Vinyl Chloride Production

Capstone Design Project
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Executive Summary

This project presents the design of a vinyl chloride plant with a capacity of 6.4 billion pounds per year located in Taft, LA. The capacity of the plant is based on comparing several different capacities' return on investment and net present worth. Applying different trends to the historical demand data allowed for the prediction of the capacities. The vinyl chloride product is 99.8 mol% pure, this composition allows for polymer feedstock applications. The total capital investment for the plant is \$65.1 million. The plant produces a total net profit of \$27.5 million per year. Extensive Monte Carlo simulations show that a 6.4 billion pound capacity has a 68% chance of having a positive net present worth. A major focus of the design is to maximize safety and minimize environmental impact while maintaining profitability. The VCM plant produces a number of by-products resulting in eight waste streams. The Clean Air and Clean Water Acts, enforced by the Environmental Protection Agency, regulate the procedure by which we dispose of the different waste streams. An integrated waste treatment system utilizing incineration, absorption, caustic scrubbing and activated carbon adsorption is developed in order to avoid releasing any hazardous waste into the environment. The total capital investment of the waste treatment system is \$667,000. The increase in environmental awareness increases the total equipment cost from \$14.5 million to \$15.28 million, and decreases the total net profit per year to \$26.2 million.

Section 1: Introduction

Chlorinating hydrocarbons is the basic idea behind the production of vinyl chloride monomer (VCM). Chlorinated hydrocarbons (CHCs) are much more resilient to biodegradation, unlike simple hydrocarbons. This is due mainly to the inherent strength of the C-Cl bond. Consequently, man-made CHCs are beginning to accumulate in the environment. However, production of VCM is essential to the production of polyvinyl chloride (PVC). Construction materials made of PVC are light, low-maintenance, and long lasting. PVC products are highly resistant to weathering, petroleum products, and UV radiation. PVC, a flame resistant material, has been examined extensively in regards to fire prevention. There are so many positive aspects of using PVC that it is imperative that it be produced. Many CHCs are created during the production of PVC; this is a growing concern. Therefore, VCM needs to be produced in a way that will minimize or totally eliminate the release of CHCs into the environment.

The goal of this project is to design an environmentally friendly, safe, and economically profitable vinyl chloride production plant. Environmental friendliness requires that the design go beyond the minimum compliance regulations while maintaining plant profitability. Plant safety includes addressing deviations from normal operation that may have adverse effects on employees or the surrounding community. The project is divided into five interrelated parts; process design, market analysis, environmental awareness, plant safety, and plant economics. The market analysis section includes a method for determining the optimal location of the plant as well as an investigation of the future demand for vinyl chloride. The process design section includes the thermodynamic system, kinetic data, balanced process for the production of VCM, process simulations, and heat integration of the heat exchangers. The environmental awareness section includes an evaluation of all the waste streams, along with an evaluation of several waste treatment methods in addition to justification for the waste treatment system that was selected. The plant safety section includes a detailed hazardous operations study of the P&ID design of the VCM plant. The last section, plant economics, includes a detailed economic analysis of the VCM plant, which quantifies the total capital investment, net present worth, and other major economical variables.

Section 2: Available Processes

Vinyl chloride was first produced using the process of dehydrating ethylene dichloride (EDC) with alcoholic caustic potash. However, the first effective industrial process was based on the hydrochlorination of acetylene. Until the late 1940s, this process was used almost exclusively (21).

The normal method of producing acetylene was from calcium carbide. “The high-energy requirement for carbide production was a serious drawback to the continuing mass production of vinyl chloride by this method” (21). However, as ethylene became more plentiful in the early 50’s, commercial processes were developed to produce vinyl chloride from chlorine and ethylene via EDC, namely, the balanced ethylene route. Today the balanced ethylene is responsible for well over 90% of the world’s vinyl chloride production. “This process has been refined and the scale of operation has greatly increased, but no fundamentally new processes have achieved commercial viability” (21). Although this is true, it is still necessary to examine the alternative processes and determine if they can still be utilized.

All current production plants for vinyl chloride depend on the use of a C_2 hydrocarbon feedstocks, specifically, acetylene, ethylene, or ethane. Commercial operations using these compounds are confined to gas-phase processes. “Manufacture from acetylene is a relatively simple single-stage process, but the cost of acetylene is high” (21). Ethane is by far the least expensive C_2 hydrocarbon, but it cannot be converted to vinyl chloride with high selectivity (21).

2.1 Vinyl Chloride from Acetylene

The process that produces vinyl chloride from acetylene employs the use of a catalyst. Most of the time the catalyst used is mercuric chloride deposited on active carbon. In this process the feed gases are purified, dried, and mixed at the entrance to the tubular fixed bed reactors, which are packed with mercuric chloride on active carbon pellets as catalysts. Usually, a slight excess of HCl is used over stoichiometry. “About 99% conversion of acetylene and 98% conversion of HCl are achieved. The selectivity to vinyl chloride is good – more than 98% -- and the only significant side reaction is the further addition of HCl to vinyl chloride to form 1,1-dichlorethane” (21).

The major issue with this process is that fact that the catalyst used, mercuric chloride, is a very volatile compound. It is so volatile that much of the development work on this process has been devoted to this problem (21). Consequently, the acetylene route is currently of little commercial importance.

2.2 Vinyl Chloride from Ethane

Many attempts have been made to develop a process that will use ethane to directly produce vinyl chloride. This is due to relative inexpensiveness of ethane. The major problem associated with the use of ethane is its molecular symmetry. In particular, the addition of chlorine to ethane gives rise to a wide product spectrum (21). “The most promising routes appear to be those based on high temperature oxychlorination that use special catalysts to achieve a worthwhile selectivity to vinyl chloride and useful major by-products such as ethylene, ethyl chloride, and EDC” (21). The ethylene may be chlorinated to EDC and recycled along with the ethyl chloride. Although possible, this process has not progressed beyond the conceptual stage. This is due to the fact that the oxychlorination reactor design presents a severe challenge in terms of materials of construction because the reaction temperature may go up to $500^{o}C$ (21). At this temperature chlorine becomes very aggressive to most construction materials.

2.3 Vinyl Chloride from Ethylene

Ethylene can be converted to vinyl chloride in a single stage, i.e., without isolating the intermediate ethylene dichloride by either chlorination or oxychlorination routes, as is the case with the balanced ethylene route. Direct chlorination routes require a high temperature and a large excess of ethylene to minimize soot formation (21). The patent literature recommends using inert fluid beds for heat transfer and diluting gases in the feeds. Substantial amounts of vinyl chloride are formed when the oxychlorination reactor is operated above 350°C.

The common problems with the direct routes of production are poor selectivities to vinyl chloride and substantial production of chlorinated by-products, many of which have no direct commercial utility (21). "This has substantially hindered the industrial application of direct-conversion processes" (21).

Section 3: Process Design

3.1 Thermodynamics

A large number of chemical species are present in the vinyl chloride plant. Generally most of the compounds are non-ideal and somewhat polar. The modified Suave-Redlich Kwong (SRK) equation of state was used to simulate the vinyl chloride plant. This equation of state handles polar-nonpolar systems well (17). It is recommended for hydrocarbon and water mixtures, as is the case in the production of vinyl chloride. The modified SRK equation of state does not accurately predict liquid densities; therefore, liquid density estimations were made using Rackett correlation (17). This correlation was selected because of its accurate prediction of hydrocarbon liquid densities (17).

3.2 Balanced Process Overview

The process chosen for vinyl chloride production is a combination of two processes, direct chlorination and oxychlorination. This process is referred to as the balanced process. Direct chlorination by itself is a process that operates at lower temperatures and produces fewer by-products when compared to oxychlorination. Oxychlorination is used in vinyl chloride production because it consumes the hydrochloric acid (HCl), a major by-product of vinyl chloride production. Currently, nearly 95% of the world's supply is produced using the balanced process. The main reactions in this process are:

Direct chlorination	$CH_2CH_2 + Cl_2 \rightarrow ClCH_2CH_2Cl$	Eqn. (1)
Oxychlorination	$CH_2CH_2 + 2\ HCl + \frac{1}{2}\ O_2 \rightarrow ClCH_2CH_2Cl + H_2O$	Eqn. (2)
EDC pyrolysis	$2\ ClCH_2CH_2Cl \rightarrow 2\ CH_2CHCl + 2\ HCl$	Eqn. (3)
Overall reaction	$2\ CH_2CH_2 + Cl_2 + \frac{1}{2}\ O_2 \rightarrow 2\ CH_2CHCl + H_2O$	Eqn. (4)

3.3 Balance Process Outline

The five main processes used in the production of vinyl chloride monomer (VCM) are: (1) direct chlorination of ethylene to form EDC, (2) oxychlorination of ethylene to form from recycled HCl and oxygen, (3) purification of EDC, (4) thermal cracking of EDC to form VCM and HCl, and (5) the purification of VCM. These processes are shown in Figure 1.

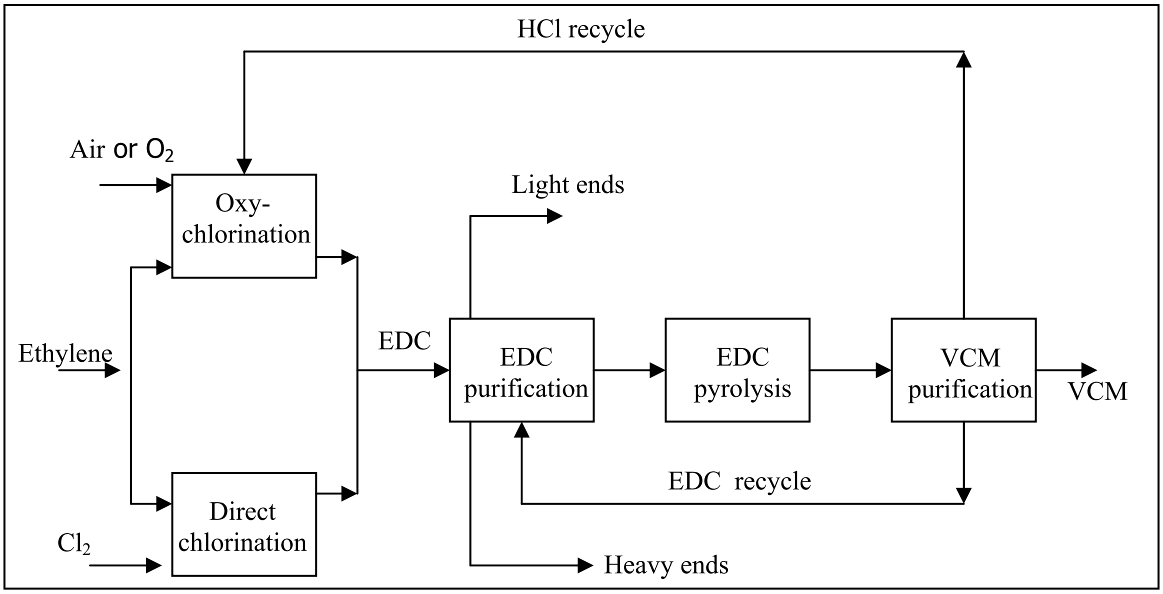

Figure 1: Vinyl Chloride Plant PFD

3.4 Direct Chlorination Reactor Design

Ethylene and chlorine combine in a homogeneous catalytic reaction to form EDC. Normally, the reaction rate is controlled by mass transfer, with absorption of ethylene as the limiting factor (9). Due to high selectivity, ferric chloride is the common catalyst of choice for chlorination of ethylene. The catalytic reaction utilizes an electrophilic addition mechanism. The catalyst polarizes chlorine (Eqn. 5) and then the polarized chlorine molecule acts as an electrophilic reagent to add Cl^- to the double bond of ethylene (Eqn. 6).

$$FeCl_3 + Cl_2 \leftrightarrow FeCl_4\text{-}Cl^+ \qquad \text{Eqn. (5)}$$

$$FeCl_4\text{-}Cl^+ + CH_2CH_2 \rightarrow FeCl_3 + ClCH_2CH_2Cl \qquad \text{Eqn. (6)}$$

The direct chlorination reaction was modeled using kinetics from Wachi and Morikawa (22). This kinetic data provided rate constants that are used to determine reaction rates. A plug flow reactor molar continuity equation (Eqn. 7) was numerically integrated to determine consumption of reactants and production of products. A slight excess of ethylene is fed to the column to maximize conversion of chlorine. Table 1 presents the conversion and selectivity parameters predicted by the reactor modeling. These results compare well to values obtain from Laskhmanan (11).

$$\frac{dF_k}{dz} = \nu r A_t \qquad \text{Eqn. (7)}$$

where: Fk is molar flow rate, z is tube length, ν is stoichiometric coefficient, r is rate of reaction, and At is tube area.

Table 1: Direct Chlorination Reactor Modeling Results

	Modeling Results	Literature Values
Conversion of ethylene	99.93%	99.94%
Selectivity to EDC	99.8%	99.4%

Kirk-Othmer and Laskhmanan both state that 1,1,2-trichloroethane is the main by-product of direct chlorination (9,11). Homolytic dissociation of chlorine forms this by-product. Oxygen inhibits the free radical reactions that produce 1,1,2-trichloroethane. Because of this, addition of pure oxygen to the chlorine in a ratio of 0.5% of the chlorine feed is commonly performed to reduce by-product formation. Wachi and Morikawa suggest that HCl is a by products as well, but only in small amounts (22). See Table 2 for complete direct chlorination product formation developed from the reactor model.

Table 2: Direct Chlorination Reactor Effluent Flow Rates (lb-mol/hr)

EDC	2682
Trichloroethane	5
HCl	0.5
Ethylene	18
Chlorine	8

The direct chlorination reaction is exothermic ($\Delta H = -180$kJ/mol), thus requiring heat removal for temperature control (9). Early reactor design had the operating temperature of the reactor at 50-60 ^{0}C. It is now desired to recover the heat of reaction to lower plant energy cost. A widely used method involves operating the reactor at the boiling point of EDC, allowing the pure vapor product to vaporize, and then either recovering heat from the condensing vapor, or replacing one or more EDC fractionation column reboilers with the reactor itself (9). Our reactor design approach is to operate the reactor at higher pressures to raise the boiling point of EDC. This causes more efficient heat transfer to occur, utilizing the higher reactor temperatures while the product remains in the liquid phase. The reactor material type depends on the temperature and product formation. Temperature control is achieved by cooling water flowing on the shell side of the PFTR; therefore, carbon steel is used to fabricate the shell of the reactor. Stainless steel tubes are required because of the corrosive HCl produced by the reaction. Table 3 presents a complete breakdown of direct chlorination reactor parameters.

Table 3: Direct Chlorination Reactor Parameters

Reactor Temperature (^{o}C)	120
Reactor Pressure (psig)	15
Reactor Volume (ft^3)	90
Tube Diameter (in)	2
Tube Length (ft)	115
Residence Time (hr)	0.018

3.5 Direct Chlorination Process Simulation

The direct chlorination reactor modeling results are transferred to Pro II for a process simulation. The liquid reactor effluent is sent to a caustic scrubber to remove aqueous waste, which contain HCl and chlorine. The EDC product from the caustic scrubber is now ready for EDC purification.

3.6 Direct Chlorination Control and Instrumentation

Reactant flow to the direct chlorination reactor is controlled by control valves that receive their corresponding signal from the ethylene flow transmitter. This control scheme ensures the proper ratio of reactant flow rates into the reactor. The direct chlorination reactor temperature is controlled by the flow rate of the cooling fluid. Temperature transmitters on the tube side of the reactor ensure proper temperature control. The caustic scrubber is controlled by ratio control that is used to adjust NaOH flow based on product pH and feed flow rate. See Figure 2 for the direct chlorination P&ID. Appendix A contains corresponding stream and equipment tag numbers and descriptions.

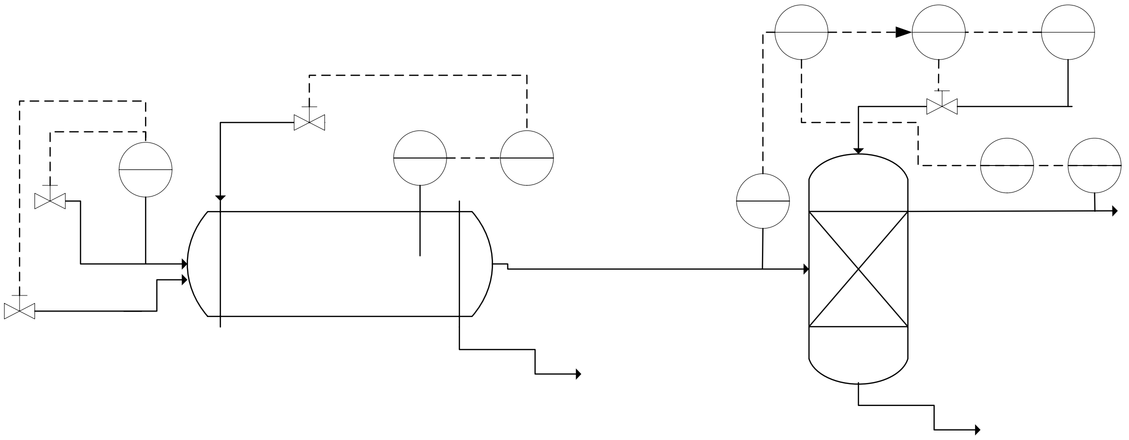

Figure 2: Direct Chlorination PFD

3.7 Oxychlorination Reactor Design

The reaction is modeled by using kinetic data obtained from a series of articles by Sai Prasad (2001), and Gel'Perin (1979, 1983, 1984). Sai Prasad presents seven reactions that make up the oxychlorination reaction (19). Gel'Perin provides more extensive by product formation kinetic data for the reaction (5,6,7). Table 4 presents the oxychlorination reactions and their stoichiometric equations.

Table 4: Oxychlorination Reactions

Set	Reaction	Stoichiometry
R-1	DCE formation	$C_2H_4 + 2CuCl_2 \rightarrow C_2H_4Cl_2 + 2CuCl$
R-2	TCE formation	$C_2H_4 + 3CuCl_2 \rightarrow C_2H_4Cl_3 + 3CuCl + 0.5H_2$
R-3	C_2H_4 combustion	$C_2H_4 + 3O2 \rightarrow 2CO_2 + 2H_2O$
R-4	CuCl oxidation	$2CuCl + 0.5O_2 \rightarrow CuO\text{-}CuCl_2 \rightarrow CuO + CuCl_2$
R-5	$CuCl_2$ regeneration	$CuO + 2HCl \rightarrow CuCl_2 + H_2O$

Along with these five main oxychlorination reactions, nine other by-product formation reactions were modeled. Equation 7 was numerical integrated to determined reactant consumption and product formation. Figure 3 shows the reactant consumption and product generation versus reactor tube length. These values are determined by the reactor model. Table 5 presents the numerical results from the oxychlorination reactor model.

