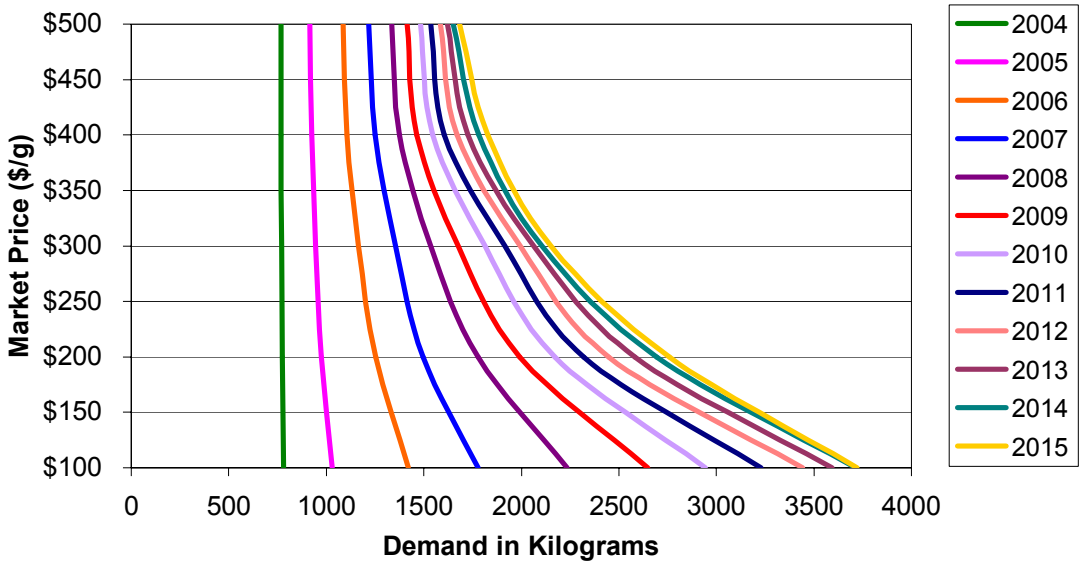


Figure A.12: Forecasted Demand Curves for SWNT

A.4 Market Equilibrium

The point at which the supply and demand curves intersect is the equilibrium point. When a market is at equilibrium, the quantity demanded is equal to the quantity supplied[50]. The supply and demand curves for each year were plotted on the same graph in order to determine the equilibrium price and quantity. The supply and demand curves for 2005 are shown in Figure A.13.

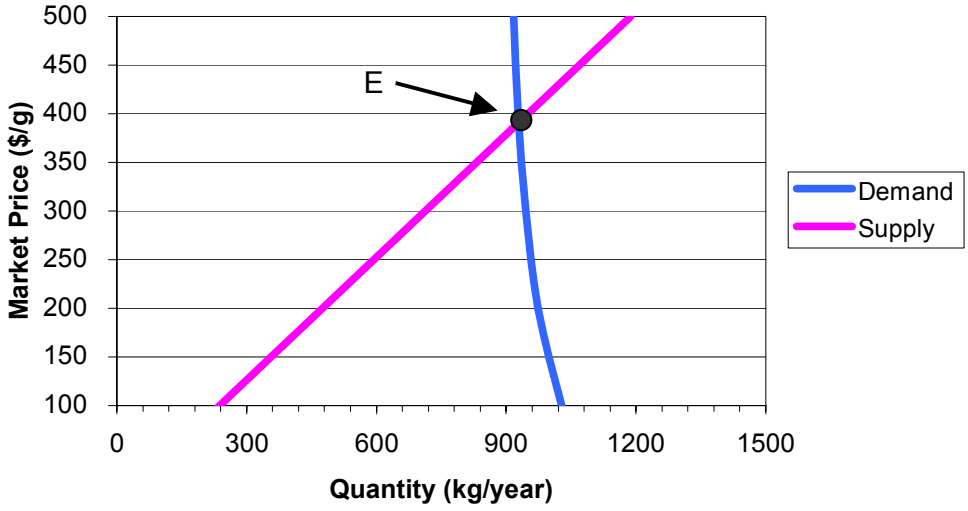


Figure A.13: Equilibrium for 2005 Demand and Supply Curves

The equilibrium price and quantity were determined by the intersection of the supply and demand curves for each year through 2015. The equilibrium quantity is plotted against time in Figure A.14. The demand is shown to increase at a nearly linear rate over the next ten years.

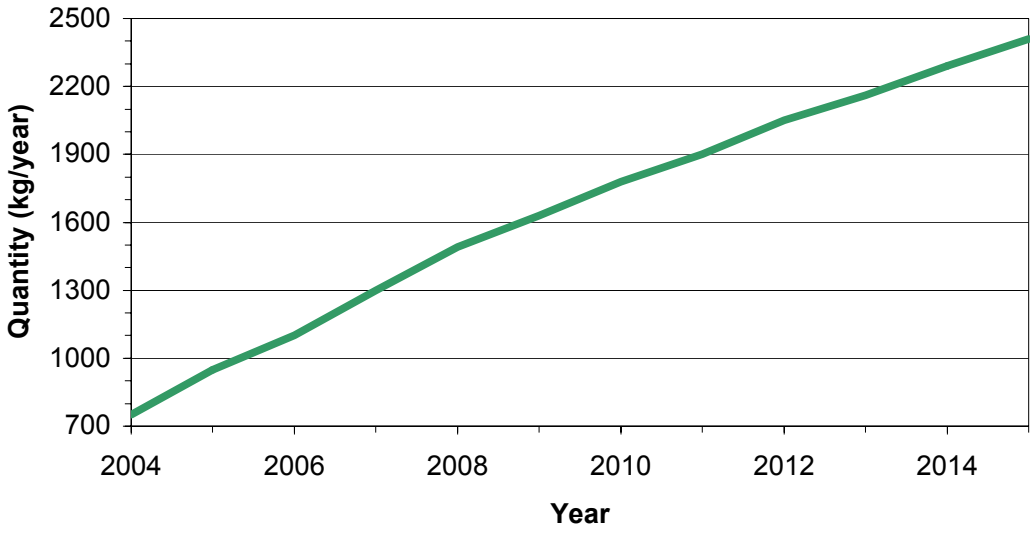


Figure A.14: Projected Equilibrium Quantities

Figure A.15 shows the resulting equilibrium prices for SWNT from 2004 to 2015. The price is forecasted to decrease considerably from about $460 per gram in 2004 to $250 per gram in 2015.

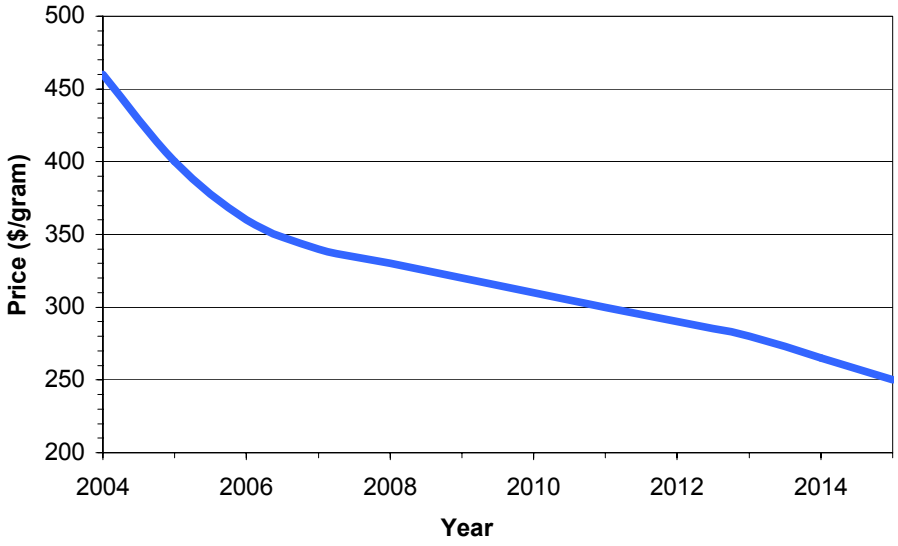


Figure A15: Projected Change in Equilibrium Price

APPENDIX B

HIPCO EQUIPMENT SPECIFICATIONS

Reactor

The reactor consists of a bundle of 100 identical tubes. The specifications for each tube are given in the table below.