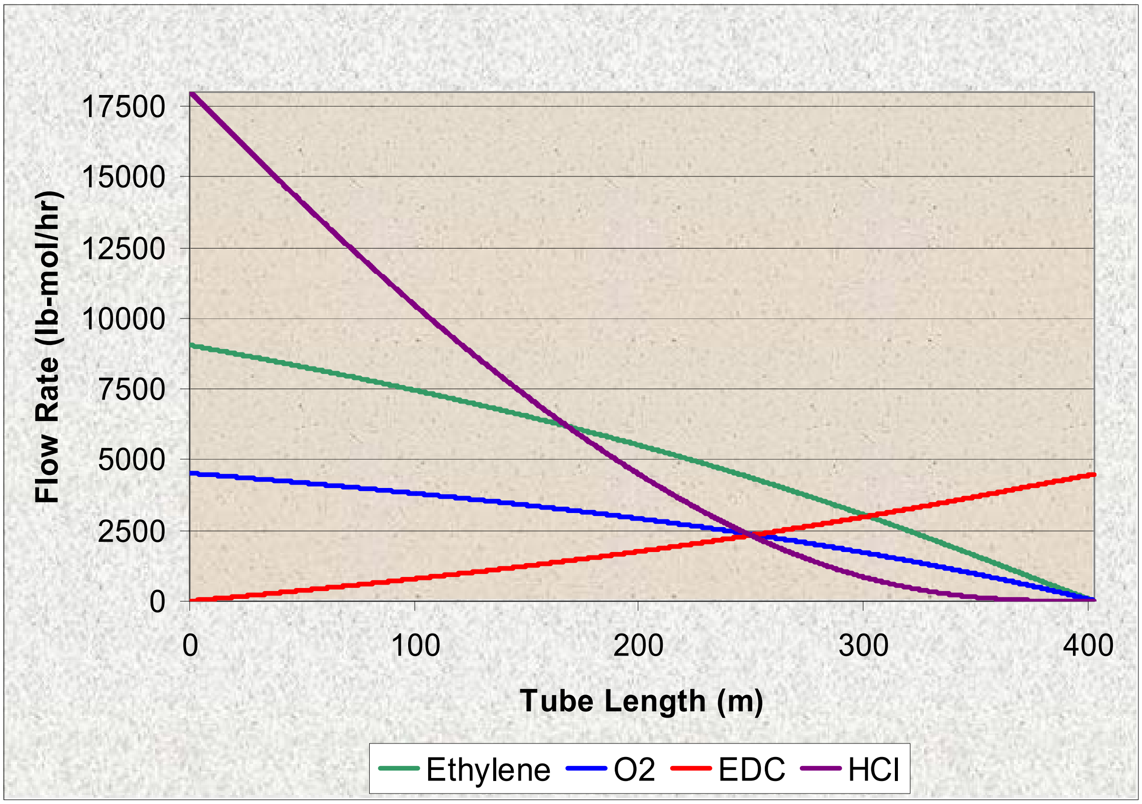

Figure 3: Oxychlorination Reactor

Table 5: Oxychlorination Reactor Effluent Flow Rates (lb-mol/hr)

EDC	1341	Cloral	0.25
Water	1341	CCl_4	1.25
TEC	1.26	Methyl Chloride	0.12
CO_2	140	Chloroform	0.11
Ethylene	5.5	Chloroethane	0.11
Oxygen	2.76	Chloroprene	0.10
HCl	0.015	Vinyl Acetylene	0.09
Acetylene	0.13	Dichloromethane	0.10

The oxychlorination reactor is a PFTR with the cupric chloride catalyst packed in the tubes while cooling water flows on the shell side for temperature control. Some oxychlorination processes utilize a fluidized bed reactor, but no heat recovery is possible with these reactors. See Appendix B-4 for a description of oxychlorination fluidized bed reactors. Oxychlorination is highly exothermic (ΔH = -239 kJ/mol). Ethylene oxychlorination is normally conducted at temperatures of 225-325 ^{o}C and at pressures of 1-15 atmospheres (McPherson, 1979). Operating the reactor at higher temperatures allow for heat recovery which result in plant energy savings. Plant wide heat integration is discussed in section 3.18. Table 6 presents the reactor parameters determine for the reactor model results. An increase in by-product formation is observed with increasing reactor temperature. This is due to an increase in oxidation of ethylene to carbon oxides and increased cracking of EDC. Kinetic data obtained from Gel'Peri, determine the chloro-hydrocarbon byproducts rate increased from 0.012 to 0.178 with a temperature increase of 350 to 400 ^{o}C (5). High temperature (>350 ^{o}C) can also cause catalyst deactivation from sublimation of $CuCl_2$.

Table 6: Oxychlorination Reactor Parameters

Reactor Temperature (^{o}C)	305
Reactor Pressure (psig)	58
Reactor Volume (ft^3)	461
Tube Diameter (in)	2
Tube Length (ft)	1320
Residence Time (hr)	0.05

3.8 Air Based or Pure Oxygen Based Oxychlorination Process

The oxychlorination process requires air or pure oxygen as a reactant. Many older designs utilize air as a reactant due to the low cost and availability. Recent oxychlorination process design selected oxygen over air for several reasons. The main advantage is the reduction in nitrous oxide (NO_x) formation as well as other by-products composed of nitrogen. In a typical oxychlorination process a small amount of reactor off gas is purged from the reactor to prevent accumulation of impurities, such as, carbon oxides, nitrogen, argon, and un-reacted hydrocarbons. These impurities can form in the oxychlorination reactor or enter the process as impurities in the feed. Utilizing pure oxygen in the oxychlorination process accounts for a substantial decrease in reactor off gas. A major reduction of vent gases can be accomplished using the oxygen based oxychlorination process. This greatly reduces the treatment cost for the vent gas. These many advantages off set the cost of utilizing pure oxygen; therefore, many air based oxychlorination process have been converted to the oxygen.

3.9 Air Based and Pure Oxygen Based Oxychlorination Simulations

Pro II simulations were performed for both air based and pure oxygen based oxychlorination. The air based simulation processes 17000 lb-mol/hr of nitrogen which passes through the reactor, caustic scrubber, and flash vessels it is then vented to the atmosphere. The addition of this nitrogen results in a waste treatment problem. The nitrogen will form NO_x in the oxychlorination reactor which produced a vent stream that is subject to incineration; the addition of nitrogen in this vent stream will dramatic increase the formation of nitrous oxides. For this reason air based oxychlorination will not be used. Oxygen based provides a much more environmentally friendly design. Waste treatment will be discussed in more detail in section 4.

3.10 Oxychlorination Process Simulation

The oxychlorination reactor modeling results are transfered to Pro II for the process simulation. The liquid reactor effluent is processed by a caustic scrubber to remove aqueous waste that includes HCl. The EDC product is then cooled by a heat exchanger and flashed to remove any oxygen and light impurities present in the effluent. The EDC product from the flash is now ready for EDC purification. See Figure 3 for the oxychlorination process flow diagram.

3.11 Oxychlorination Control and Instrumentation

Reactant flow to the oxychlorination reactor is controlled by control valves that receive their corresponding signal from the ethylene flow transmitter. This control scheme ensures the proper ratio of reactant flow rates into the reactor. The direct chlorination reactor is controlled by the flow rate of the cooling fluid. Temperature transmitters on the tube side of the reactor ensure proper temperature control. The caustic scrubber is controlled by ratio control that is used to adjust NaOH flow based on product pH and feed flow rate. Heat exchanger E-104 is controlled by a temperature control on the process stream controlling cooling fluid flow rate. See Figure 4 for the oxychlorination P&ID. Appendix A contains corresponding stream and equipment tag numbers and descriptions.

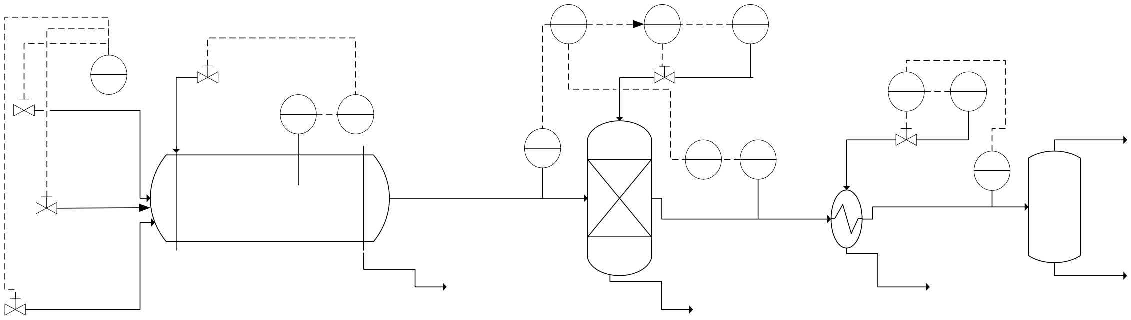

Figure 4: Oxychlorination Process PFD

3.12 Ethylene Dichloride Purification Simulation

Ethylene dichloride from direct chlorination, oxychlorination, and the recycle stream from the cracking step must be purified before pyrolysis. The EDC must be purified to 99.5 wt%. Initially, the combined EDC is washed with water in a wash tower. This is done to remove a majority of the water produced by the oxychlorination reaction. Also, the $FeCl_3$ catalyst can be removed by washing with water, in conjunction with EDC from the oxychlorination process (9). Ferric chloride is highly soluble in water; therefore, separation is not a problem. The $FeCl_3$ can then be removed by adsorption on activated carbon (13). Process water treatment is discussed in Section 4.2. The EDC is then purified by two distillation columns. The first column, referred to as the lights column, removes water and low boiling point impurities. The bottoms from the lights column, which have lower volatility, are combined with the pyrolysis feed purge; these two streams combine to form the feed of the heavies column. The second feed is a purge stream from the quench section of the plant. The pure EDC composition is 99.3%, and is the overhead product of the heavies column. The lights column consists of 17 theoretical trays, operates with a reflux ratio equal to three, and operates at a top tray pressure of 185 psig with a 22 psig pressure drop. The heavies column consists of 30 theoretical trays, operates with a reflux ratio of one, and operates at a top tray pressure of 80 psig and has a 15 psig pressure drop.

3.13 Ethylene Dichloride Purification Control and Instrumentation

The lights column is controlled by an overhead and bottoms control loop. The bottoms control loop utilizes a low select switch control steam flow rate. A differential pressure controller and a composition controller each call for a certain steam flow rate. The smallest flowrate is selected by the low select switch. The differential pressure controller has a set point equal to the maximum tray pressure drop and the composition controller's set point is the desired composition of the bottoms. The overhead control loop utilizes a level controller on the reflux drum to control the reflux ratio. The heavies column is controlled by an overhead and bottoms control loop. The bottoms temperature is controlled by the steam flow rate to the reboiler. In the overhead control loop the level control of the reflux drum is established by the distillate flow rate, reflux ratio is adjusted by the composition controller in order to control distillate composition. See Figure 5 for the oxychlorination P&ID. Appendix A contains corresponding stream and equipment tag numbers and descriptions.

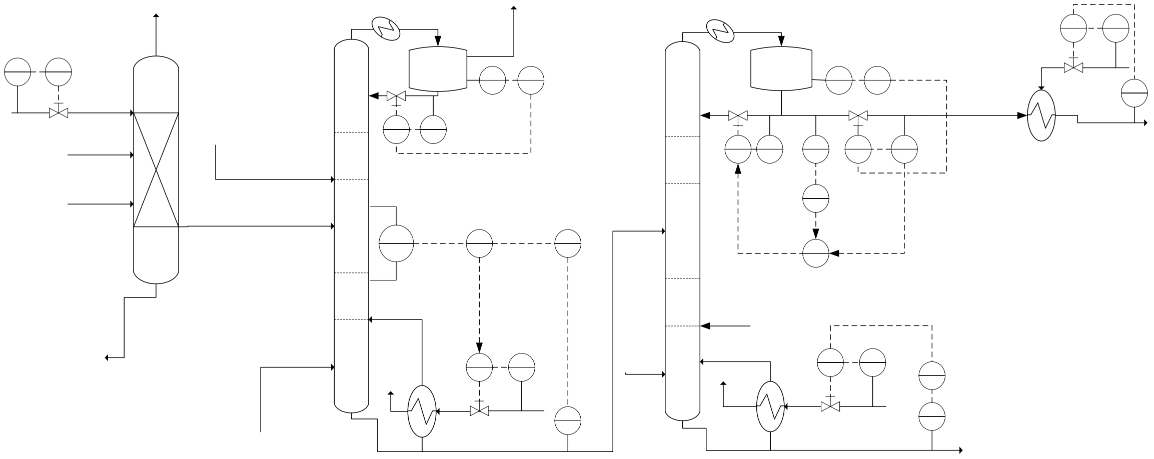

Figure 5: EDC Purification Section

3.14 EDC Cracking and Quench Design

Pyrolysis (thermal cracking) of EDC produces vinyl chloride. Pyrolysis of EDC is an endothermic reaction (ΔH = 71 kJ/mol) that is carried out in a furnace. The furnace consists of four main sections: a radiation section, a convection section, a shock section, and a stack. The radiation section, also referred to as the firebox, contains the tubes, burners, and tube sheets. The heat required for endothermic reaction is supplied by combustion of fuel from the firebox burners. The fire box operates at 500 ^{o}C. The convection and shock sections utilize combustion gases to preheat the feed before entering the firebox. The combustion gases are then released to the atmosphere by way of the furnace stack. The main reaction which yields vinyl chloride and hydrogen chloride is a homogeneous, first order free-radical chain mechanism, see equation 8.

Several by products are produced through free-radical and molecular mechanism, see equations 8-16.

$ClCH_2CH_2Cl \leftrightarrow C_2H_3Cl + HCl$ Eqn. (8)
$C_2H_3Cl \leftrightarrow C_2H_2 + HCl$ Eqn. (9)
$H\cdot + HCl \leftrightarrow H_2 + Cl\cdot$ Eqn. (10)
$Cl + C_2H_4 \leftrightarrow HCl + C_2H_3\cdot$ Eqn. (11)
$C_2H_3\cdot + C_2H_2 \leftrightarrow C_4H_5\cdot$ Eqn. (12)
$C_4H_5\cdot \leftrightarrow H\cdot + C_4H_4$ Eqn. (13)
$C_4H_5\cdot + HCl \leftrightarrow C4H6 + Cl$ Eqn. (14)
$C_4H_5\cdot + C_2H_2 \leftrightarrow C_6H_7\cdot$ Eqn. (15)
$C_6H_7\cdot \leftrightarrow c\text{-}C_6H_7\cdot$ Eqn. (16)
$c\text{-}C_6H_7\cdot \leftrightarrow H + C_6H_6$ Eqn. (17)

It is very difficult to verify the formation and amount of by products (11). Also it is very difficult to obtain kinetics parameters of the reactions involved (11). The pyrolysis kinetics were obtained from the following sources Choi, Weissmann, and Kurtz (3,23,10). Using the kinetic data and conversion of EDC data given by Kirk-Othmer and Choi the cracking furnace was modeled and then a conversion reactor was used in the Pro II process simulation (9,3). Conversion of EDC is maintained at 50-55%. Operating the furnace at a higher conversion decreased the selectivity to vinyl chloride. One way to increase conversion while maintaining high selectivity is to allow a small amount, 1200 ppm of carbon tetrachloride (CCl_4), a oxychlorination by-product, to enter with the feed. This increases free chlorine radical formation, which increases conversion to 60%. The Pro II simulation determined a selectivity of vinyl chloride to 98.8% at a conversion of 60%. This corresponds well to literature values of 99.9% selectivity at 54% conversion with no CCl_4 present in feed. The effluent from the reactor must be quenched quickly to avoid coke formation and heavy tar formation (9). Re-circulating liquid streams quenches the reactor effluent. Next, two separate flash drums are needed to flash the effluent. From this the effluent will now be ready for vinyl chloride purification. Figure 5 presents the process flow diagram for the EDC cracking and quench sections of the vinyl chloride plant.

3.15 EDC Cracking and Quench Control and Instrumentation

The EDC cracking furnace fuel gas flow rate is controlled by a ratio control of effluent flow rate and temperature. A cascade controller system is used to control the heat exchangers. See Figure 6 for the oxychlorination P&ID. Appendix A contains corresponding stream and equipment tag numbers and descriptions.

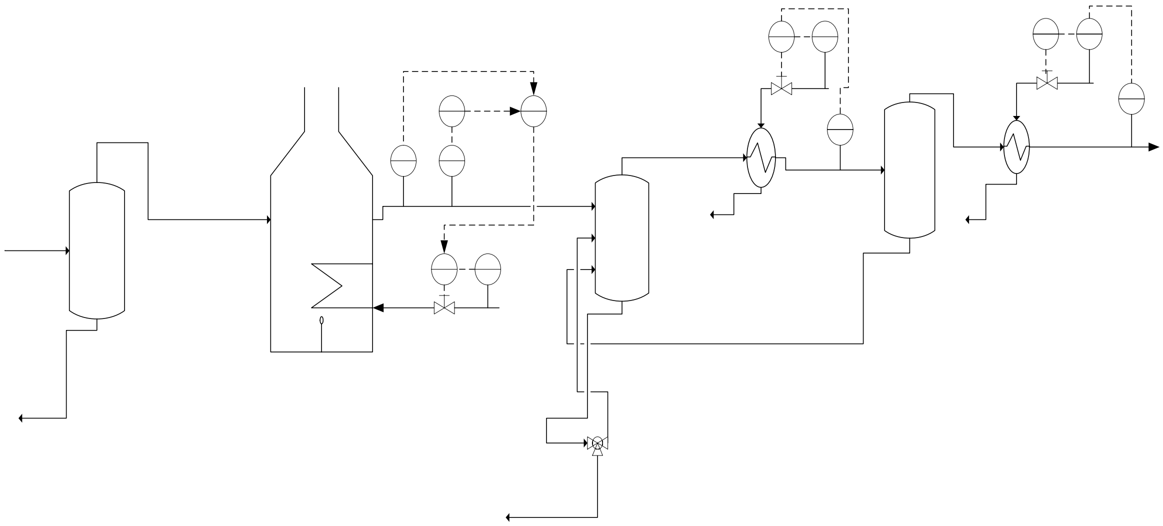

Figure 6: EDC Cracking and Quench Section

3.16 Vinyl Chloride Purification

Two distillation columns are used to separate vinyl chloride from EDC, HCl and remaining by-products. The first column, HCl column, distills the hydrogen chloride mixture to a pure overhead product. This HCl is recycled to the oxychlorination reactor. The HCl column consists of 42 trays and operates at a top tray pressure of 135 psig with a column pressure drop of 10 psig. The bottoms product of the HCl column is fed to the second column, the VCM column. The VCM column consists of 20 trays and operates at a top tray pressure of 65 psig with a column pressure drop of 10 psig. A VCM product of 99.9 wt% is produced as the overhead product of the VCM column. The bottoms of the VCM column are recycled to the lights column for re-purification.

3.17 VCM Purification Control and Instrumentation

The HCl column is controlled by a overhead and bottoms control loop. The bottoms control loop utilizes a low select switch control steam flow rate. A differential pressure controller and a composition controller each call for a certain steam flow which ever is the smallest is selected by the low select switch. The differential pressure controller has a set point equal to the maximum tray pressure drop and the composition controller's set point is the desired composition of the bottoms. The overhead control loop utilizes a level controller on the reflux drum to control the reflux ratio. The VCM column is controlled by an overhead and bottoms control loop. The bottoms temperature is controlled by the steam flow rate to the reboiler. In the overhead control loop the level control of the reflux drum is established by the distillate flow rate, reflux ratio is adjusted by the composition controller in order to control distillate composition. See Figure 7 for the oxychlorination P&ID. Appendix A contains corresponding stream and equipment tag numbers and descriptions.

S21

S20

V-103

S49

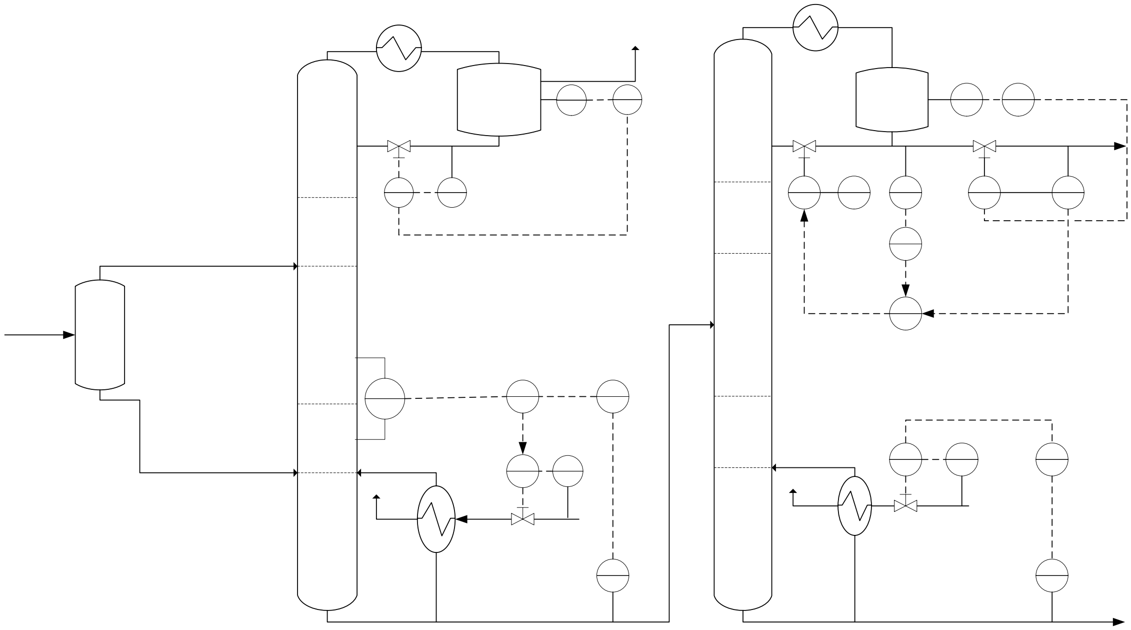

Figure 7: VCM Purification Section

3.18 Heat Integration Design

The vinyl chloride plant process design includes a heat-integrated network. Based on the stream data and the temperature targets that are required for the process a table cascade was constructed to find the minimum utilities. The ΔT_{min} of the system equals 10 ^oF. Table 7 shows the stream data for the vinyl chloride plant. Table 8 presents a table cascade diagram

Table 7: Stream Data

	Stream	Initial T (F)	Target T (F)	T_S*	T_T*	Cp (BTU/lb-F)	m (lb/hr)	F*Cp (Btu/hr-F)
Hot	E1	588	248	583	243	0.2881	5.64E+05	1.62E+05
Cold	E2	316	318	321	323	0.3316	1.99E+06	6.60E+05
Hot	E3	263	90	258	85	0.2363	2.03E+06	4.79E+05
Hot	E4	254	25	249	20	0.2321	1.98E+06	4.59E+05
Cold	Furnace	299	932	304	937	0.285	1.98E+06	5.65E+05
Hot	T2 (Cond)	316	310	311	305	0.3316	3.98E+06	1.32E+06
Cold	T3(Rebolier)	173	197	178	202	0.381	3.75E+06	1.43E+06
Cold	T4(Reboiler)	309	311	314	316	0.334	2.40E+06	8.01E+05

S30

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S32

Table 8: Cascade Table Diagram

Temperature (F)	Δ Hint	Hot Utility (BTU/hr)
937		3.08E+08
	2.00E+08	
583		1.08E+08
	1.05E+08	
323		4.13E+06
	2.12E+06	
321		2.01E+06
	2.01E+06	
316		0.0000
	-9.98E+05	
314		9.97E+05
	9.65E+05	
311		3.28E+04
	-5.60E+06	
305		5.63E+06
	4.02E+05	
304		5.23E+06
	-7.47E+06	
258		1.27E+07
	-5.78E+06	
249		1.84E+07
	-6.61E+06	
243		2.50E+07
	-3.86E+07	
202		6.36E+07
	2.28E+07	
178		4.08E+07
	-8.76E+07	
85		1.28E+08
	-2.99E+07	
		1.58E+08
		Cold Utility (BTU/hr)

From the cascade diagram the minimum hot utility is 308 MMBtu/hr and the minimum cold utility is 158 MMBtu/hr. These utilities include all heat exchangers, furnace, and the heavies columns condenser, HCl column reboiler, and VCM column reboiler. The heavies column pressure was increased from 60 to 80 psig to increase the condenser temperature which then allowed for heat transfer to the HCl and VCM column reboilers. The pinch temperature is equal to 316 ^{o}F. See Appendix B-3 for corresponding grand composite curve of the heat integrated system. The overall energy requirements of the plant, including all equipment, reduced from 1247 to 903 MMBtu/hr for the hot utility and a corresponding reduction of cold utility from 652 MMBtu/hr to 308 MMBtu/hr. Refer to Table B2 in Appendix B for the optimal network design.

Section 4: Waste Treatment

4.1 Vapor and Liquid By-Product Treatment

Many waste by-products are formed during the production of vinyl chloride. These by-products can be very harmful to the environment as well as to human health. Because of this, these by-products must be either eliminated or reduced. It is unreasonable to think that all the by-products can be totally eliminated; they can only be reduced into other compounds. In order to reduce these by-products, a waste treatment method has been implemented.

The by-products formed in the process are found in waste streams arising from EDC Purification and Pyrolysis, as well as the Direct Chlorination Caustic Scrubber, and the Oxychlorination Reactors. These waste streams come in two forms, liquid and vapor. The vapor wastes contain more contaminants than the liquid wastes and this is due to the fact of the high temperatures with which the reactors are run.

Many different treatment techniques that could reduce the by-products are available. These treatment techniques are examined for their technical feasibility in regards to the process. These treatments include condensation, absorption/scrubbing, flaring, and catalytic and thermal incineration. Condensation is the liquefication of contaminants by the use of low temperatures. That is, the compounds to be removed from the gas phase are cooled to a temperature at which their partial pressure in the gas stream surpasses their dew point so that they turn to liquids (8). The liquids are then packaged and are prepared for either selling or disposal. “Flaring is another combustion technique that involves the direct burning of an organic stream in an open flame” (8). Catalytic incineration involves the burning of the by-products using a catalyst. Thermal incineration involves the burning of combustible wastes. After examining each one of these treatments it was found that using one single treatment method would not be sufficient in significantly reducing the waste streams. In fact, other waste streams are created as a result of using the treatments by themselves.

From here it was then decided to implement a treatment method that incorporated a combination of the single treatments. A treatment method that incorporated incineration, absorption, and scrubbing technologies was selected. Figure 8 shows this treatment method.

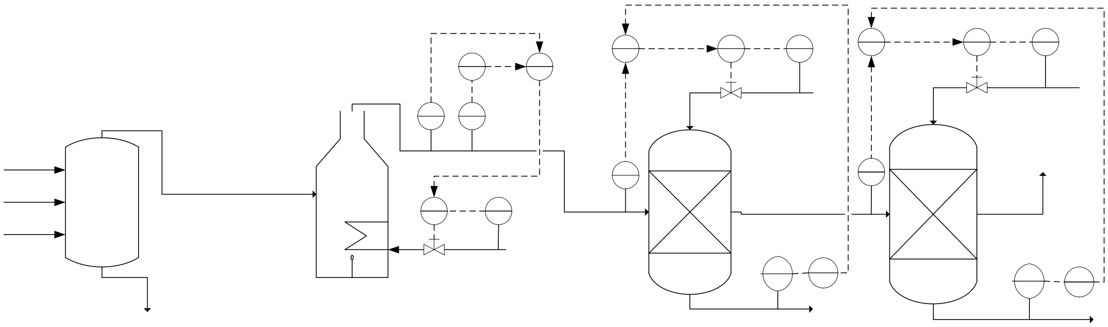

Figure 8: Waste Treatment Section

The first step in this treatment method is to send all the liquid and vapor wastes to the incinerator, where they are all combusted at a temperature of 1127 °C. The organic compounds in the waste streams contain chlorine attached to them. "These elements create complications by adding extra products of combustion" (43). By inspection it was found that carbon dioxide (CO_2), water (H_2O), hydrochloric acid (HCl), chlorine gas (Cl_2), nitrous oxides (NO_x), and chlorooxides (ClO_x) would be formed. A thermodynamic analysis was then performed on all the combustion reactions to determine what actual products would form and be present at equilibrium. From here it was determined that the ClO_x would actually be more prevalent than the Cl_2 and HCl. Although this is true, the ClO_x will not be present after incineration. This is simply because the ClOx is very unstable. Chlorooxides actually dissociate and donate chlorine and oxygen anions. These chlorine and oxygen anions then attach to hydrogen to form the aforementioned HCl and H_2O. Therefore, as a result of the incineration process, CO_2, H_2O, HCl, Cl_2, and NO_x are formed. These products are then sent to an absorption column. This column uses water as a solvent and removes HCl and H_2O from the stream. From here the remaining products are sent to another absorption column, this one using NaOH as the solvent. Here the NaOH removes the Cl_2 and forms a solution of sodium chloride and sodium hypochlorite, which is sold to an industrial bleach production company. The CO_2 is then sent to where it will be sequestered. The NO_x in our system must be accounted for. The NO_x production is very minimal and in fact it is negligible. The NO_x is actually only about 7×10^{-4} percent of the waste streams. Tables 9, 10, and 11 show the design parameters of this waste treatment method.

Table 9: Auxiliary Fuel Needed.

Waste Stream Flow Rate (kg/hr)	Auxiliary Fuel Flowrate O_f (kg/hr)
4596	**150**

Table 10: Column Specifications for Absorption Column

Design Parameters	Values
Solvent Flowrate	**45000 lbs/hr**
Column Diameter	**4.5 ft**
N_{OG}	**12 trays**
H_{OG}	**.83 ft**
Height of Packing	**10 ft**

Table 11: Column Specifications for Caustic Scrubber

Design Parameters	Values
Solvent Flowrate	**154,000 lbs/hr**
Column Diameter	**5.7 ft**
N_{OG}	**20 trays**
H_{OG}	**.75 ft**
Height of Packing	**15 ft**

4.2 Process Water Treatment

The water stream from the water wash drum needs to be treated before it can be disposed. The contaminants of this water stream can be seen in Table 12. The EPA enforces strict regulations for release into the environment. However, the costs associated with obtaining water will be reduced by treating the stream and recycling it back to the system.

Table 12: Water Stream Data

	Water Wash Drum(L/hr)
Water	41,000
NaCl	0
HCl	200
Chloral	26
EDC	680
CCl4	180
TCE	170

All of the chemicals can be removed from the water by adsorption, aeration (air stripping), or by boiling. Since the water is being recycled back to the system the only feasible solution is using adsorption. The EPA considers liquid phase granular activated carbon adsorption the best available control technology. Activated carbon adsorption is often favored because it has the following characteristics:

- The ability to remove more than 99% of contaminants
- Simple design and operation
- No waste by-products requiring costly disposal
- Safe process that has the ability to operate at low pressure and temperature with minimal toxic gases and dangerous chemicals.

The activated carbon treatment system was designed using design equations that can be found in Appendix E. The results for the column are shown in Table 13.

Table 13: Adsorption Column Specifications

Carbon Mass	21000 lb
Adsorber Volume	170 ft3
Adsorber Area	36 ft2
Velocity	7 ft/min
Contact Time	27 min
Equilibrium Saturation	19 days

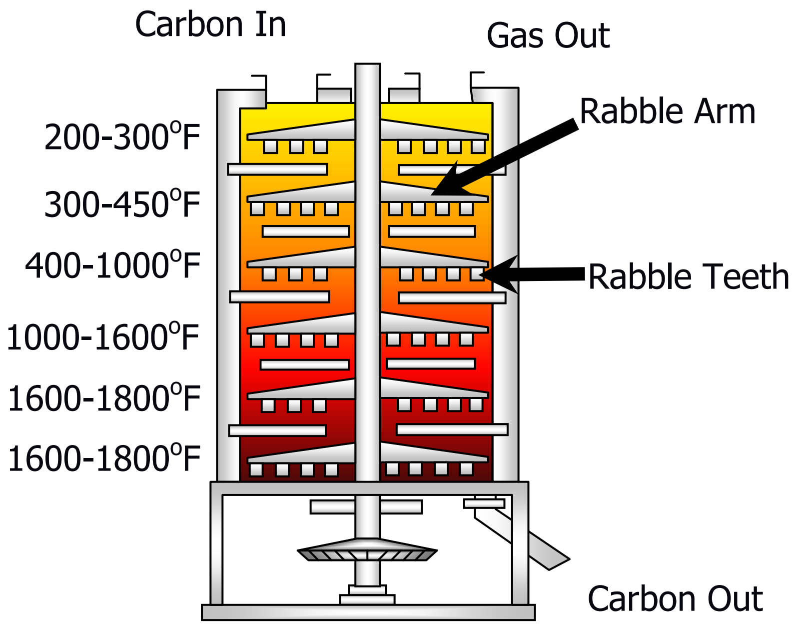

Figure 9: Carbon Regeneration Column

The system was designed to remove 100% of the contaminants.

When the carbon has reached the saturation point (19 days), it will need to be regenerated. Therefore, carbon regeneration column will be installed (see Figure 9). Thermal regeneration is the process of removing adsorbed contaminants in carbon, using thermal desorption and high temperature treatment. The 3 major variables involved are furnace temperature, residence time and carbon loading. Residence time can be changed by varying the rabble arm speed. Hearths 1-2, seen in figure 9, (200-450 ^{o}F) are included for water evaporation and physical desorption of VOCs. Hearth 3 (400-1000 ^{o}F) is included for the pyrolysis of non VOCs and carbonization of residue. Hearths 4 and 6 (1000-1800 ^{o}F) are included for uniform distribution of temperature. Hearth 5 (1600-1800 ^{o}F) is the hearth in which activation occurs.

Section 5: HAZOP

The purpose of HAZOP studies is to reduce the possibility of work related injuries. Due to the processing and handling of hazardous materials, the vinyl chloride plant has many inherent dangers. The first step of the HAZOP study is to subdivide the plant into sections and plan the sequence. The whole process is divided into small sessions. Each session will have one or two major equipment such as flask, column, reactor or heat exchanger. The plant will be divided from upstream to downstream. Secondly, all the deviations were studied to find out all he causes as well as the consequences. Knowing the causes and consequences, additional safety equipment might be added to the plant. All the actions that should be done to improve safety and to guide others in case the problem happens were also suggested. All the details on the HAZOP studies for this VCM plant can be found in appendix C.

Section 6: Plant Location

The plant will be located in Taft, Louisiana. The decision making process utilized a factor rating maximization method. This method takes several attributes of a potential location into consideration when comparing it to other locations. These attributes or factors are ranked according to their importance to the success of the plant. These factors are all placed into the same scale so as to not distort the weight of a factor that inherently has larger values than others.

The factors chosen for this location decision are raw materials, particularly distance between ethylene and chlorine and abundance, total tax rates, including corporate income tax, property tax, and sales tax, wages, utilities, and land cost. All of these attributes have values that can be compared between the different location options.

There are two heuristics that need to be followed in order to obtain the locations that are to be compared.

- It is imperative that the location be within close proximity of ethylene and chlorine. No more than 20 miles, as the resulting transportation costs will substantially reduce the profitability of the VCM plant.
- The ethylene and chlorine plants should be separate from existing VCM plants in order to minimize the effects of competition. This is also an important factor as far as emissions are concerned, simply because more plants in a certain area will decrease the quality of the air in that area.

Applying both heuristics results in two possible locations, Taft, LA, and Corpus Christi, TX. These locations are compared using the above factors. The attributes are given relative weighting factors, which are represented as percentages, adding up to 100%. There are 6 factors considered, thus there are six weighting factors assigned. The highest percentage is 30% and is given to the distance between the ethylene and chlorine locations. This importance is illustrated in the first heuristic. The next highest percentage of 25% is given to the abundance of raw material plants. More raw materials are desirable when considering future expansion. The tax rates are given the next highest percentage of 20%. The tax rates are an important annual cost that becomes significant when applied to the amount of revenue generated from the selling of VCM product. The fourth most important factor is the difference in wages. Wages vary from region to region, and are an ongoing cost associated with operating a plant. Wages are given a weight of 12%. The utility costs are less than the salaries paid to employees, thus the weight percentage given to it is lower, at 8%. Lower, however, does not mean that it will not have a significant impact on the operating cost of the plant if overlooked. The last consideration is the cost of the land in each of the locations. This is least important aspect of the six, and is given the lowest weight of 5%. The land cost does not affect the operating cost, and is merely a one-time cost. All of the other considerations will continually affect the amount of profit that is made.

Each location has a unique value for each of the categories stated above. However, some of these values are different orders of magnitude compared to others. Multiplying the weight percentages by the actual values will give misleading results. For example, the values for land costs in TX and LA are $640 and $1270 per acre, respectively. These are much higher than the values for utilities, which are $3.50 and $3.30 per MMBTU. Therefore, if a minimum value is desired, the land cost will contribute a significantly higher value when multiplied by the weight percentage. This is misleading, because it gives a lot more weight to the land cost over the utility cost which is a much more significant value. In order to make sure that the correct amount of weight is given to each value, the percentages of each value within each factor must be calculated in order to create a situation where all factors are compared on the same scale. For example the percentage value for the land cost in TX is 34%, and the land cost in LA is 66%. These percentages can be used, because they represent the value as it is related to the other value. There is however, one drawback of using the relative percentages. This occurs when the values are not necessarily better if they are lower. A lower land cost is more desirable than a higher land cost, however being located near three chlorine plants is more beneficial than being located near only 1. It is for this reason that the raw material abundance factor must be treated differently. These percentage values must be switched. Therefore, if the number of chlorine plants near Taft, LA is 3, and the number of chlorine plants near Corpus Christi, TX is 1, then the percentage values for this factor are 75% and 25%, respectively. However this shows an advantage to the location with less chlorine plants in close proximity, so the results are not accurate. Thus, the percentages need to be switched, so the 75% will be assigned to Taft, LA, and 25% will be assigned to Corpus Christi, TX. All aspects are now on the same scale and are ready to be summed into one value. The lowest value will provide the location that will provide the most profitable environment. Table 14 below shows both locations' values for each factor.

Table 14: Table of values and factor ratings used for plant location.

Factor	Weight %	Taft, LA			Corpus Christi, TX		
		Value	%	Factor Value	Value	%	Factor Value
Raw Materials							
Distance (miles)	30	3	0.15	0.045	17	0.85	0.255
# Plants	25						
Chlorine		3	0.25	0.063	1	0.75	0.188
Ethylene		1	0.50	0.125	1	0.50	0.125
Taxes	20						
Corporate Income (%)		8	1.00	0.200	0	0.00	0.000
Sales		4	0.39	0.078	6.25	0.61	0.122
Property		25	0.42	0.085	34	0.58	0.115
Wages	12	0.95	0.48	0.058	1.03	0.52	0.062
Utilities ($/MMBTU)	8	3.5	0.51	0.041	3.3	0.49	0.039
Land ($/acre)	5	1270	0.66	0.033	640	0.34	0.017
			Total	**0.727**		**Total**	**0.923**

The lowest total factor value represents the location with the most potential for a profitable environment. In this case Taft, LA will be the location of the environmentally safe vinyl chloride plant.

Section 7: Risk Analysis and Probability

Predicting how long the project will last, how much it costs, or how much it profits is almost impossible, and a single point study can be dangerously misleading. Risk analysis using Monte- Carlo simulation can answer question such as: "How confidence are we that profits will be more than three million dollars?" or "What are the chances that this specific plant capacity will end up losing money?". In this specific project, the objective of doing risk analysis is to choose a plant capacity that has the highest net present worth and lowest chance of losing money. Three different plant capacities: 4.09 billion, 6.44 billion and 10.5 billion VCM production per year were studied. Forecasting prices for raw materials as hydrogen chloride, chlorine, oxygen and product vinyl chloride monomer was carried out to predict the prices for the future years. Then economic and risk analysis was done on all three to choose the most reliable and beneficial capacity for the plant.