Table B.1 Specifications for Reaction Tubes

Tube specification		
stainless steel type 304 sched. 80		
Inner diameter	2.5	cm
Outside diameter (page204 high P)	3	cm
Heated Length	20	cm
Total tube Length	60	cm
Out side surface area	188	cm^2
Cold injector (32ppm $Fe(CO)_5$)		
304 stainless steel pipe		
inner diameter	1	mm
Outside diameter	1.2	mm
copper nozzle	1	mm inner diameter
Hot injector		
Chromium steels (30%Cr)		
inner diameter	1.5	in.
Outside diameter	2.75	in.
length	36	in.
6 channels		
inner diameter	0.375	in.
Outside diameter	0.45	in.
6 orifices	1.00	mm diameter

The following table was used to determine the overall cost of the reactor based on the sizes and materials of the individual parts. Additional equipment prices are also listed in the table.

Table B.2 Breakdown of Equipment Cost for SWNT's Production Plant

1 tube					
	Amount	**Cost**	**Length (m)**	**d (in)**	**Cost**
Cold injector	1	$45/m	0.3	0.5	$13.50
reaction tube	1	$75/m	0.6	1	$45.00
Hot injector (includes cost of boring channels	1	$70/m	0.9144	2.5	$63.30
Cost of boring holes	6	$8/hole	1	3/8	$48.00
ceramic orifice	6	$8.10/orifice		0.125	$48.60
ceramic nozzle	1	$8.10/nozzle		0.125	$8.10
Total cost of 1 tube					$226.50
Insulator wall	1	$2,400.00			**$2,400.00**
Material	foaming insulator	$40/m			
Ai, inner area	0.1				
Thickness **Sub-system Name**	**Amount**				**Cost**
reactor	1				**$75,050.00**
compressor	1				**$60,000.00**
SILIPORITE® Molecular Sieves (remove CO_2)	1	Type 4A or 5A			**$10,000.00**
nano filter	1	batch size = $1m^3$			**$1,300.00**
Equipment cost					**$109,409.00**

APPENDIX C

CoMoCat PROCESS DESIGN

C.2.1 Plant Design

This section gives the plant design for single wall nanotube production facility using the CoMoCat process. A detailed study of the process was performed with literature research, calculations on Excel spread sheet and GAMS mathematical model.

The equipment costs vary with the production rate, the values presented are priced for a capacity of 360 kilogram SWNT's per year.

C.2.2 Process description

This method is based on the controlled reaction of carbon monoxide (CO) on a solid catalyst, under conditions that result in high yield and selectivity towards SWNT as opposed to other less desired forms of carbon, such as graphite nanofibers. Because the electronic and optical properties of single-walled carbon nanotubes depend on tube structure, a major goal in nanotube production is to control the distribution of nanotube diameters and chiralities in the product. With CoMoCat unique production method, the product composition depends on catalyst design and parameters that precede the reaction process and nanotube growth. Adjustment of these parameters allows fine control over the specific catalyst activity and, therefore, of the nanotube structures.