7.1 Forecasting of Prices

Prices for the previous 20 years were taken into consideration for forecasting. The changes in prices for these materials are all increasing. The trend of chlorine can be seen in Figure 10.

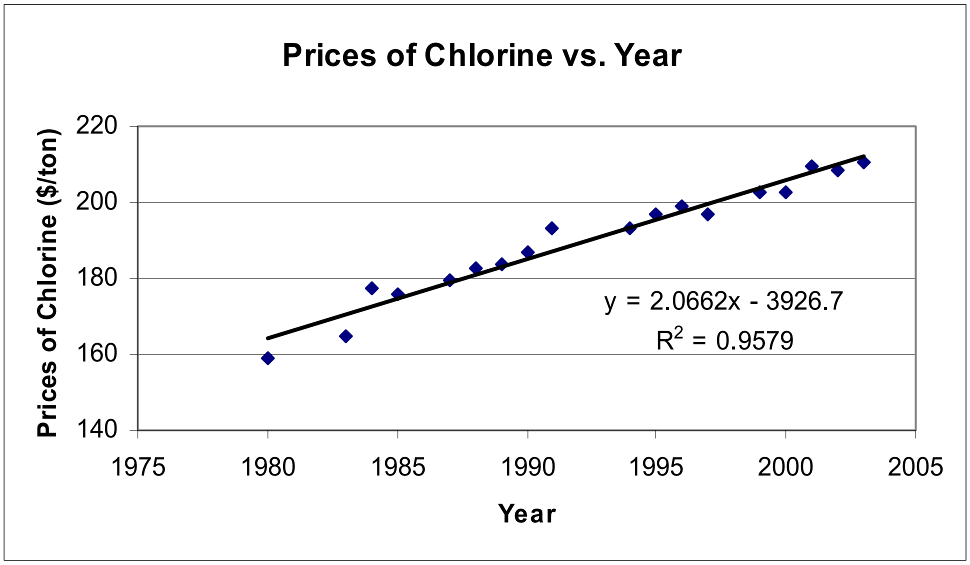

Figure 10: Trend in changing chlorine price

From the chart, the price of chlorine was found to have a linear relationship with the year. The mean of this graph was extended in order to predict future prices. However, merely using the mean values of the plot is not sufficient, so the prices were estimated by generating random numbers of the mean and standard deviation. Nearly one thousand cases were evaluated, with each giving different prices of the raw materials and product.

Prices for 2004-2011 were calculated to range from \$212 to \$225/ton. The same method was performed to forecast the prices of ethylene, oxygen and vinyl chloride. All the forecasted values are shown in table 15. These values will be used as the base values for doing economic analysis and risk analysis.

Table 15: Forecasted prices of raw materials product

Year	Ethylene \$/ton	Chlorine \$/ton	Oxygen \$/ft3	VCM \$/ton
2004	492.55	212.21	0.00144	499.19
2005	499.39	214.14	0.00144	506.19
2006	506.22	216.07	0.00143	513.18
2007	513.06	218.00	0.00142	520.18
2008	519.90	219.93	0.00141	527.18
2009	526.73	221.86	0.00140	529.17
2010	533.57	223.79	0.00139	535.17
2011	540.41	225.72	0.00138	543.17
Std. Dev	24.17	10.56	0.00010	26.15

7.2 Brief Economic Analysis

A brief economic analysis was done for the aforementioned capacities with a project lifetime of 20 years. For this general analysis, most of the components of total product cost (i.e. direct cost, fixed charges, overhead costs, and general expenses) were based on the percentages given in Peter and Timmerhaus (16). A more detailed analysis will be discussed for the chosen plant capacity in the section 8.

Table 16: Economic results for different capacities

Plant Capacity	4.09E9 lb/yr	6.44E9 lb/yr	1.05E10 lb/yr
TCI	\$47,110,219	\$68,886,317	\$77,154,892
NPW	\$133,739,890	\$284,828,289	\$161,759,443
ROI	0.24	0.25	0.20

The total capital investment is proportional to the plant capacity. As plant capacity increases, costs in all areas increase, which causes the total capital cost to increase. However, the net present worth and rate of return on investment reach a maximum at a plant capacity of 6.44 billion lb/yr. The net present worth and rate of return on investment are criteria, which is used to determine which capacity is the best.

7.3 Risk Analysis and Probability

The steps for the risk analysis are shown in the following figure:

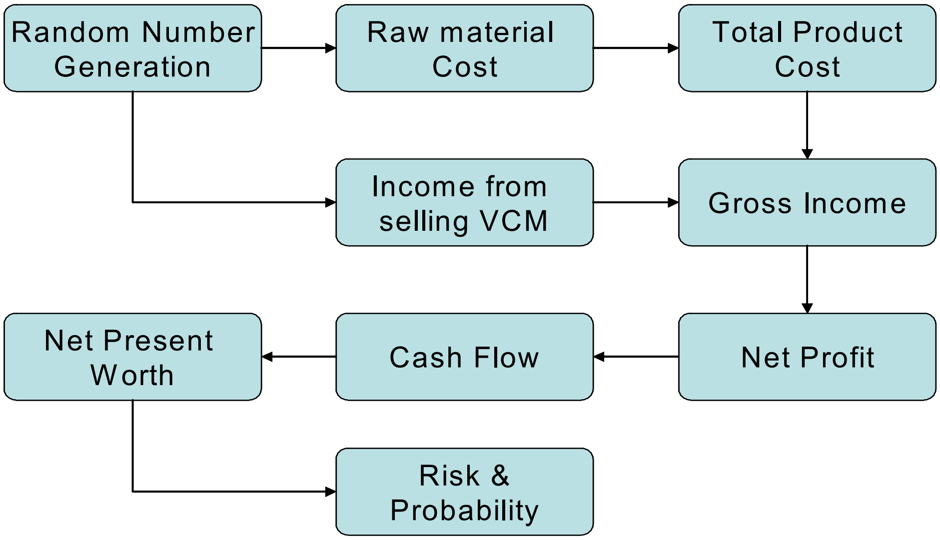

Figure 11: Procedure of Risk Analysis

Gross income depends on the total production cost and income from selling vinyl chloride. The amount of raw materials and VCM production for each year is different for different years until the demand meets maximum capacity of the plant. Therefore, the cost and income are different for each plant capacity. The detailed flow rates are shown in table 17.

Table 17: Flow rates of raw materials and VCM for different years

Year	Ethylene Lb-mol/hr	Chlorine lb-mol/hr	Ethylene lb-mol/hr	Oxygen lb-mol/hr	VCM lb-mol/hr
2004	2700	2690	2700	1350	3602
2005	4200	4190	4200	2100	5521
2006	5600	5590	5600	2800	7355
2007	7400	7390	7400	3700	9551
2008	9050	9040	9050	4525	11888
2009	10800	10790	10800	5400	14322
2010	12750	12740	12750	6375	16535
2011	14700	14690	14700	7350	18972

Net present worth is calculated based on cash flow method, which uses the following equation:

$$NPW = \sum_{k=1}^{n-1} \frac{CF_k}{(1+i)^k} + \frac{CF_n + V_S + I_W}{(1+i)^n} - TCI$$

Eqn. (18)

From approximately a thousand trials, the probability of having the net present worth at a specific value can be calculated. Figure 12 shows the probabilities of different net present worth for three different capacities. A plant capacity of 10.5 billion lbs/year shows a high probability of having positive net present worth, but it also shows a high probability of having negative net present worth. It will be very risky if this option is chosen. The probability of making money with a plant capacity of 4.09 billion lbs/year is lower than the probability of losing money. This is illustrated in the Figure 12. A plant capacity of 6.44 billion lbs/yr shows the most preferred probability function, which has a high chance of making money and a low chance of losing money.

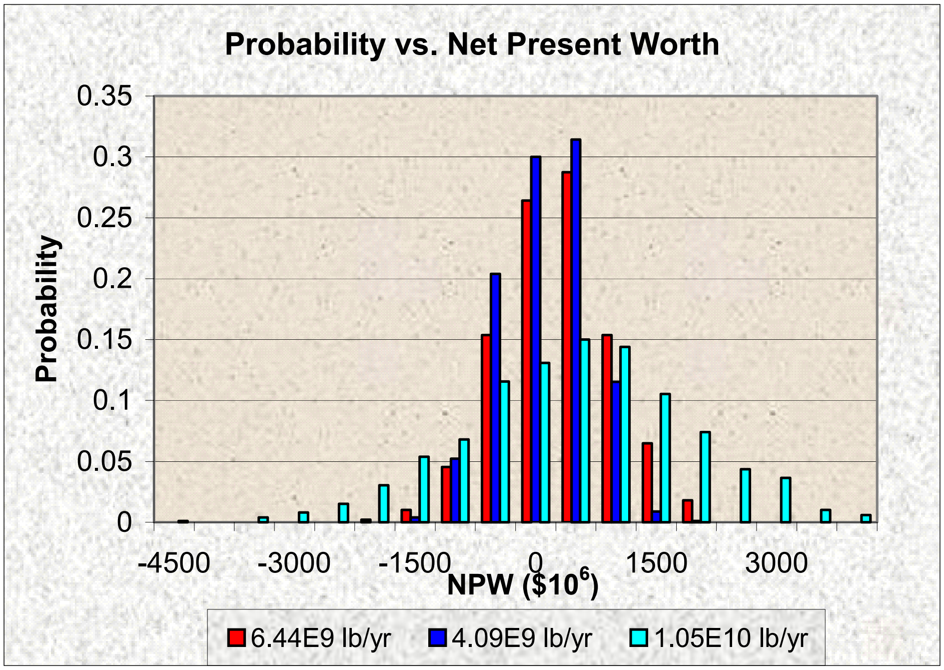

Figure 12: Probability vs. NPW for three different capacities

The risk curves are also constructed using the net present worth values that were calculated. The risk curves show a 36% chance of losing money for the 10.5 billion lbs/year capacity, 31.7% for the 6.44 billion lbs/yr capacity and 41% chance for the 4.09 billion lbs/year capacity. The 6.44 billion lbs/yr curve is the most preferred capacity since it has the lowest risk. See Figure 13 for the associated risk at different plant capacitates.

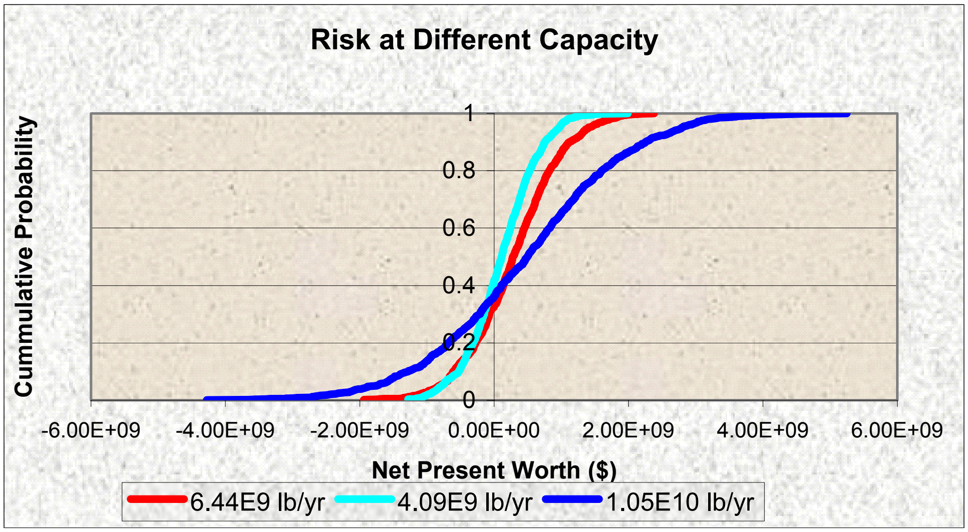

Figure 13: Risk of different capacities

7.4 Plant Capacity Selection

Economics in addition to probability and risk analysis showed that the plant capacity of 6.44 billion pounds of VCM per year is the best one. It has the highest net present worth of $286 million, highest rate of return of 0.25 and lowest risk of losing money, 31.7%.

Section 8: Economic Analysis

The total plant cost was approximated from the total capital investment, total product cost, and environmental cost. The capital investment from the total equipment cost was found using the "Ratio Factor" method described in Peters and Timmerhaus (16). The production cost is the cost associated with plant operation. The environmental cost includes installing and running the incineration unit and the adsorption system. The total equipment cost for the capacity of 6.4 billion pounds per year was found to be $15.3 million, with a total capital investment of $69.85 million. The plant has the potential to make profit of up to $26.2 million/year in the next five years. The net present worth associated with this plant was found to be around $265 million with a rate of return of 24 percent.

8.1 Equipment Cost

The major equipment for this plant consists of four heat exchangers, four distillation towers, seven flash tanks, three reactors, two carbon adsorption columns, regeneration unit, incineration unit, absorption column, and a scrubbing column. The equipment price values were determined using the flow rate, capacities, diameter, and surface area to purchase cost found in Peters and Timmerhaus.

For the heat exchangers, the overall heat transfer area (U) was assumed from the hot or cold fluid used for each heat exchanger (16). Using the duty and log-mean temperature difference; the surface area for each heat exchanger was determined.

Table 18: Heat Exchanger Cost

Heat Exchangers							
Heat Exchangers	Cooling/Heating	LMTD (F)	U (Btu/h*ft^2*F)	Duty	Area (ft^2)	Cost ($) 1990	Cost ($) 2003
E1	Cooling	866.45	112	70.67	728.24	9,000	10,260
E2	Cooling	756.27	112	196.23	2316.70	19,000	21,660
E3	Cooling	632.34	112	312.45	4411.76	28,000	31,920
E4	Cooling	592.17	112	392.84	5923.13	35,000	39,900
						91,000	**103,740**

Using the graph of surface area to purchased cost from figure 15-16 in P&T, the cost of the heat exchangers was estimated (16). However, these prices are not current; therefore to update the price, the Marshall and Swift index values were used. As shown in the table 18, the cost of the heat exchangers for year 2003 was found to be $103,740.

Using the correlation of column diameter to cost per tray from figure 16-25 in P&T, the cost of trays in the distillation tower (including installation cost) was estimated. The total cost of the towers was found to be around $3.6 million.

Table 19: Distillation Tower Cost

Distillation Towers						
Tower	Number of Trays	Diameter (in.)	Diameter (ft.)	Cost/Tray	Cost ($) 1990	Cost ($) 2003
T1	15	234	19.5	13000	195,000	222,300
T2	28	324	27	50000	1,400,000	1,596,000
T3	40	264	22	30000	1,200,000	1,368,000
T4	18	216	18	20000	360,000	410,400
					3,155,000	**3,596,700**

The capacities of the flash tanks were obtained from the flow rates. To estimate the cost of the flash tank, the correlation of flow rates to purchase cost from figure 14-56 in P&T was used. The total cost of the flash tanks for 2003 was around $230 thousand.

Table 20: Flash Tank Cost

Flash Tanks							
Tanks	Inlet (ft^3/hr)	Residence Time (hrs)	Capacity (gallons)	Cost ($)1990	Vapor Rate(ft^3/hr)	Liquid Rate (ft^3/hr)	Cost ($) 2003
F1	911.58	0.24	1636	7000	386.525	1.586	7980
F2	301.37	0.24	541	4000	3363.366	284.587	4560
F3	14763.59	0.24	26504	35000	2362.634	13400.93	39900
F4	6073.89	0.24	10904	21000	6092.577	5057.013	23940
F5	2553.39	0.24	4584	16000	12553.337	0	18240
F6	27564.94	0.24	49485	59000	2858.02	26174.15	67260
F7	30820.93	0.24	55330	60000	0	31242.7	68400
				202000			**230,280**

For reactor sizing, both oxy-chlorination and direct chlorination reactors were treated as plug flow tubular reactors (PFTR). Plug flow tubular reactors can be considered shell and tube heat exchangers. The overall heat transfer area (U) was assumed from the hot or cold fluid used for each reactor. Using the duty and log-mean temperature difference (from pro II), the surface area for each reactor was determined. The cost of these reactors was determined using the correlation of surface area to purchase cost.

Table 21: Reactors Cost

Reactors					
Types	**Output Stream**	**Residence Time**	**Capacity**	**Cost (\$) (1990)**	**Cost (\$) (2003)**
DC	3444.032	0.0178	458.5522	27000	30780
OC	3737.495	0.243	6793.4204	110000	125400
Duty (MM Kcal/hr)				9.12E+06	10,396800
Cracking	159.6			**9257000**	**10,552,980**

The third reactor, known as cracking reactor, was treated like a furnace. From the duty (from pro II) of the reactor, the cost of the reactor was estimated. As shown in the table 21, the cost of the towers was found to be around \$10.5 million.

8.2 Waste Treatment Units

The environmental costs include all of the costs associated with removing toxic contaminants from the waste streams that are released to the environment. These costs are necessary because the EPA regulates the chemicals that can be harmful to humans. The cost of the adsorption column was determined using capacity to price correlation. Adding all the equipments, the total equipment cost was found to be a \$15.3 million. The possible uncertainties in estimating the price of equipments were (+/-) 5 %.

Table 22: Adsorption System and Incineration Unit Cost

Adsorption System			Incineration Unit		
Capacity (gallons)	**Cost (\$) 1990**	**Cost (\$) 2003**	**Capacity (\$) m^3/hr**	**Cost(\$) 1990**	**Cost (\$) 2003**
1279.52	550,000	660000	25.2	117000	140400

8.3 Total Capital Investment

A large sum of money must be supplied to purchase and install the equipment. Capital investment estimation is necessary to estimate necessary investment for the vinyl chloride plant. The total capital consists of fixed-capital investment and working capital.

Table 23: Total Capital Investment

Total Capital Investment		
Total Equipment Cost		**\$15,284,100**
Variables	**Description**	**Cost (\$)**
Equipment Installed	47% of TEC (P&T)	7,183,527
Incineration Unit (install)	Flow Rate Correlation	10,500
Instrumentation & Control	18% of TEC (P&T)	2,751,138
Piping (installed)	50% of TEC (P&T)	7,642,050
Electrical (installed)	11% of TEC (P&T)	1,681,251
Total		**19,268,466**
Building Cost		
Office	\$45/ft^2 (Brick Building) in 3000 ft^2	135,000
Process Building (5-Unit)	\$15/ ft^2 (Steel Building)in 4500 ft^2/Unit	375,000
Service Building	\$45/ ft^2 (Brick Building) in 2000 ft^2	90,000
Storage Building	\$15/ ft^2 (Steel Building)in 4000 ft^2/Unit	62,500
Maintenance Unit/Shop	\$45/ ft^2 (Brick Building) in 1500 ft^2	67,500
Administration/Accounting	\$45/ ft^2 (Brick Building) in 2500 ft^2	112,500
Environment/Research	\$45/ ft^2 (Brick Building) in 3000 ft^2	135,000
Total		**977,500**
Yard Improvement		
Site Cleaning	\$4400/acre (total of 50 acres)	220,000
Grading	\$465/acre (total of 10 acres)	4,650
Fencing	\$9/ft (total of 9000 ft)	81,000
Walkways	\$4.50/ ft^2 (total of 5000 ft^2)	22,500
Total		**328,150**
Land Cost	\$1270/acre (total of 50 acres)	**63,500**
Total Direct Plant Cost		**35,921,716**
Engineering & Supervision	32% of TEC (P&T)	4,890,912
Construction Expenses	41% of TEC (P&T)	6,266,481
Contractor's Fee	21% of TEC (P&T)	3,209,661
Contingency	42% of TEC (P&T)	6,419,322
Total Indirect Cost		**20,786,376**
Working Capital	86% of TEC (P&T)	**13,144,326**
Total Capital Investment	Direct+Indirect+Working Capital	**69,852,418**

For this vinyl chloride plant, the total capital cost was determined by applying the factor estimation (“Ratio Factor”) method described in Peters and Timmerhaus (16). However, these factors were altered based on our plant capacity. As shown in table 20, the building construction, yard improvement and land costs were determined based on our plant capacity. The costs associated with the building were found to be around \$977 thousand dollars. The total capital investment for our plant was estimated to be \$69.8 million. The possible accuracy for estimating capital investment was (+/-) 15 % when using this method.