In the CoMoCAT method, nanotubes are grown by CO disproportionation (decomposition into C and CO_2) at 700-950ºC in flow of pure CO at a total pressure ranging from 1 to 10 atm. The CO disproportionation reaction shown below is the exothermic Boudouard reaction.

$$2CO \rightarrow C\,[SWNT]_{(s)} + CO_{2\,(g)}$$
$$\Delta H = -172.42\ KJ/mol$$

This process is able to grow a significant amount of SWNT in several minutes, keeping selectivity towards SWNT better than 90 %. The difference of this technology with the rest of the catalytic decomposition methods is based on the stabilization of highly dispersed Cobalt (Co) species on a solid substrate. The effect of having Co stabilized is dramatic. It avoids the formation of large metallic particles. These large metallic particles, present in all of the competing methods have the disadvantage of getting encapsulated in graphite layers, which remain in the product and are extremely difficult to remove. By contrast, in the CoMoCAT process, Cobalt atoms are initially in the form of cobalt molybdate and only begin to agglomerate under the reaction conditions and their growth is delayed by the interaction with the substrate. The CoMoCat process has the essential ability to produce SWNT of different diameters by varying the operating temperature or the gas composition.

C.2.3 Plant Description

The flow sheet of the process is shown in Figure C.2.1. In this process the raw materials include commercial grade carbon monoxide (CO), cobalt and molybdenum (Co: Mo) as catalyst and silica (SiO2) as support. The commercial grade CO is 99.5 % pure. The inert gases used in this process are hydrogen (H_2), helium (He) and oxygen/air mixture (Air/O_2).