8.4 Total Product Cost

The operating cost and revenue generated from products are the most important aspects of running a plant. These costs are grouped under total product cost, which in turn is divided into manufacturing cost and general cost. The manufacturing cost consists of direct product cost, fixed cost and plant overhead cost. The general expenses include administrative expenses, distribution and marketing expenses, and quality control cost. The table below shows the cost associated with total product cost.

8.5 Direct Product Cost

The direct product cost includes the cost of raw materials, operating labor, direct supervisory and clerical, utilities, maintenance and repairs, and operating supplies.

For any plant, operating labor cost contributes a major portion to the total product cost. In table 24, the detailed cost associated with the specific types of labor is shown. These values are obtained from taking an average of the individual salaries, which were determined by the U.S. Department of Labor. It should be noted that all non-essential laborers (e.g. janitors, security officers, etc.) were excluded in the determination of the average salaries. The total labor cost for our plant was found to be $5.14 million per year.

Table 24: Operating Labor Cost

Employee	# of Employee	$/yr	Total ($/yr)
Plant Chairman	1	105000	105000
Managers			
Plant Manager	1	80000	80000
Unit Managers	5	73000	365000
Operational Engineers			
Computer Programmer	1	62890	62890
Computer Engineer	2	74310	148620
Chemical Engineers	5	72780	363900
Process Engineers	5	73000	365000
Electrical Engineers	3	68630	205890
Environment Engineers	3	62000	186000
Industrial Engineers	3	61900	185700
Mechanical Engineers	2	63500	127000
Maintenance Engineers	2	30000	60000
Operator	30	68000	2040000
Supervisor	5	70000	350000
Administration			
Financial Manager	1	60000	60000
Production Manager	1	68000	68000
Sales Manager	1	60000	60000
Accounting			
Budget Analysts	2	53000	106000
Financial Analysts	1	62000	62000
Tax Prepares	2	33000	66000
Auditor	2	35000	70000
Total			**5,137,000**

Another major cost associated in estimating direct product cost is the cost associated with utilities. The cost of utilities, such as steam (for hot utility) and cooling water (for cold utility) depends on the plant capacity and raw material consumption. The price of the hot utility depends upon the price of natural gas. The price of the hot and cold utility was found to be \$3.3/MMBTU and \$0.5/MMBTU, respectively. As shown in Table 25, the overall utility cost was found to be \$20.5 million per year. To maintain the efficiency of the plant, regular maintenance and repair is necessary. Assuming 2% of the fixed capital investment (P&T), the maintenance and repair cost was found to be around \$1.1 million per year. The operating cost for our plant was estimated to be \$170 thousand dollars per year.

Table 25: Net Profit

Summary of Annual Costs along with the Total Product Cost (2008)			
		Working Capital	**\$13,144,326**
		Fix Capital Investment (\$)	**\$56,708,092**
		Total Capital Investment (\$)	**\$69,852,418**
	Manufacturing Cost	**Assumption**	**\$/yr**
	Direct Product Cost	**Assumption**	**\$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Carbon, Methane	1,553,971,400
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	\$3/MMBTU heating, 930 MMBTU/hr	19,154,400
	Cold Utility	\$0.5/MMBTU/cooling, 448 MMBTU/hr	1,492,378
4	Maintenance and Repair	2% of Fixed Capital Investment	1,134,162
5	Operating Supplies	15% of Cost for Maintenance and Repair	170,124
	Sub Total		**1,581,059,464**
	Fix Charges	**Assumption**	**\$/yr**
1	Capital Cost or Depreciation	Sinking Fund Method for Project life to be 20 yrs	3,155,987
2	Local Taxes	1% of Fix Capital Investment	567,081
3	Insurance	0.8% of Fix Capital Investment	453,665
	Sub Total		**4,176,733**
	Overhead Costs	40% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**1,587,290,996**
	General Expenses	**Assumption**	**\$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	1,581,059
	Sub Total		**2,351,609**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**1,589,642,606**
Gross Income			
		Assumptions	**\$/yr**
1	Selling Price of Vinyl Chloride	\$527/ton, 11888 lb-mol/hr, 24 hr/day, 365 days/yr	1,631,006,997
	Gross Income (G)	Selling Price - Total Production Cost	**41,364,391**
Net Profit (P)			
		Assumption	**dollars (\$)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of F	**1,629,249**
2	**Net Profit (P)**	G-D-(G-D)*tax	**26,225,194**
	Annual Cash Flow	Cash flow for the first year	**27,854,443**
3	**Net Present Worth (NPW)**	Function of cash flow, TCI, working capital	**265,926,784**
5	**Paid Out Time (POT)**	FCI-Salvage value/Average Cash Flow	**1.83**
6	**Rate of Return (ROI)**	Cash flow method	**0.238**

8.6 Fixed Cost

Regardless of whether manufacturing processes are under operating conditions or not, certain expenses are always associated with any existing plant. This cost is called the fixed cost. The cost associated with fixed charges includes: depreciation, local taxes and insurance. These costs represent a percentage of the capital investment. The depreciation was determined using the sinking-fund method for a project life of twenty years. As shown in Table 25, the fixed costs were estimated to be $4.2 million per year.

8.7 Overhead Cost

Other expenses required for plant operation include overhead costs. These costs include safety services, non-manufacturing machineries, interplant communications, transportation, and shipping and receiving facilities. Assuming the overhead cost to be 40% of the total operating labor, which includes supervision and maintenance, the plant overhead cost was found to be $2.05 million per year.

8.8 General Expenses

General expenses include administration cost, distribution and marketing cost, and quality control cost. The administration cost includes salaries and wages for administrators, accountants, secretaries, typists, office supplies and outside communications. The distribution and marketing cost is the cost associated with selling the products. The sum total of all the above costs comes out to be $2.3 million per year.

Summing the total manufacturing cost and general expenses, the total product cost was estimated to be $1.59 billion per year. The approximate accuracy for estimating the total product cost was up to (+/-) 15 %. However, alternative methods for cost calculation should be taken into account to verify our result.

8.9 Total Net Profit

Net profit is a function of gross income, depreciation and taxes. Using the price mentioned in Table 25, the selling price of the product was found to be $1.6 billion per year. Subtracting the total product cost from the selling price, the gross profit was estimated to be $41.4 million per year. Taking depreciation and taxes from the gross income, the net profit for vinyl chloride plant was estimated to be $26.2 million per year.

To analyze the profitability, the net present worth, pay out time, and rate of return was evaluated. Assuming the project life is for twenty years, and interest rate to be five percent, the net present value was estimated using equation 18. For a capacity of 6.4 billion pound per year, the net present worth of the plant was calculated to be $2.66 billion with a pay of time of 2 years. Thus, this project is considered to be profitable.

The rate of return can be found based on the following equation:

$$TCI = \sum_{k=1}^{n} CF_k (1+r)^{-k} + (V_s + I_w)(1+r)^{-n} \qquad \text{Eqn. (19)}$$

TCI= total capital investment
CF= cash flow

Vs= salvage value
R= rate of return

The rate of return on investment was determined using discounted cash flow method. Using above equation the rate of return on investment for the capacity of 6.4 billion pound per year was found to be 23.7%.

Table 26: Economic Uncertainties

Cost Uncertainties	Percent
Total Equipment Cost	+/-5
Total Capital Investment	+/-10
Total Product Cost	+/-15
Environment Cost	+/-15

Table 26 estimates the uncertainties involved in calculating economics. The error associated for equipment cost will most likely be contributed to human error, which is likely to be (+/-) 5%. Since the total product cost is a function of total capital investment, the error associated with this cost was (+/-) 15%.

Section 9: The Environmental Impact Effect on Profit

Traditionally, cost optimization has been the most important aspect of plant design, however, due to an increase in environmental awareness, plant design should minimize or completely eliminate the production of waste material. Designing a plant with minimal environmental effects costs more money than merely designing a VCM plant with no regard for the environment. In order to study the effects of environmental impact on the profit, there must be a tool to quantify it. The Waste Reduction Algorithm (WAR) algorithm is the tool employed to quantify the environmental impact. K.S. Telang of the University of Louisiana developed the WAR algorithm in 1998. The WAR algorithm is used to study the effects of environmental impact on profit.

The WAR algorithm is based on the pollution index methodology of the Environmental Protection Agency (EPA). This methodology defines pollution indices that can be used to compare different plant designs. Variations in furnace temperature and variations in oxygen and air usage will provide the different plant designs needed for comparison. There will be a cost associated with each variation; this cost will be subtracted from the amount of profit, calculated to be \$27.5 million.

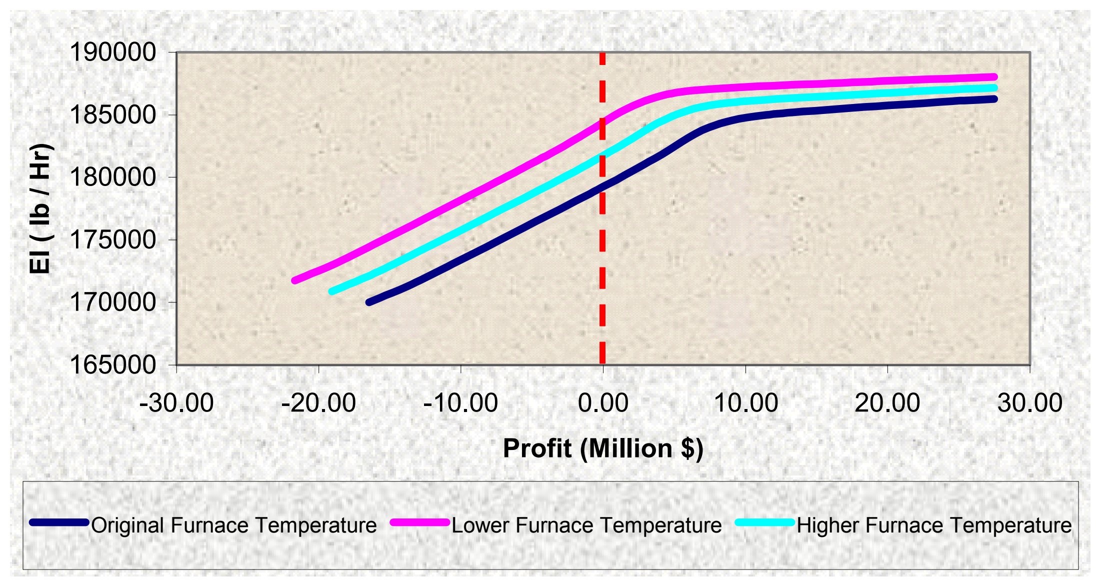

Figure 14: Profit vs. E.I. for three furnace temperatures

The first set of environmental impacts was calculated using a furnace temperature of 500°C; the furnace is the unit that cracks EDC into VCM. There are three areas that oxygen can be used in order to lower the amount of nitrous oxide emissions, the incineration unit, the furnace, and the combustion of methane for hot utility use. Each area uses a different amount of natural gas in order to perform its function. The natural gas combustion reaction produces carbon dioxide. However, if the oxygen used in the combustion reaction comes from an air stream, nitrous oxides are also formed. The environmental impact of these two pollutants can be assessed for each variation in design. Thus, the amount of oxygen used and the temperature specified have a cost associated with them, and this cost is the manipulated variable. The dependent variable is the environmental impact. A graph can be produced from the environmental impact and the cost associated with that environmental impact, which can be seen in Figure 14.

There are eight points that make up each line. These points are presented in table 23. The values for the other temperatures can be seen in Appendix I.

Table 23: Environmental impact parameters

Oxygen Used					
Incinerator	Furnace	Hot Utility	O_2 Cost ($/hr)	Profit ($million)	E.I.
-	-	-	0	27.5	186300
X	-	-	458	23.5	186000
-	X	-	1833	11.4	183000
X	X	-	2290	7.4	180500
-	-	X	2725	3.6	178000
X	-	X	3183	-0.4	175000
-	X	X	4558	-12.5	172300
X	X	X	5016	-16.5	170000

The points with the highest environmental impact, closer to the top of table 23, are represented in figure 13 as the furthest points to the right. This data only represents the original furnace temperature data.

In order to calculate the E.I. seen in table 23, the mass flow rates of all of the components must be known, as well as their respective environmental impact potentials. The environmental impact potentials include acidification factors, global warming potentials, and ozone-depletion potentials. The equation used to calculate the E.I. can be seen below.

$$I_i = \sum_j M_j^{(i)} \sum_k x_{kj} \psi_k \qquad \text{Eqn. (20)}$$

Where I_i is the total impact flow in the input or output, Mj is the mass flow rate of the stream j, and x_{kj} is the mass fraction of chemical k in that stream. Ψ_k is the characteristic potential impact of chemical k. The total E.I. is in units of lb impact/time, which for this case will be lb impact/hr.

The WAR algorithm is a tool used to quantify the E.I. of different designs. The design variations include change in furnace temperature, and change in oxygen usage. These changes in design do not produce enough change to implement them. This is due mainly to the fact that the only potentially harmful compounds are carbon dioxide and nitrogen oxides. They are emitted in abundance when fuel is gas is burned in the furnace, incinerator, and for the hot utilities. The nitrogen oxides are essentially the component that is being removed. As can be seen in the figure, a lot of capital is required per year, which significantly reduces the amount of profit earned. It is not financially reasonable to change the temperature in order to reduce the amount of environmental impact; it is also not reasonable to increase the amount of oxygen used in the system. Another method for reducing the amount of environmental impact is required.

Sequestering CO_2 was evaluated in order to determine if it could be employed to reduce the amount of environmental impact. Whereas variation in design, the method studied previously, merely lowered the amount of emissions, sequestration will eliminate the impact totally.

The idea behind sequestration is to help reduce increasing CO_2 concentrations in the atmosphere by placing them in into other mediums. Enhanced Oil Recovery (EOR) and brine aquifers are two applications of sequestration. EOR is a process that pumps CO_2 into an existing oil well, in order to increase production by increasing pressure. This method has the advantage of being able to increase revenue by selling the CO_2, but the operating costs of liquefying, must be liquefied for transportation, are higher than the revenue gained. This creates a need for another system for eliminating CO_2 emissions from our plant.

Brine aquifers are located beneath the shale layer of the earth. These layers are beneath the oil reservoirs, and those are beneath the potable water layer. The depth of the brine aquifer in Taft, LA is approximately 3100 ft. At this depth, the CO_2 needs to be at a pressure of 1000 psi at the wellhead, which will allow it to be the required 2000 psi when it reaches the brine aquifer. The capital associated with sequestration is a function of flow rate. The capital investment required for injected the CO_2 emissions into the brine aquifers is $11.4 million dollars. This will increase the total capital investment of the plant to $26.7 million. The operating cost of this injection system is $116,000/yr. This will not significantly reduce the total net profit of the project, as the profit is $26 million dollars. This is most cost efficient method for disposing of CO_2. The calculations are shown in Appendix J.

Section 10: Conclusion

This project presents the design of a vinyl chloride plant with a capacity of 6.4 billion pounds per year located in Taft, LA. The capacity of the plant is based on comparing several different capacities' return on investment and net present worth. Applying different trends to the historical demand data allowed for the prediction of the capacities. The vinyl chloride product is 99.8 mol% pure, this composition allows for polymer feedstock applications. The total capital investment for the plant is $65.1 million. The plant produces a total net profit of $27.5 million per year. Extensive Monte Carlo simulations show that a 6.4 billion pound capacity has a 68% chance of having a positive net present worth. A major focus of the design is to maximize safety and minimize environmental impact while maintaining profitability. The VCM plant produces a number of by-products resulting in eight waste streams. The Clean Air and Clean Water Acts, enforced by the Environmental Protection Agency, regulate the procedure by which we dispose of the different waste streams. An integrated waste treatment system utilizing incineration, absorption, caustic scrubbing and activated carbon adsorption is developed in order to avoid releasing any hazardous waste into the environment. The total capital investment of the waste treatment system is $667,000. The increase in environmental awareness increases the total equipment cost from $14.5 million to $15.28 million, and decreases the total net profit per year to $26.2 million.

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APPENDIX A

Table A1. Stream Definitions for P&ID figures

Stream	Description	Stream	Description
S1	Ethylene	S37	HCl Feed to Oxy Reactor
S2	Chlorine	S38	NaCl Solution
S3	Ethylene	S39	Purified Water
S4	Oxygen	S40	Vapor Waste
S5	DC Reactor Effluent	S41	EDC Recycle
S6	Oxy Reactor Effluent	S42	Incinerator Flue gas
S7	DC Product	S43	Water
S8	Oxy Caustic Wash Effluent	S44	CO2 + Cl2 + Nox
S9	Oxy Caustic Wash Effluent	S45	Water & HCl
S10	Oxy Product	S46	Caustic Solution
S11	Vent	S47	Vapor Emissions
S12	Water	S48	NaCl Solution
S13	Water Wash Vent	S49	Furnace Feed Purge
S14	Water Decant	S50	Cooling Water
S15	EDC Purification Feed	S51	Cooling Water Return
S16	Light Ends	S52	Cooling Water
S17	EDC minus light ends	S53	Cooling Water Return
S18	Purified EDC	S54	Caustic Solution
S19	Heavy Ends	S55	NaCl Solution
S20	Purified EDC (vapor)	S56	Caustic Solution
S21	Cracking Furnace Feed	S57	NaCl Solution
S22	Furnace Effluent	S58	Cooling Water
S23	Furnace Effluent Quech	S59	Cooling Water Return
S24	Quench Bottoms	S60	Steam
S25	Quench Product	S61	Condensate
S26	Overhead Quench Product	S62	Furnace Fuel
S27	Quench Bottoms	S63	Cooling Water
S28	Quench Purge	S64	Cooling Water Return
S29	Quench Recycle	S65	Cooling Water
S30	VCM Purification Feed	S66	Cooling Water Return
S31	VCM Purification Feed (vapor)	S67	Steam
S32	VCM Purification Feed (liquid)	S68	Condensate
S33	HCl Recycle	S69	Steam
S34	VCM minus HCl	S70	Condensate
S35	VCM Prdouct	S71	Incinerator Fuel
S36	EDC Recycle		

Table A2. Equipment Definitions for P&ID figures

Tag Number	Equipment	Equipment Description
R-100	Direct Chlorination Reactor	PFTR, cooling fluid flowing shell side, ferric chloride catalyst
R-200	Oxychlorination Reactor	PFTR, cooling fluid flowing shell side, cupric chloride catalyst
F-100	EDC Cracking Furnace	furnace with tubes in radiation section
V-100	DC Caustic Scrubber	HCL is absorbed by NaOH, random packing used
V-101	Oxy Caustic Scrubber	HCL is absorbed by NaOH, random packing used
V-102	Oxy Flash	Used to separate light impurities for the system
V-103	Furnace Feed Flash	Vapor is charged to furnace, liquid recycled
V-104	Furnace Quench Flash 1	Quench Furnace effluent to prevent by product formation
V-105	Furnace Quench Flash 2	Quench Furnace effluent to prevent by product formation
V-106	HCl Column Feed Flash	Separates feed to liquid and vapor to utilize energy savings (3% reduction in reboiler duty)
V-107	Vent Flash	Used to recover EDC from waste streams
V-108	HCl Absorber	
V-109	Caustic Absorber	Absorbers Cl2
V-110	HCl Storage Tank	Stores the recycle HCl
V-111	Carbon Adsorption Column	Removes impurities from the water streams
V-112	Water Wash	Flash used to remove water generated by oxy, before the effluent is sent to the distillation columns. Removes water extractable impurities, i.e. chloral
T-100	Lights Column	17 theoretical trays, reflux ratio equal to 3, top tray pressure of 185 psig with a 22 psig pressure drop. Dia 6.5 ft H = 30ft
T-101	Heavies Column	30 theoretical trays, reflux ratio of 1, top tray pressure of 80 psig and has a 15 psig pressure drop.Dia 9 ft H = 56ft
T-102	HCl Column	42 trays and a top tray pressure of 135 psig with a column pressure drop of 10 psig. Dia 7.3 ft H = 80ft
T-103	VCM Column	20 trays, top tray pressure of 65 psig with a column pressure drop of 10 psig. Dia 6 ft H = 36ft
I-100	Waste Incinerator	Burns by products
E-100	Furnace Preheater	charge is heated to allow vapor feed to furnace, A = 2316 ft^2
E-101	Furnace Effluent Cooler 1	Quench Furnace effluent to prevent by product formation, A = 4411 ft^2
E-102	Furnace Effluent Cooler 2	Quench Furnace effluent to prevent by product formation, A = 5623 ft^2
E-104	Oxy Reactor Effluent Cooler	Cools reactors effluent, A = 728 ft^2

APPENDIX B

B-1. Reactor Modeling Procedure

Direct Chlorination Reactor Model:

$$\frac{dF_k}{dz} = \nu r_i A_t \rightarrow dF_k = \nu r_i A_t dz \qquad \text{Eqn (7)}$$

From Wachi and Morikawa
$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$ Reaction 1
$C_2H_4Cl_2 + Cl_2 \rightarrow C_2H_3Cl_3 + HCl$ Reaction 2

$R_1 = k_1[C_2H_4][Cl_2]$ where: $k_1 = 0.132 m^3 mol^{-1} s^{-1}$
$R_2 = k_2[C_2H_4][Cl_2]^2$ where: $k_2 = 0.0239\ m^6 mol^{-2}\ s^{-1}$

Based on initial reactant parameters equation 7 is numerical integrated to find reactant consumption and product formation. See attached Excel file "Direct Chlorination Reactor" for the complete reactor model and corresponding data.

Oxychlorination Reactor Model:

Table B1 Oxychlorination Reactions

Set	Reaction	Stoichiometry
R-1	DCE formation	$C_2H_4 + 2CuCl_2 \rightarrow C_2H_4Cl_2 + 2CuCl$
R-2	TCE formation	$C_2H_4 + 3CuCl_2 \rightarrow C_2H_4Cl_3 + 3CuCl + 0.5H_2$
R-3	C_2H_4 combustion	$C_2H_4 + 3O2 \rightarrow 2CO_2 + 2H_2O$
R-4	CuCl oxidation	$2CuCl + 0.5O_2 \rightarrow CuO\text{-}CuCl_2 \rightarrow CuO + CuCl_2$
R-5	$CuCl_2$ regeneration	$CuO + 2HCl \rightarrow CuCl_2 + H_2O$

$R_1 = k_1 \rho_s p^1 S^1$
$R_2 = k_2 \rho_s p^1 S^1$
$R_3 = k_3 \rho_s p^1 p^2$
$R_4 = k_4 \rho_s p^2 S^2$
$R_5 = k_5 \rho_s p^3 S^3$

Where: k_j = rate constant for reaction j ($mol/m^3\ \sigma\ M\Pi\alpha$)
ρ_s = bulk density of catalyst support (kg/m^3)
S = concentration of cupric chloride (mol/kg of the support)
p^i = partial pressure of species i (MPa)

$k_i = A_i \exp(-E_i/RT)$ where $A_i = (S^i)(k_o)$

Table B2: Oxychlorination Kinetic Data (from Sai Prasad 2001)

Reaction	Frequency Factor A_i	Activation Energy E_i (KJ/mol)
1	1.849E8	97.72E3
2	1.672E8	111.3E3
3	7.759E13	129.7E3
4	3.446E8	86.97E3
5	8.329E13	144.3E3

Based on initial reactant parameters equation 7 is numerical integrated to find reactant consumption and product formation. Total pressure of reactor is 0.5 MPa, the density of the cupric chloride catalyst is 100 kg/m^3. See attached Excel file "Oxychlorination Reactor" for the complete reactor model and corresponding data.

Nine by product formation reaction were modeled using kinetic data obtained from Gel'Perin 1979, 1983, 1984.

Table B3: EDC Pyrolysis Kinetic Data

EDC Pyrolysis Reactions	Log A (L/mol s)	Act. Energy (kcal/mol)
$ClCH_2CH_2Cl \leftrightarrow C_2H_3Cl + HCl$	13.6	58
$C_2H_3Cl \leftrightarrow C_2H_2 + HCl$	13.5	69
$H\cdot + HCl \leftrightarrow H2 + Cl\cdot$	9.7	3.2
$Cl + C_2H_4 \leftrightarrow HCl + C_2H_3\cdot$	11	7
$C_2H_3\cdot + C_2H_2 \leftrightarrow C_4H_5\cdot$	8.8	4.7
$C_4H_5\cdot \leftrightarrow H\cdot + C_4H_4$	14	41.4
$C_4H_5\cdot + HCl \leftrightarrow C4H6 + Cl$	9.9	1
$C_4H_5\cdot + C_2H_2 \leftrightarrow C_6H_7\cdot$	9.6	6.9
$C_6H_7\cdot \leftrightarrow c\text{-}C_6H_7\cdot$	11.5	8
$c\text{-}C_6H_7\cdot \leftrightarrow H + C_6H_6$	14	15

Reaction of the EDC pyrolysis components was based on the following kinetic data and used in a Pro II simulation to find the actual reactant consumption and product formation.

B-2. Pro II Simulations

Pro II simulations were performed for various design parameters for the entire process minus the direct chlorination and oxychlorination reactors. The following table show what the different attached simulation files contain.

Table B4 Pro II Simulations

Pro II Simulation File Name	Description
2004-oxygen	Capacity of 1.98 billion lb/yr of VCM, oxygen based oxychlorination
2005-oxygen	Capacity of 3 billion lb/yr of VCM, oxygen based oxychlorination
2006-oxygen	Capacity of 4.09billion lb/yr of VCM, oxygen based oxychlorination
2007-oxygen	Capacity of 5.23billion lb/yr of VCM, oxygen based oxychlorination
2008-oxygen	Capacity of 6.44 billion lb/yr of VCM, oxygen based oxychlorination
2008-Air	Capacity of 6.44 billion lb/yr of VCM, air based oxychlorination
2008-low oxy	Capacity of 6.44 billion lb/yr of VCM, oxygen based oxychlorination, low oxychlorination reactor temperature
2008-hign F T	Capacity of 6.44 billion lb/yr of VCM, oxygen based oxychlorination, high furnace temperature
2008-low F T	Capacity of 6.44 billion lb/yr of VCM, oxygen based oxychlorination, low furnace temperature
2009-oxygen	Capacity of 7.72 billion lb/yr of VCM, oxygen based oxychlorination
20010-oxygen	Capacity of 9.08 billion lb/yr of VCM, oxygen based oxychlorination
20011-oxygen	Capacity of 10.5 billion lb/yr of VCM, oxygen based oxychlorination
20012-oxygen	Capacity of 12 billion lb/yr of VCM, oxygen based oxychlorination

B-3. Heat Integration

The pinch method was used to find the minimum utilities for the entire plant. These utilities include all heat exchangers, furnace, and the heavies columns condenser, HCl column reboiler, and VCM column reboiler. The remaining equipment as not integrated due to temperature constraints of the system. The stream data presented in Table 7 was used to develop a table cascade diagram from this initial diagram the final cascade diagram was constructed see Table 8. Figure B1 presents the grand composite curve for the system. Figure B2 presents the optimal heat exchanger network.

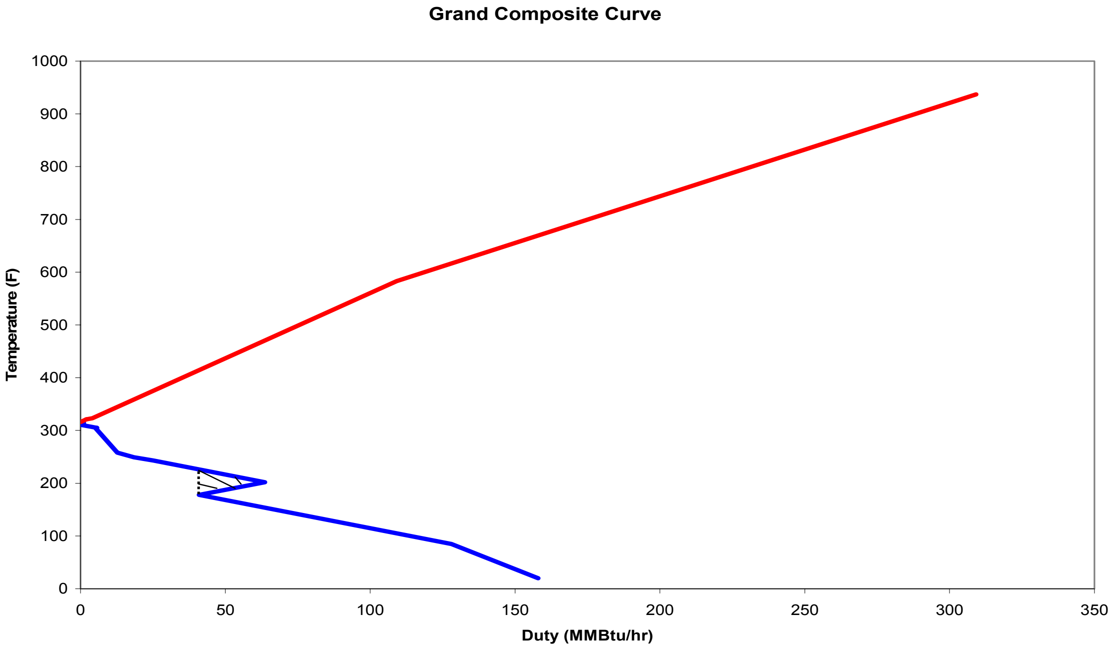


Figure B1: Grand Composite Curve

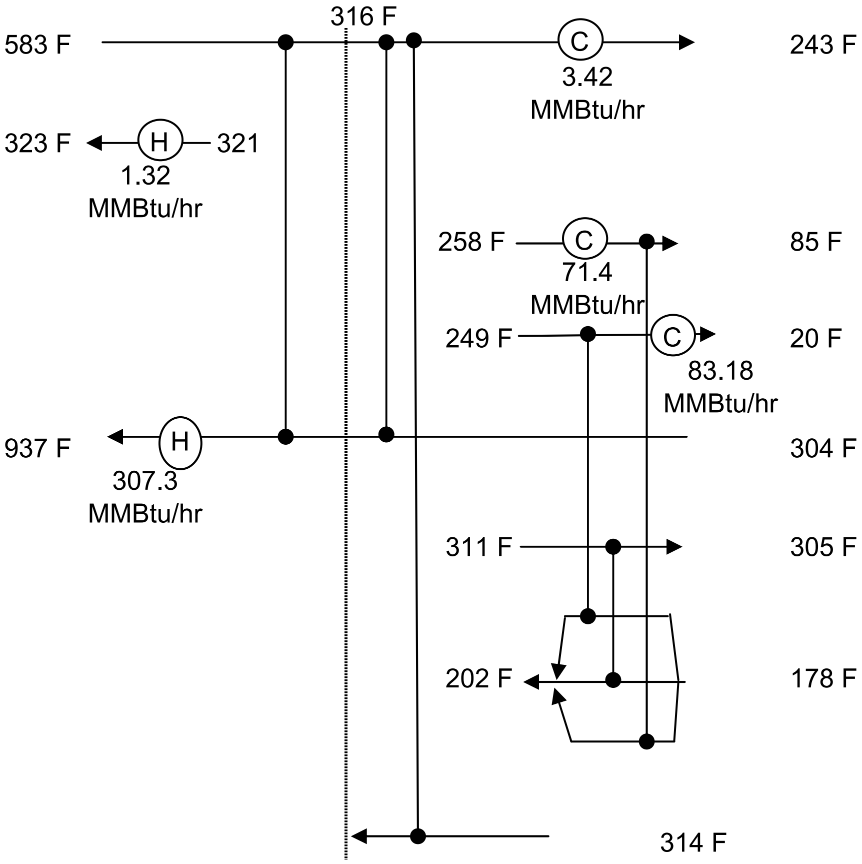


Figure B2. Optimal Network

B-4. Oxychlorination Fluidized Bed Reactor Design

Fluidized-bed reactors are vertical cylindrical vessels with internal equipment that allows for adequate fluidization, heat removal, and feed distribution. Fluidization allow for proper contact between the reactants and the catalyst. Controlling heat transfer is also an advantage of fluidized-bed reactors. Typical operating temperatures are 220-245 ^{o}C and operating pressures of 22-73 psig. Operating at these conditions allows for internal equipment to be fabricated out of a corrosion resistant alloy while utilizing a carbon steel shell. One problem dealing with fluidized-bed reactors is a phenomenon known as catalyst stickiness. Catalyst stickiness is particle agglomeration, which is characterized by declining fluidization quality that can result in a collapsed bed. Oxychlorination catalyst stickiness is brought on by adverse operating conditions that promote the formation of growths of cupric chloride in the surface on individual catalyst particles, which leads to increasing inter-particle interactions and agglomeration (9). Stickiness can be avoided by utilizing proper catalyst mixtures that exhibit proper fluidization characteristics over a wide range of operating conditions (9)

APPENDIX C
HAZOP

The complete HAZOP analysis is included next.

Section	Item	Intention	Parameter	Deviation	Cause	Consequence	Safe guard	Action
1	Reactor R-100	Designed for direct chlorination reaction.	Inlet Flowrate (stream 1 and 2)	No	Leaking or blocking in the inlet pipes	Release of toxic chemicals (ethylene and chlorine) to environment, the pipes might explode at the blocking point.	Sensor, alarm; flow controller	Check the conditions of the inlet pipes immediately. Shut down the system after 15 min if there's no flow.
				More	Increase in flowrate of the streams	Increase pressure; mixer does not function properly; might lead to explosion; release of toxic chemicals to environment	Flow controller allows the maximum capacity of 95%, pressure control	Adjust flow control. In case failure of the valve, shut down the system.
				Less	Blocking or leaking in the pipes	Release of toxic chemicals (ethylene and chlorine) to environment, the pipes might explode at the blocking point.	Alarm, flow controller	Alarm at 50% of normal flow; Flow controller shut down the system if the flow goes to 15%
				Reverse	Blocking in outlet stream, failure in controls	No achievement of products, pushing the feed back, possible release chemicals to environment.	Alarm, flow controller	Immediately shut down the system. Check the pipes and equipments.

Section	Item	Intention	Parameter	Deviation	Cause	Consequence	Safe guard	Action
1	Reactor R-100		Pressure	Higher	Increase in inlet flowrate; decrease in outlet flowrate (outlet blocking)	Explosion; Release of chemicals to environment.	Pressure and level control.	Adjust the controller; check the conditions of the system.
			Temperature	Higher	Too much heat transferred into the reactor; bad insulated walls; not enough cooling water	Products' composition changes. Possible explosion. Destroy the reactor. Possible leaking of chemicals to environment	Temperature controller; Alarm when temperature goes over 200oC.	Temperature controller. Might consider composition controller. Check the system and equipments. Shut down if can not find the reason and temperature is unstable.
				Lower	Heat is not provided for the reactor	Changing in composition of the products.	Composition controller; Alarm when temperature goes under 70oC	Adjust the controller, add heat to the reactor. Shut down if temperature keeps decreasing.
2	DC Caustic Scrubber	Remove aqueous waste, including water and HCl	Pressure	Higher	High inlet flowrate. Blocking of outlet streams.	Failed function. Don't have expected results. Possible leaking and explosion.	Alarm, Flow controller, Pressure Controller	Don't run at high inlet flowrate. Check the equipment periodically. Shut down the system when pressure goes too high.
			Flow	More	High inlet flowrate. Blocking of outlet streams.	Failed function. Don't have expected results. Possible leaking and explosion.	Alarm, Flow controller.	Don't run at high inlet flowrate. Check the equipment periodically. Shut down the system when pressure goes too high.
				No	Blocking or Leaking; Running out of feed.	Release of chemicals to surrounding. Pressure build up at blocking region	Alarm when there's an increase of toxic chemicals in vented gas or waste liquid. Alarm when there's no flow.	Checking the equipment periodically. Check back the feed. Shut down after 30 minute of no flow.
				Reverse	Blocking in outlet stream, failure in controls	No achievement of products, pushing the feed back, possible release chemicals to environment.	Alarm, flow controller	Immediately shut down the system. Check the pipes and equipments.

Section	Item	Intention	Parameter	Deviation	Cause	Consequence	Safe guard	Action
3	Reactor R-101	Designed for oxychlorination reaction	Inlet Flowrate (stream 3 and 4)	No	Leaking or blocking in the inlet pipes	Release of toxic chemicals (HCl, EDC, etc.) to environment, the pipes might explode at the blocking point.	Sensor, alarm; flow controller	Check the conditions of the inlet pipes immediately. Shut down the system after 15 min if there's no flow.
				More	Increase in flowrate of the streams	Increase pressure; mixer malfunction properly; might lead to explosion; release of toxic chemicals to environment	Flow controller allows the maximum capacity of 95%, pressure control	Adjust flow control. In case failure of the valve, shut down the system.
				Less	Blocking or leaking in the pipes	Release of toxic chemicals (ethylene and chlorine) to environment, the pipes might explode at the blocking point.	Alarm, flow controller	Alarm at 50% of normal flow; Flow controller shut down the system if the flow goes to 15%
				Reverse	Blocking in outlet stream, failure in controls	No achievement of products, pushing the feed back, possible release chemicals to environment.	Alarm, flow controller	Immediately shut down the system. Check the pipes and equipments.
			Pressure	Higher	Increase in inlet flowrate; decrease in outlet flowrate (outlet blocking)	Explosion; Release of chemicals to environment.	Pressure and level control.	Adjust the controller; check the conditions of the system.
			Temperature	Higher	Too much heat transferred into the reactor; bad insulated walls	Products' composition changes. Possible explosion. Destroy the reactor. Possible leaking of chemicals to environment	Temperature sensor; Alarm when temperature goes over 200oF.	Temperature controller. Might consider composition controller. Check the system and equipments. Shut down if can not find the reason and temperature is unstable.
				Lower	Heat is not provided for the reactor	Changing in composition of the products.	Composition controller; Alarm when temperature goes under 70oC	Adjust the controller, add heat to the reactor. Shut down if temperature keeps decreasing.

Section	Item	Intention	Parameter	Deviation	Cause	Consequence	Safe guard	Action
4	Oxy Caustic Scrubber V-101	Remove aqueous waste (hydrogen chloride) from the input stream	Pressure	Higher	High inlet flowrate. Blocking of outlet streams. Increase in temperature	Failed function. Don't have expected results. Possible leaking and explosion.	Pressure Controller , Alarm if pressure goes over 100 psig	Don't run at high inlet flowrate. Check the equipment periodically. Shut down the system when pressure goes too high.
			Flow	More	High inlet flowrate. Blocking of outlet streams.	Failed function. Don't have expected results. Possible leaking and explosion.	Alarm, Flow controller.	Don't run at high inlet flowrate. Check the equipment periodically. Shut down the system when pressure goes too high.
				No	Blocking or Leaking; Running out of feed.	Release of chemicals to surrounding. Pressure build up at blocking region	Alarm when there's an increase of toxic chemicals in vented gas or waste liquid. Alarm when there's no flow.	Checking the equipment periodically. Check back the feed. Shut down after 30 minute of no flow.
				Reverse	Blocking in outlet stream, failure in controls	No achievement of products, pushing the feed back, possible release chemicals to environment.	Alarm, flow controller, and level control should be used.	Immediately shut down the system. Check the pipes and equipments.
			Temperature	Higher	Affection from insulation's condition. Increase temperature of inlet stream	Changing expected products. Might lead to explosion and leaking.	Sensor, temperature control.	Choosing proper insulation material. Vented system. Adjust immediately.