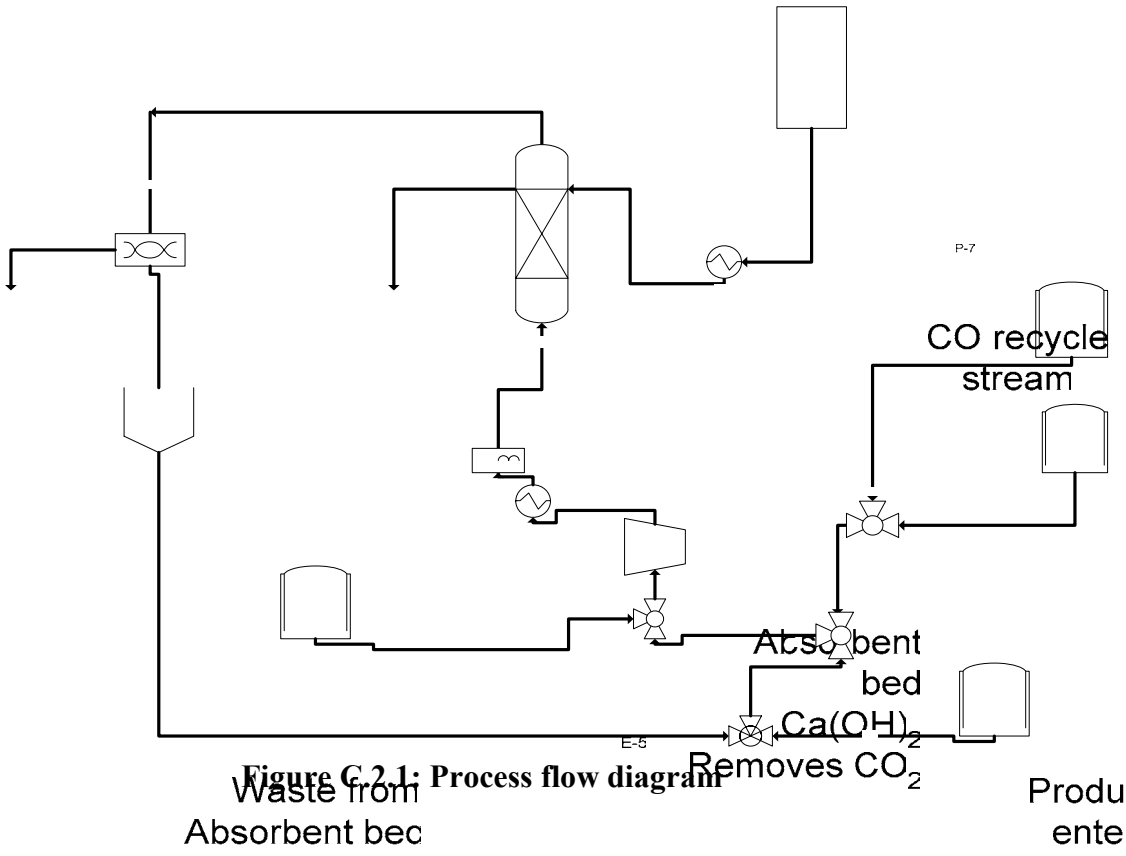


Figure C.2.1: Process flow diagram

In the process the reaction conditions to which the catalytic particles are exposed are highly controlled at different stages. The ability to regulate temperature and reactive concentrations is important to obtain the high selectivity necessary to produce SWNT's. The yield of nanotubes is affected by the reaction temperature (700°C -950°C), catalytic gas pressure (70 psi), space velocity (30,000particles/hr) and reaction time (3 min-1 hr) and by pretreatment conditions. The detailed production method were described in section 3.2.

C.2.4 Nanotube purification

The flow sheet of the purification process is shown in Figure C.2.2. In this process raw materials include commercial grade sodium hydroxide NaOH, oxygen O_2 and hydrochloric acid HCl. In purification method support SiO_2 is dissolved by treatment with a base (2 M NaOH). The catalytic particles are sonicated in 2 M NaOH for 5 hr at preferred temperature from 22°C to 70°C. This step eliminates 99 % of the SiO_2, most of

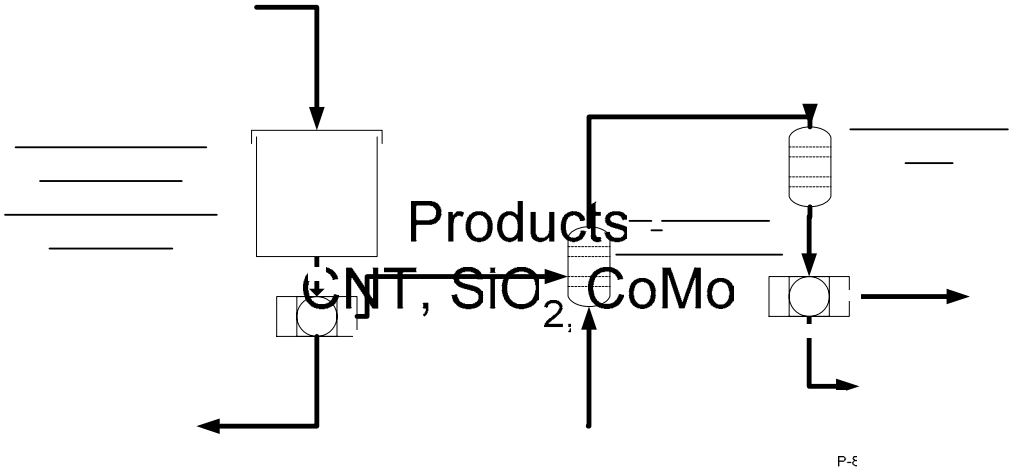


Figure C.2.2 Purification process flow diagram

the Mo 90% and 40% of Co. After this treatment, the sample is further oxidized in air at 200-250°C. Finally the catalytic particles (CNT's, CoMo and O_2) are sonicated in acid solution HCl. In this step the metal catalyst particles are dissolved. The total removal of metal is about 95%-99%. After purification, the nanotubes are farther treated in handling process. The flow sheet of the handling process is shown in Figure C.2.3.

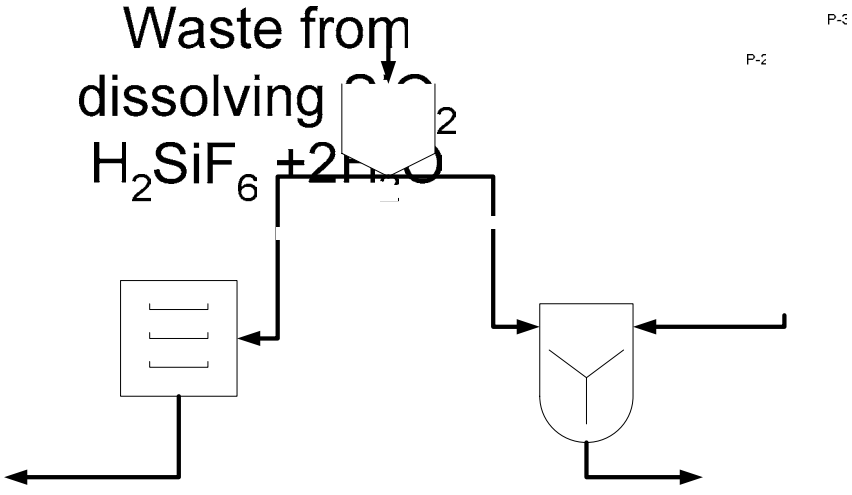


Figure C.2.3 Handling Process Flow Diagram

Handling process shown on flow diagram above produce freeze-dried web and stable suspension. The freeze- dried webs are produced by heating SWNT's to the triple point in the gel drying bed. The stable suspension is produced by mixing SWNT's with water H_2O and sonicating. The delivering forms of SWNT are produced by CoMoCat production plant can be seen in Figure C.2.4.

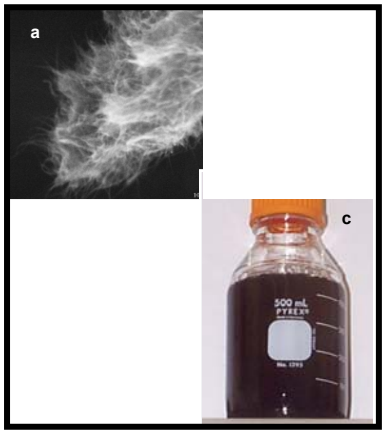


Figure C.2.4 Forms of SWNT's

C.2.5 Equipment Cost

Total equipment cost was determined by the sum of individual equipment costs. Table C.2.1 lists the necessary equipment and prices for each.

Table C.2.1 Equipment Cost

Purchased Equipment	**Cost**
Heater gass	$11,000.00
Heatr catalyst	$15,000.00
Filrter	1,300.00
Sonicating Beds	11,500.00
Gel drying bed	10,000.00
Insulator wall	$5,000.00
Reactor	$30,800.00
Compressor	$50,300.00
SILIPORITE® Molecular Sieves (remove CO_2)	$10,000.00
Total Equipment cost	**$144,900.00**

The total capital investment was calculated by adding indirect costs and direct costs. The calculated values can be seen in Table C.2.2.

Table C.2.2 Total Capital Investment

Investment	Costs
Indirect Costs	$604,872.62
Direct Costs	$1220903.40
Fixes capital investment	$1,825,776.02

APPENDIX D

MATHEMATICAL MODEL RESULTS

Results from Mathematical Model
Table D.1: Total Capital Investment

Estimation of TCI

Component	Basis for Estimate	$
Direct Cost		
Onsite		
Purchased Equipment:		
Reactor		$75,050.00
Compressor		$60,000.00
Molecular Sieve		$10,000.00
Nanotube filter		$1,300.00
Vacuum Oven	Cole-Parmer: electronic control, 0.67 ft^3	$2,700.00
Furnace	Cole Parmer 800W	$2,000.00
Vacuum Pump		$500.00
Ultrasonic processor	Cole-Parmer: 1500 W, 10 L cap. (100L/h)	$7,940.00
Total purchased equipment		*$159,490.00*
delivered equipment	10% of purchased cost	$23,923.50
pruchased equiment installation	*Subtotal: delivered equipment*	$63,796.00
instrumentation$Controls(installed)	47% of delivered equipment	$95,694.00
Piping(isntalled)	36% of delivered equipment	$49,441.90
Electrical systems(installed)	68% of delivered equipment	$39,872.50
Buildings(land and constructions)	11% of delivered equipment	$639,593.50
Yard improvements	18% of delivered equipment	$39,872.50
Service facilities	10% of delivered equipment	$87,719.50
Total Direct Cost		$1,207,343.40
Engineering and supervision		$25,000.00
Construction expenses		$250,000.00
Legal expenses		$9,170.68
Contractor's fee		$150,000.00
Contingency		$80,701.94
Advertising		$10,000.00
Marketing		$5,000.00
Total Indirect Cost		**$529,872.62**
Fixed Capital Investment		**$1,737,216.02**
Working Capital	15% of TCI	**$306,567.53**
Total Capital Investment		**$2,043,783.55**