Section	Item	Intention	Parameter	Deviation	Cause	Consequence	Safe guard	Action
5	Heat Exchanger E-104	Exchange heat between hot streams and cold streams.	Temperature	Higher	Decrease in cooling water flowrate, Increase in CW's temperature	Too much heat is added to the streams, cannot get desired temperature. Might lead to burning.	Sensor, temperature and flow control.	Check the temperature periodically, increase cooling water flowrate if necessary
				Lower	Too much cooling water.	Might freeze some of low boiling point chemicals; therefore block the pipes, cause leaking and breaking.	Sensor, temperature and flow control.	Decrease flowrate of cooling water. Check functions of the equipments.
	Oxy Flash V-102	Remove aqueous waste, including water and HCl	Pressure	Higher	High inlet flowrate. Blocking of outlet streams.	Failed function. Don’t have expected results. Possible leaking and explosion.	Alarm, Flow controller, Pressure Controller	Don't run at high inlet flowrate. Check the equipment periodically. Shut down the system when pressure goes too high.
			Flow	More	High inlet flowrate. Blocking of outlet streams.	Failed function. Don’t have expected results. Possible leaking and explosion.	Alarm, Flow controller.	Don't run at high inlet flowrate. Check the equipment periodically. Shut down the system when pressure goes too high.
				No	Blocking or Leaking; Running out of feed.	Release of chemicals to surrounding. Pressure build up at blocking region	Alarm when there's an increase of toxic chemicals in vented gas or waste liquid. Alarm when there's no flow.	Checking the equipment periodically. Check back the feed. Shut down after 30 minute of no flow.
				Reverse	Blocking in outlet stream, failure in controls	No achievement of products, pushing the feed back, possible release chemicals to environment.	Alarm, flow controller	Immediately shut down the system. Check the pipes and equipments.

Section	Item	Intention	Parameter	Deviation	Cause	Consequence	Safe guard	Action
6	Column T-100	Separate EDC from byproducts. Reflux Ratio =3, 185 psig, 22 psig pressure drop	Flow	Overfilled	Outlet stream does not drain, too much liquid coming back to column,	Column malfunction. Leaking: EDC and toxic organic compounds. Harmful to people.	Flow controller, alarm when output flow rate goes under 70% set point	Lower select switch. Shut down if the outlet stream does not drain. Check pipe conditions for blocking
			Reflux Ratio	Decreased	Changing in outlet conditions. Failure of valve system.	Cannot get expected separation.	Flow controller	Check with the controller to see if there's anything wrong.
			Vapor Flow	More	More heat added to reboiler.	Foaming Entrainment Weeping/Dumping; Flooding. Reduce efficiency.	Composition and flow controller.	Balance the heat duty of condenser and reboiler.
	Reboiler		Temperature	Too high	Too much input energy	Build up pressure inside the reboiler. Might lead to explosion. Release of chemical to environment.	Temperature controller.	Reduce heat to design level. Shut down if the reboiler is not working properly. Might use dual-reboiler option to keep the system working.
	Compressor	Compress the liquid and vapor stream	Pressure	Higher	Flowrate is increased, temperature increased.	Can lead to explosion. Release of chemicals to environment.	Pressure control on the column, flow control	Decrease the inlet flowrate. In case malfunctioning of the equipment, shut down the system.
6	Compressor		Temperature	Higher	Energy input changes, temperature of feed increases.	Pressure build up, lead to explosion and consequences.	Temperature control.	Keep the temperature of the compressor at proper temperature.
7	EDC Cracking Furnace, F100	Crack the EDC. Yields vinyl chloride and HCl	Temperature	Higher	Too much fuel supplied to the furnace, inlet flowrate decreases	Cannot get desired products; pressure build up, lead to explosion, releases of chemicals.	Flow controller, alarm when fuel flow rate is 20% more than set point	Check the flowrate; change set point if necessary, check pipes/ equipment function. Shut down if temperature is too high.
				Lower	Not enough heat provided; inlet flowrate is too high	Effect the conversion of product	Flow controller. alarm when fuel flow rate is 20% lower than set point	Check valves, set point, pipes, increase fuel flow or decrease inlet flow
8	Tank V110	Store and recycle hydrogen chloride	Level	Overfilled	Too much flow in, blocking in outlet pipe, valve malfunctioning	Build up pressure, lead to explosion, release toxic chemical	Level controller, alarm when tank is filled up to 95% capacity	Check pipes, valves' conditions. Decrease the inlet flowrate.

APPENDIX D
By-Product Treatment

Auxiliary Fuel Flowrate (Q_F)

The following equation is an energy balance over the incineration unit (2). It equates the amount of heat provided by the fuel to the amount of heat required for combustion of the waste streams. This equation allows for the amount of auxiliary fuel to be calculated.

Qf = Qw (X/Y) where,

X = 1.1Cpo(Tc – Tr) – Cpi(Ti – Tr) – hw
Y = hf – 1.1Cpo(Tc-Tr) where,

Cpo = mean heat capacity of exhaust stream
Tc = combustion temperature
Tr = reference temperature (usually S.T.P.)
Cpi = mean heat capacity of inlet streams
Ti = temperature of inlet waste streams
hw = heat content of waste streams
hf = heat content of fuel

Amount of Solvent (L)

The following equation is a material balance on the solute over the whole absorption column. This equation allows for the amount of liquid solvent to be calculated.

L = G*(Yi – Yo)/(Xo – Xi) where,

G = vapor flowrate
Yi = amount of pollutant per amount of pollutant free vapor entering the column
Yo = amount of pollutant per amount of pollutant free vapor leaving the column
Xi = amount of pollutant per amount of pollutant free solvent entering the column
Xo = amount of pollutant per amount of pollutant free solvent leaving the column

Column Diameter (D_T)

The following equation is a manipulation of this continuity equation: Flowrate = velocity*Flow Area*Density. This equation allows for the column diameter to be calculated.

$$D_T = \frac{4VM_v}{fU_f\pi(1 - A_d / A)\rho_v}$$ where,

V = vapor flowrate
Mv = molecular weight of vapor
f = fraction of flooding
Uf = flooding velocity

Ad/A = area occupied by the downcomer over the cross sectional area of the column
pv = vapor density

Overall Height of Transfer Unit (H_{OG})

The following equation is a manipulation of a differential material balance for the solute over a differential height of packing. This equation allows for the overall height of a transfer unit to be calculated.

HOG = G/KyaS where,

G = vapor flowrate
Kya = overall gas mass transfer coefficient
S = overall cross sectional area of the column

Number of Theoretical Stages (N_{OG})

The following equation is also a manipulation of a differential material balance for the solute over a differential height of packing. This equation allows for the number of theoretical stages to be calculated.

$$N_{OG} = \frac{\ln\{[(A-1)/A][(Y_i - KX_i)/(Y_O - KX_i)] + (1/A)\}}{(A-1)/A}$$ where,

A = absorption factor
Yi = amount of pollutant per amount of pollutant free vapor entering the column
Yo = amount of pollutant per amount of pollutant free vapor leaving the column
Xi = amount of pollutant per amount of pollutant free solvent entering the column
Xo = amount of pollutant per amount of pollutant free solvent leaving the column
K = equilibrium constant

Height of Packing (H_{pack})

The following equation is used to determine the height of packing.

Hpack = NOG*(HOG)

APPENDIX E

Calculations for Carbon Adsorption Tower

Equations for the design of activated carbon adsorption tower

1. Minimum amount of carbon in the mass bed

$$\frac{X}{M} = Kc^{\frac{1}{n}}$$

X = amount of carbon adsorbed (mg)
M = mass of carbon (g)
c = equilibrium concentration in solution after desorption (mg/L)
K = Freundlich constant
n = Freundlich number

2. Volume of the granular activated carbon bed

$$V = \frac{M}{AD \times .85}$$

V = Volume of granulated activated carbon bed (ft^3)
AD = Apparent density of carbon (lb/ft^3)
M = Mass of carbon (lbs)

3. Equilibrium saturation (maximum usable life of the carbon)

$$D = \frac{M \times L}{MR}$$

D = Equilibrium saturation (days)
M = Mass of carbon bed (lbs)
L = Loading (lb organic/lb carbon)
MR = Mass flow rate of contaminants (lbs/day)

4. Hydraulic loading

$$HL = \frac{VF}{A}$$

HL = Hydraulic loading (gpm/ft^2)
VF = Volumetric flow rate of water (gpm)
A = Area (ft^2)

5. Superficial contact time

$$CT = \frac{V}{VF}$$

CT = Superficial contact time (min)
V = Volume (gallons)
VF = Volumetric flow rate (gpm)

APPENDIX F

Economic Analysis Plant Capacity of 4.09 billion lb VCM/yr

Table F1: Cash flow for the first year 2004

Summary of Annual Costs along with the Total Product Cost (2004)			
		Working Capital	**$7,378,262**
		Fix Capital Investment ($)	**$36,891,312**
		Total Capital Investment ($)	**$47,110,219**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	441,621,989
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	5,952,438
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	458,836
4	Maintenance and Repair	2% of Fixed Capital Investment	737,826
5	Operating Supplies	9% of Cost for Maintenance and Repair	110,674
	Sub Total		**454,018,763**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	2,053,120
2	Local Taxes	1% of Fix Capital Investment	368,913
3	Insurance	0.8% of Fix Capital Investment	295,130
	Sub Total		**2,717,163**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**458,790,727**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	454,019
	Sub Total		**1,224,569**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**460,015,295**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	467,949,440
	Gross Income (G)	Selling Price - Total Production Cost	**7,934,144**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,059,904**
2	**Net Profit (P)**	G-D-(G-D)*tax	**4,536,998**
3	**Annual Cash Flow**	Cash flow for the first year	**5,596,903**

Table F2: Cash flow for the second year (2005)

	Summary of Annual Costs along with the Total Product Cost (2005)		
		Working Capital	**$7,378,262**
		Fix Capital Investment ($)	**$36,891,312**
		Total Capital Investment ($)	**$47,110,219**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	695,483,017
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	9,049,413
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	697,520
4	Maintenance and Repair	2% of Fixed Capital Investment	737,826
5	Operating Supplies	9% of Cost for Maintenance and Repair	110,674
	Sub Total		**711,215,450**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	2,053,120
2	Local Taxes	1% of Fix Capital Investment	368,913
3	Insurance	0.8% of Fix Capital Investment	295,130
	Sub Total		**2,717,163**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**715,987,413**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	711,215
	Sub Total		**1,481,765**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**717,469,178**
	Gross Income		
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	727,307,700
	Gross Income (G)	Selling Price - Total Production Cost	**9,838,522**
	Net Profit (P)		
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,059,904**
2	**Net Profit (P)**	G-D-(G-D)*tax	**5,793,888**
3	**Annual Cash Flow**	Cash flow for the first year	**6,853,792**

Table F3: Cash flow of the maximum capacity (2006)

Summary of Annual Costs along with the Total Product Cost (2006)			
		Working Capital	**$7,378,262**
		Fix Capital Investment ($)	**$36,891,312**
		Total Capital Investment ($)	**$47,110,219**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	938,435,745
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	12,283,800
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	947,726
4	Maintenance and Repair	2% of Fixed Capital Investment	737,826
5	Operating Supplies	9% of Cost for Maintenance and Repair	110,674
	Sub Total		**957,652,771**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	2,053,120
2	Local Taxes	1% of Fix Capital Investment	368,913
3	Insurance	0.8% of Fix Capital Investment	295,130
	Sub Total		**2,717,163**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**962,424,735**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	957,653
	Sub Total		**1,728,203**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**964,152,937**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	982,302,700
	Gross Income (G)	Selling Price - Total Production Cost	**18,149,763**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,059,904**
2	**Net Profit (P)**	G-D-(G-D)*tax	**11,279,307**
3	**Annual Cash Flow**	Cash flow for the first year	**12,339,211**

Table F4: NPW and ROI

n	Year	Cash Flow		NPW ($)	$CF_{k/}(1+r)^{k}$
1	2004	5.597E+06	5.330E+06	**1.34E+08**	4530496
2	2005	6.854E+06	6.217E+06		4490833
3	2006	1.234E+07	1.066E+07		6544574
4	2007	1.271E+07	1.046E+07		5456531
5	2008	1.309E+07	1.026E+07		4549376
6	2009	1.348E+07	1.006E+07		3793037
7	2010	1.389E+07	9.870E+06		3162440
8	2011	1.430E+07	9.682E+06		2636681
9	2012	1.473E+07	9.497E+06		2198329
10	2013	1.518E+07	9.317E+06		1832854
11	2014	1.563E+07	9.139E+06		1528140
12	2015	1.610E+07	8.965E+06		1274085
13	2016	1.658E+07	8.794E+06		1062267
14	2017	1.708E+07	8.627E+06		885663.8
15	2018	1.759E+07	8.462E+06		738421.1
16	2019	1.812E+07	8.301E+06		615657.7
17	2020	1.866E+07	8.143E+06		513303.9
18	2021	1.922E+07	7.988E+06		427966.5
19	2022	1.980E+07	7.836E+06		356816.6
20	2023	2.039E+07	7.687E+06		297495.4

Inflaction	0.03	**TCI**	47110219
Interest rate	0.05		
ROI	0.2353841		

APPENDIX G

Economic Analysis Plant Capacity 6.44 billion lb/yr.

Table G1: Cash flow of 2004

Summary of Annual Costs along with the Total Product Cost (2004)			
		Working Capital	**$11,007,612**
		Fix Capital Investment ($)	**$55,038,060**
		Total Capital Investment ($)	**$68,886,317**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	441,621,989
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	5,952,438
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	458,836
4	Maintenance and Repair	2% of Fixed Capital Investment	1,100,761
5	Operating Supplies	9% of Cost for Maintenance and Repair	165,114
	Sub Total		**454,436,139**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,063,044
2	Local Taxes	1% of Fix Capital Investment	550,381
3	Insurance	0.8% of Fix Capital Investment	440,304
	Sub Total		**4,053,729**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**460,544,668**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	454,436
	Sub Total		**1,224,986**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**461,769,654**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	467,949,440
	Gross Income (G)	Selling Price - Total Production Cost	**6,179,785**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,581,269**
2	**Net Profit (P)**	G-D-(G-D)*tax	**3,035,021**
3	**Annual Cash Flow**	Cash flow for the first year	**4,616,290**

Table G2: Cash flow of 2005

Summary of Annual Costs along with the Total Product Cost (2005)			
		Fix Capital Investment ($)	**$55,038,060**
		Total Capital Investment ($)	**$68,886,317**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	695,483,017
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	9,049,413
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	697,520
4	Maintenance and Repair	2% of Fixed Capital Investment	1,100,761
5	Operating Supplies	9% of Cost for Maintenance and Repair	165,114
	Sub Total		**711,632,825**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,063,044
2	Local Taxes	1% of Fix Capital Investment	550,381
3	Insurance	0.8% of Fix Capital Investment	440,304
	Sub Total		**4,053,729**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**717,741,354**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	711,633
	Sub Total		**1,482,183**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**719,223,537**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	727,307,700
	Gross Income (G)	Selling Price - Total Production Cost	**8,084,163**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,581,269**
2	**Net Profit (P)**	G-D-(G-D)*tax	**4,291,910**
3	**Annual Cash Flow**	Cash flow for the first year	**5,873,179**

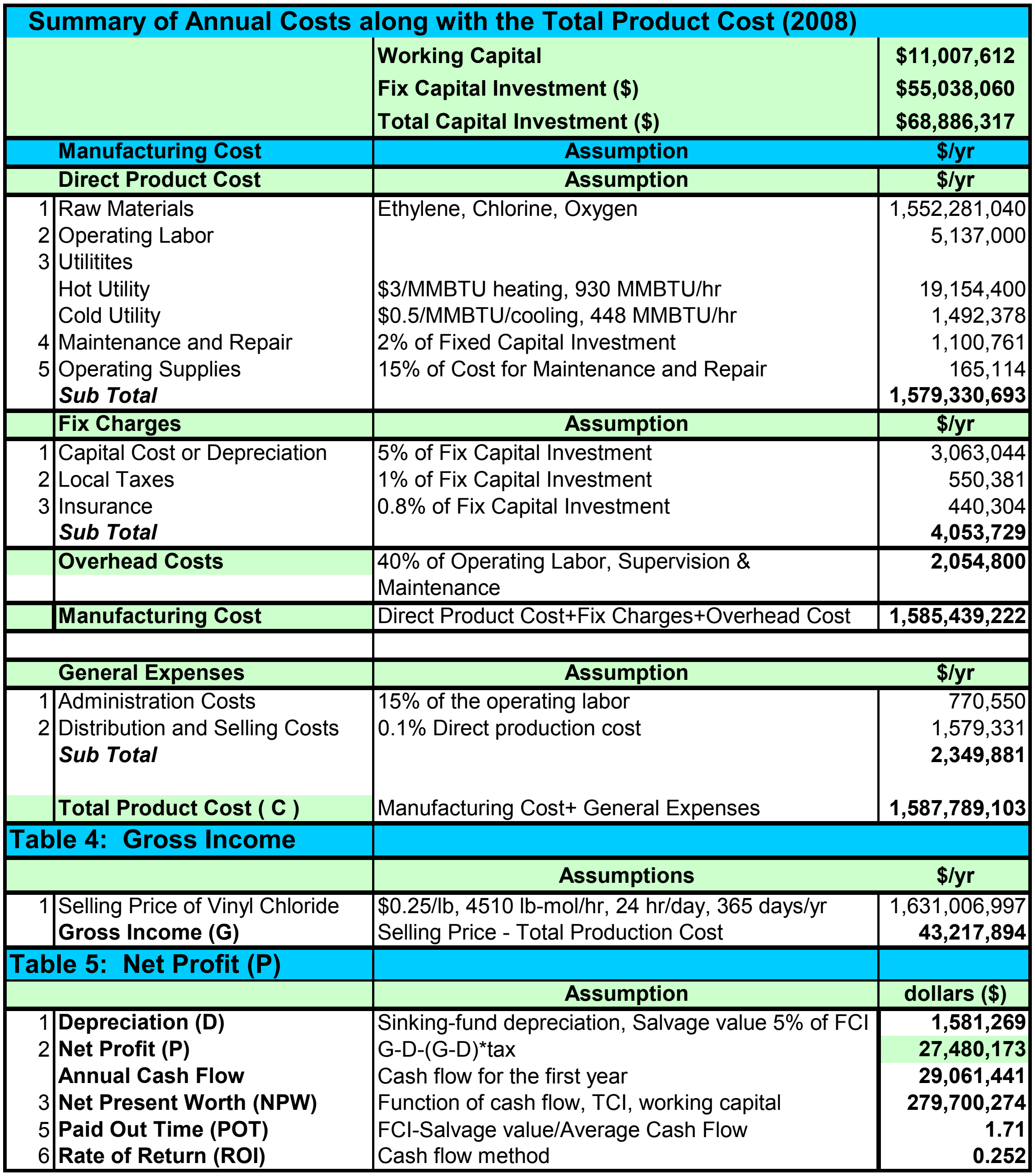
Table G3: Cash Flow of 2006

Summary of Annual Costs along with the Total Product Cost (2006)			
		Fix Capital Investment ($)	**$55,038,060**
		Total Capital Investment ($)	**$68,886,317**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	938,435,745
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	12,283,800
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	947,726
4	Maintenance and Repair	2% of Fixed Capital Investment	1,100,761
5	Operating Supplies	9% of Cost for Maintenance and Repair	165,114
	Sub Total		**958,070,147**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,063,044
2	Local Taxes	1% of Fix Capital Investment	550,381
3	Insurance	0.8% of Fix Capital Investment	440,304
	Sub Total		**4,053,729**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**964,178,676**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	958,070
	Sub Total		**1,728,620**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**965,907,296**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	982,302,700
	Gross Income (G)	Selling Price - Total Production Cost	**16,395,404**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,581,269**
2	**Net Profit (P)**	G-D-(G-D)*tax	**9,777,330**
3	**Annual Cash Flow**	Cash flow for the first year	**11,358,598**