Table D.2: Annual Total Product Cost

Component	Basis for Estimate	Cost ($/yr)
I. Manufacturing cost		
A. Direct production costs		
1. Raw materials		
$Fe(CO)_5$		$ 209
CO	Commercial Grade	$ 177
Argon	liquid (230 psi)	$ 393,300
Filter Paper	Millipore (Grade 102) 3μm pore	$ 500
Filter Paper	Cole-Parmer 1μm pore	$ 1,500
	Subtotal:	***$ 395,686***
2. Operating labor		$ 2,000,000
3. Direct supervisory and clerical	15% of operating labor	$ 300,000
4. Utilities		$ 2,589,499
5. Maintenance and repair	6% of FCI	108256.5609
6. Operating supplies	15% of maintenance and repair	$ 5,611
7. Laboratory charges	15% of operating labor	$ 52,560
8. Patents and royalties	15% of total product cost	$ 860,758
	Variable cost	***$ 5,916,685***
B. Fixed charges		
1. Capital costs		
Property taxes	2% of FCI	$ 36,086
Insurance	1% of FCI	$ 18,043
sub-total		***$ 54,128***
C. Overhead costs	60% of labor & supervision	***$ 1,380,000***
II. General expenses		
A. Administration costs	20% of labor & supervision	$ 88,074
B. Distribution and selling costs	5% of total product cost	$ 286,919
C. Research and development	10% of total product cost	$ 573,839
sub-total		***$ 948,832***
Total annual product cost		$ 8,695,331
	Unit cost ($/gram)	**$ 23.82**

MATHEMATICAL MODEL

```
option optcr= 0.001;
option iterlim = 1e9;

file res/gam 2941.xls/;
put res;

Sets i plants/ Texas, Oklahoma,California, Illinois, NY/
*i plants/ California, Texas, Oklahoma, Illinois, NY, Massachusetts/
    j markets / M1/
    tp time periods / 1,2,3,4,5,6,7,8,9,10/

scalar totalyears  lifespan of plant /10/;

Parameters
            year(tp)
/1 1
2 2
3 3
4 4
5 5
6 6
7 7
8 8
9 9
10 10
/

taxprop(i) property taxes

/
California 30
Texas 25
NY 34
*Massachusetts 30
Illinois 33.33
Oklahoma 15/

;

Alias (tp,tpp);

Scalar maxcap maximum capacity of plant kg /400/;
Scalar int rate of return /0.15/   ;
Scalar Vs salvage value percenta of fci /.15/ ;
```

```
Scalar Iw working capital percentage of fci /.2/  ;
Scalar maxinitcapital max invesetment/15000000/  ;
Scalar eqcost equipment cost for 1 kg capacity /715000/;
Scalar opfixed opering cost utility /2000000/;
Scalar operkg operating per kg /23820/;

;

Variables
rmc(i,tp) raw material costs
tc(i,tp) total costs
r(i,tp) revenue
cf(i,tp) cash flow
capadd(i,tp) capacity of plant
fci(i,tp) fixed capital investment
tci(i,tp) total capital investment
op(i,tp)
totx(tp)
npw
x(i,j,tp) amount sold
totcap(i,tp)
built(i)
capmint(i,tp)
bilt(i,tp)
capimp(i,tp)
repay(tp)
add1(i,tp)
;

binary variables

bi(i,tp) plant constructed
bc(i,tp) plant expanded;

positive variables x, rmc, tc, op, r, repay, capadd, bilt, fci, tc, capimp;

Equations
costs(i,tp)
Operatingcosts(i,tp)
totalcost(i,tp)
revenue(i,tp)
cappimprove(i,tp)
cappimprove2(i,tp)
maxcapacity(i,tp)

fixedcicon(tp)
```

```
fixedci(i,tp)
totalci(i,tp)
cashflow(i,tp)

netpresentworth
build(i)
numplants
capimprov(i,tp)

capimprove2(i,tp)
capimprove3(tp)
Capacity(i,tp)

prodsupply(i,tp)
totalproduct(tp)
demand1(i,tp)
demand(j,tp)
capimp1(i,tp)
add(i,tp)
;

costs(i,tp)..                    rmc(i,tp) =e= raw1(i,tp)*capadd(i,tp) +
                raw2(i,tp)*capadd(i,tp) + raw3(i,tp)*capadd(i,tp)+
                capadd(i,tp)*(raw4(i,tp) + capadd(i,tp)*(raw5(i,tp));
Operatingcosts(i,tp)$(ord(tp) gt 1)..   op(i,tp) =e=  opfixed*bilt(i,tp) + 194.2*capadd(i,tp);
totalcost(i,tp)..                tc(i,tp) =e=  rmc(i,tp) + op(i,tp)+ capimp(i,tp) ;
revenue(i,tp)..                  r(i,tp) =e=  sum(j,marketprice(j,tp)*x(i,j,tp));
capimp1(i,tp)..                  capimp(i,tp) =e=  0.1*r(i,tp)+.07*r(i,tp);



Capacity(i,tp)..                 capadd(i,tp) =g= SUM(j,x(i,j,tp));
cappimprove(i,tp)..              capadd(i,tp) =l= 1000*bc(i,tp);
cappimprove2(i,tp)..             capadd(i,tp) =g= 65*bc(i,tp);

maxcapacity(i,tp)..              totcap(i,tp) =e= sum(tpp$(ord(tpp) le  (ord(tp) -1)),
capadd(i,tpp));

fixedcicon(tp)..            sum(i,tci(i,'1')) =l= maxinitcapital;
fixedci(i,tp)..      fci(i,tp) =e= 2000000*bi(i,tp) + 26000*bc(i,tp) + 353.43*capadd(i,tp);
totalci(i,tp)..           tci(i,'1') =e= fci(i,'1')/0.85;

cashflow(i,tp)..            cf(i,tp) =e= (r(i,tp) - (r(i,tp) - (1/6)*(sum(tpp $ (ord(tpp) le
ord(tp) and ord(tpp) gt (ord(tp)-6)),fci(i,tpp))))*taxprop(i)/100);
```

```
netpresentworth..                    npw =e= sum(i,( sum(tp,cf(i,tp)/power((1+int),
year(tp))))+(Vs+Iw)*sum(tp,fci(i,'1')/power((1+int),totalyears))- tci(i,'1'));
build(i)..                           sum(tp,bi(i,tp)) =l= 1;
numplants..                          sum(tp,sum(i,bi(i,tp))) =l=1;
capimprov(i,tp)..                    sum(tpp $ (ord(tpp) le ord(tp)), bi(i,tpp)) =e= bilt(i,tp);
capimprove2(i,tp) $ (ord(tp) gt 1)..    bc(i,tp) =l= bilt(i,tp);
capimprove3(tp)..                    sum(i,bc(i,'1')) =e= sum(i,bi(i,'1'));


prodsupply(i,tp)..              sum(j, x(i,j,tp)) =l= totcap(i,tp);
totalproduct(tp)..              totx(tp) =e= sum((j,i), x(i,j,tp));
demand1(i,tp)..         sum(j,x(i,j,'1')) =e= 0;
demand(j,tp)..          sum(i, x(i,j,tp)) =l= market(j,tp);
rev1(i,tp)..           r(i,'1') =e= 0;
add(i,tp)..             add1(i,tp) =e= r(i,tp) - tc(i,tp);

nanoplantnew.reslim = 9999999;
Model nanoplantnew/all/;
Solve nanoplantnew using mip maximizing npw;


Display  bc.l, bi.l,  rmc.l, x.l,op.l, fci.l, npw.l, capadd.l, r.l, cf.l, fci.l, tci.l, capimp.l, tc.l;
```

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