Table G4: Cash flow of 2007

Summary of Annual Costs along with the Total Product Cost (2007)			
		Fix Capital Investment ($) **Total Capital Investment ($)**	**$55,038,060** **$68,886,317**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	1,254,711,587
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	15,724,513
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	1,211,891
4	Maintenance and Repair	2% of Fixed Capital Investment	1,100,761
5	Operating Supplies	9% of Cost for Maintenance and Repair	165,114
	Sub Total		**1,278,050,866**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,063,044
2	Local Taxes	1% of Fix Capital Investment	550,381
3	Insurance	0.8% of Fix Capital Investment	440,304
	Sub Total		**4,053,729**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**1,284,159,396**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	1,278,051
	Sub Total		**2,048,601**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**1,286,207,997**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	1,292,983,501
	Gross Income (G)	Selling Price - Total Production Cost	**6,775,504**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,581,269**
2	**Net Profit (P)**	G-D-(G-D)*tax	**3,428,196**
3	**Annual Cash Flow**	Cash flow for the first year	**5,009,464**

Table G5: Cash flow of 2008



	Summary of Annual Costs along with the Total Product Cost (2008)		
		Working Capital	**$11,007,612**
		Fix Capital Investment ($)	**$55,038,060**
		Total Capital Investment ($)	**$68,886,317**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen	1,552,281,040
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 930 MMBTU/hr	19,154,400
	Cold Utility	$0.5/MMBTU/cooling, 448 MMBTU/hr	1,492,378
4	Maintenance and Repair	2% of Fixed Capital Investment	1,100,761
5	Operating Supplies	15% of Cost for Maintenance and Repair	165,114
	Sub Total		**1,579,330,693**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,063,044
2	Local Taxes	1% of Fix Capital Investment	550,381
3	Insurance	0.8% of Fix Capital Investment	440,304
	Sub Total		**4,053,729**
	Overhead Costs	40% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**1,585,439,222**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	1,579,331
	Sub Total		**2,349,881**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**1,587,789,103**
	Table 4: Gross Income		
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	1,631,006,997
	Gross Income (G)	Selling Price - Total Production Cost	**43,217,894**
	Table 5: Net Profit (P)		
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,581,269**
2	**Net Profit (P)**	G-D-(G-D)*tax	**27,480,173**
	Annual Cash Flow	Cash flow for the first year	**29,061,441**
3	**Net Present Worth (NPW)**	Function of cash flow, TCI, working capital	**279,700,274**
5	**Paid Out Time (POT)**	FCI-Salvage value/Average Cash Flow	**1.71**
6	**Rate of Return (ROI)**	Cash flow method	**0.252**

Table G6: NPW and ROI

n	Year	Cash Flow		NPW ($)	$CF_{k/}(1+r)^k$
1	2004	4.616E+06	4.396E+06	**2.80E+08**	3686482.002
2	2005	5.873E+06	5.327E+06		3745513.512
3	2006	1.136E+07	9.812E+06		5784714.459
4	2007	5.009E+06	4.121E+06		2037358.825
5	2008	2.906E+07	2.277E+07		9438706.087
6	2009	2.993E+07	2.234E+07		7763700.079
7	2010	3.083E+07	2.191E+07		6385942.984
8	2011	3.176E+07	2.149E+07		5252684.594
9	2012	3.271E+07	2.108E+07		4320535.825
10	2013	3.369E+07	2.068E+07		3553807.484
11	2014	3.470E+07	2.029E+07		2923143.828
12	2015	3.574E+07	1.990E+07		2404398.628
13	2016	3.681E+07	1.952E+07		1977710.678
14	2017	3.792E+07	1.915E+07		1626743.37
15	2018	3.906E+07	1.879E+07		1338059.212
16	2019	4.023E+07	1.843E+07		1100605.35
17	2020	4.143E+07	1.808E+07		905290.382
18	2021	4.268E+07	1.773E+07		744636.2822
19	2022	4.396E+07	1.740E+07		612492.0842
20	2023	4.528E+07	1.706E+07		503798.3807

Table G7: ROI

Inflaction	**0.03**	**TCI**	**244965.18**
Interest rate	**0.05**		
ROI	**0.2522209**		

Table G8: Probability

NPW	Probability		
($)	10.5 billion (lb/yr)	6.44 billion (lb/yr)	4.09 billion (lb/yr)
-4.5E+09	0.001014199		
-4E+09	0		
-3.5E+09	0.004056795		
-3E+09	0.00811359		
-2.5E+09	0.015212982	0	0
-2E+09	0.030425963	0.002024291	0
-1.5E+09	0.053752535	0.010121457	0.004016064
-1E+09	0.067951318	0.045546559	0.052208835
-5E+08	0.115618661	0.153846154	0.253815261
0	0.130831643	0.26417004	0.300200803
500000000	0.15010142	0.287449393	0.264257028
1E+09	0.144016227	0.153846154	0.115461847
1.5E+09	0.105476673	0.064777328	0.009036145
2E+09	0.074036511	0.018218623	0.001004016
2.5E+09	0.043610548	0	0
3E+09	0.036511156		
3.5E+09	0.010141988		
4E+09	0.006085193		
4.5E+09	3	0.003042596	

APPENDIX H

Economic Analysis Plant Capacity of 10.5 billion lb VCM/year

Table H1: Cash flow of 2004

Summary of Annual Costs along with the Total Product Cost (2004)			
		Working Capital	**$12,385,708**
		Fix Capital Investment ($)	**$61,928,539**
		Total Capital Investment ($)	**$77,154,892**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	441,621,989
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	5,952,438
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	458,836
4	Maintenance and Repair	2% of Fixed Capital Investment	1,238,571
5	Operating Supplies	9% of Cost for Maintenance and Repair	185,786
	Sub Total		**454,594,620**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,446,522
2	Local Taxes	1% of Fix Capital Investment	619,285
3	Insurance	0.8% of Fix Capital Investment	495,428
	Sub Total		**4,561,235**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**461,210,655**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	454,595
	Sub Total		**1,225,145**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**462,435,799**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	467,949,440
	Gross Income (G)	Selling Price - Total Production Cost	**5,513,640**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,779,235**
2	**Net Profit (P)**	G-D-(G-D)*tax	**2,464,707**
3	**Annual Cash Flow**	Cash flow for the first year	**4,243,942**

Table H2: Cash flow of 2005

Summary of Annual Costs along with the Total Product Cost (2005)			
		Fix Capital Investment ($) **Total Capital Investment ($)**	**$61,928,539** **$77,154,892**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	695,483,017
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	9,049,413
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	697,520
4	Maintenance and Repair	2% of Fixed Capital Investment	1,238,571
5	Operating Supplies	9% of Cost for Maintenance and Repair	185,786
	Sub Total		**711,791,306**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,446,522
2	Local Taxes	1% of Fix Capital Investment	619,285
3	Insurance	0.8% of Fix Capital Investment	495,428
	Sub Total		**4,561,235**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**718,407,341**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	711,791
	Sub Total		**1,482,341**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**719,889,682**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	727,307,700
	Gross Income (G)	Selling Price - Total Production Cost	**7,418,018**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,779,235**
2	**Net Profit (P)**	G-D-(G-D)*tax	**3,721,597**
3	**Annual Cash Flow**	Cash flow for the first year	**5,500,832**

Table H3: Cash flow of 2006

Summary of Annual Costs along with the Total Product Cost (2006)			
		Fix Capital Investment ($) **Total Capital Investment ($)**	**$61,928,539** **$77,154,892**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	938,435,745
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	12,283,800
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	947,726
4	Maintenance and Repair	2% of Fixed Capital Investment	1,238,571
5	Operating Supplies	9% of Cost for Maintenance and Repair	185,786
	Sub Total		**958,228,628**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,446,522
2	Local Taxes	1% of Fix Capital Investment	619,285
3	Insurance	0.8% of Fix Capital Investment	495,428
	Sub Total		**4,561,235**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**964,844,663**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	958,229
	Sub Total		**1,728,779**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**966,573,441**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	982,302,700
	Gross Income (G)	Selling Price - Total Production Cost	**15,729,259**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,779,235**
2	**Net Profit (P)**	G-D-(G-D)*tax	**9,207,016**
	Annual Cash Flow	Cash flow for the first year	**10,986,251**

Table H4: Cash flow of 2007

Summary of Annual Costs along with the Total Product Cost (2007)			
		Fix Capital Investment ($) **Total Capital Investment ($)**	**$61,928,539** **$77,154,892**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	1,254,711,587
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	6,289,805
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	1,211,891
4	Maintenance and Repair	2% of Fixed Capital Investment	1,238,571
5	Operating Supplies	9% of Cost for Maintenance and Repair	185,786
	Sub Total		**1,268,774,639**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,446,522
2	Local Taxes	1% of Fix Capital Investment	619,285
3	Insurance	0.8% of Fix Capital Investment	495,428
	Sub Total		**4,561,235**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**1,275,390,675**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	1,268,775
	Sub Total		**2,039,325**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**1,277,429,999**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	1,292,983,501
	Gross Income (G)	Selling Price - Total Production Cost	**15,553,502**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,779,235**
2	**Net Profit (P)**	G-D-(G-D)*tax	**9,091,016**
3	**Annual Cash Flow**	Cash flow for the first year	**10,870,251**

Table H5: Cash flow of 2008

Summary of Annual Costs along with the Total Product Cost (2008)			
		Working Capital	**$12,385,708**
		Fix Capital Investment ($)	**$61,928,539**
		Total Capital Investment ($)	**$77,154,892**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen	1,552,281,040
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 930 MMBTU/hr	19,154,400
	Cold Utility	$0.5/MMBTU/cooling, 448 MMBTU/hr	1,492,378
4	Maintenance and Repair	2% of Fixed Capital Investment	1,238,571
5	Operating Supplies	15% of Cost for Maintenance and Repair	185,786
	Sub Total		**1,579,489,174**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,446,522
2	Local Taxes	1% of Fix Capital Investment	619,285
3	Insurance	0.8% of Fix Capital Investment	495,428
	Sub Total		**4,561,235**
	Overhead Costs	40% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**1,586,105,209**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	1,579,489
	Sub Total		**2,350,039**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**1,588,455,248**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	1,631,006,997
	Gross Income (G)	Selling Price - Total Production Cost	**42,551,749**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,779,235**
2	**Net Profit (P)**	G-D-(G-D)*tax	**26,909,859**
3	**Annual Cash Flow**	Cash flow for the first year	**28,689,094**

Table H6: Cash flow of 2009

Summary of Annual Costs along with the Total Product Cost (2009)			
		Fix Capital Investment ($)	**$61,928,539**
		Total Capital Investment ($)	**$77,154,892**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	1,873,650,466
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	9,284,721
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	1,788,988
4	Maintenance and Repair	2% of Fixed Capital Investment	1,238,571
5	Operating Supplies	9% of Cost for Maintenance and Repair	185,786
	Sub Total		**1,891,285,531**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,446,522
2	Local Taxes	1% of Fix Capital Investment	619,285
3	Insurance	0.8% of Fix Capital Investment	495,428
	Sub Total		**4,561,235**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**1,897,901,566**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	1,891,286
	Sub Total		**2,661,836**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**1,900,563,402**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	1,972,390,142
	Gross Income (G)	Selling Price - Total Production Cost	**71,826,740**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,779,235**
2	**Net Profit (P)**	G-D-(G-D)*tax	**46,231,353**
3	**Annual Cash Flow**	Cash flow for the first year	**48,010,589**

Table H7: Cash flow of 2010

Summary of Annual Costs along with the Total Product Cost (2010)			
		Fix Capital Investment ($)	**$61,928,539**
		Total Capital Investment ($)	**$77,154,892**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen, Hydrochloride	2,236,955,317
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 285 MMBTU/hr	10,920,007
	Cold Utility	$0.5/MMBTU/cooling, 137.7 MMBTU/hr	2,104,152
4	Maintenance and Repair	2% of Fixed Capital Investment	1,238,571
5	Operating Supplies	9% of Cost for Maintenance and Repair	185,786
	Sub Total		**2,256,540,832**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,446,522
2	Local Taxes	1% of Fix Capital Investment	619,285
3	Insurance	0.8% of Fix Capital Investment	495,428
	Sub Total		**4,561,235**
	Overhead Costs	50% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**2,263,156,868**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	2,256,541
	Sub Total		**3,027,091**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**2,266,183,959**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	2,302,965,909
	Gross Income (G)	Selling Price - Total Production Cost	**36,781,951**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,779,235**
2	**Net Profit (P)**	G-D-(G-D)*tax	**23,101,792**
3	**Annual Cash Flow**	Cash flow for the first year	**24,881,027**

Table H8: Cash flow of 2011 (full capacity)

Summary of Annual Costs along with the Total Product Cost (2011)			
		Working Capital	**$12,385,708**
		Fix Capital Investment ($)	**$61,928,539**
		Total Capital Investment ($)	**$77,154,892**
	Manufacturing Cost	**Assumption**	**$/yr**
	Direct Product Cost	**Assumption**	**$/yr**
1	Raw Materials	Ethylene, Chlorine, Oxygen	2,607,877,975
2	Operating Labor		5,137,000
3	Utilitites		
	Hot Utility	$3/MMBTU heating, 930 MMBTU/hr	31,569,366
	Cold Utility	$0.5/MMBTU/cooling, 448 MMBTU/hr	2,433,208
4	Maintenance and Repair	2% of Fixed Capital Investment	1,238,571
5	Operating Supplies	15% of Cost for Maintenance and Repair	185,786
	Sub Total		**2,648,441,906**
	Fix Charges	**Assumption**	**$/yr**
1	Capital Cost or Depreciation	5% of Fix Capital Investment	3,446,522
2	Local Taxes	1% of Fix Capital Investment	619,285
3	Insurance	0.8% of Fix Capital Investment	495,428
	Sub Total		**4,561,235**
	Overhead Costs	40% of Operating Labor, Supervision & Maintenance	**2,054,800**
	Manufacturing Cost	Direct Product Cost+Fix Charges+Overhead Cost	**2,655,057,941**
	General Expenses	**Assumption**	**$/yr**
1	Administration Costs	15% of the operating labor	770,550
2	Distribution and Selling Costs	0.1% Direct production cost	2,648,442
	Sub Total		**3,418,992**
	Total Product Cost (C)	Manufacturing Cost+ General Expenses	**2,658,476,933**
Gross Income			
		Assumptions	**$/yr**
1	Selling Price of Vinyl Chloride	$0.25/lb, 4510 lb-mol/hr, 24 hr/day, 365 days/yr	2,681,872,397
	Gross Income (G)	Selling Price - Total Production Cost	**23,395,464**
Net Profit (P)			
		Assumption	**dollars ($)**
1	**Depreciation (D)**	Sinking-fund depreciation, Salvage value 5% of FCI	**1,779,235**
2	**Net Profit (P)**	G-D-(G-D)*tax	**14,266,711**
3	**Annual Cash Flow**	Cash flow for the first year	**16,045,946**
4	**Net Present Worth (NPW)**	Function of cash flow, TCI, working capital	**161,759,443**
5	**Paid Out Time (POT)**	FCI-Salvage value/Average Cash Flow	**3.07**
6	**Rate of Return (ROI)**	Cash flow method	**0.180**
7	**Rate of Return (ROI)**	Profit/total capital investment	**0.18**

Table H9: NPW

n	Year	Cash Flow		NPW ($)	$CF_{k/}(1+r)^{k}$
1	2004	4.244E+06	4.042E+06	**1.62E+08**	3596916.39
2	2005	5.501E+06	4.989E+06		3951391.729
3	2006	1.099E+07	9.490E+06		6688551.844
4	2007	1.087E+07	8.943E+06		5608968.686
5	2008	2.869E+07	2.248E+07		12546458.03
6	2009	4.801E+07	3.583E+07		17795172.11
7	2010	2.488E+07	1.768E+07		7816176.066
8	2011	1.605E+07	1.086E+07		4272206.228
9	2012	1.653E+07	1.065E+07		3729497.273
10	2013	1.702E+07	1.045E+07		3255729.983
11	2014	1.753E+07	1.025E+07		2842146.527
12	2015	1.806E+07	1.006E+07		2481101.604
13	2016	1.860E+07	9.865E+06		2165921.113
14	2017	1.916E+07	9.677E+06		1890778.781
15	2018	1.973E+07	9.493E+06		1650588.462
16	2019	2.033E+07	9.312E+06		1440910.116
17	2020	2.094E+07	9.134E+06		1257867.729
18	2021	2.156E+07	8.960E+06		1098077.671
19	2022	2.221E+07	8.790E+06		958586.1409
20	2023	2.288E+07	8.622E+06		836814.5656

Table H10: ROI

Inflaction	**0.03**	**TCI**	**86789944**
Interest rate	**0.05**		
ROI	**0.1798835**		

APPENDIX I

EI Data for different Design Options

Oxygen Used			Furnace Temperature = 500°C		
Incinerator	**Furnace**	**Hot Utility**	**O_2 Cost (\$/hr)**	**Profit**	**E.I.**
-	-	-	0	27.5	186300
X	-	-	458	23.5	186000
-	X	-	1833	11.4	183000
X	X	-	2290	7.4	180500
-	-	X	2725	3.6	178000
X	-	X	3183	-0.4	175000
-	X	X	4558	-12.5	172300
X	X	X	5016	-16.5	170000

Oxygen Used			Furnace Temperature = 426°C		
Incinerator	**Furnace**	**Hot Utility**	**O_2 Cost (\$/hr)**	**Profit**	**E.I.**
-	-	-	0	27.5	188023
X	-	-	657	18.2	187635
-	X	-	2032	6.2	186922
X	X	-	2688	2.2	185744
-	-	X	2924	-1.6	183244
X	-	X	3581	-5.6	180744
-	X	X	4956	-17.7	173744
X	X	X	5613	-21.7	171744

Oxygen Used			Furnace Temperature = 575°C		
Incinerator	**Furnace**	**Hot Utility**	**O_2 Cost (\$/hr)**	**Profit**	**E.I.**
-	-	-	0	27.5	187151
X	-	-	562	20.8	186817
-	X	-	1937	8.8	185960
X	X	-	2498	4.8	184872
-	-	X	2829	1.0	182373
X	-	X	3391	-3.0	179850
-	X	X	4766	-15.1	172872
X	X	X	5328	-19.1	170872

APPENDIX J

Sequestering of Carbon Dioxide

Calculation of Capital Investment of brine aquifer injection:

$$CapitalInvestment = \frac{\$27.75}{kg/hr} x Q_{\mathrm{CO_2}} = (410{,}810 kg/hr) x \left(\frac{\$27.75}{kg/hr}\right) = \$11.4 million$$

Where Q_{CO2} is the mass flow rate of the CO_2 from the system.

Calculation of operating cost of brine aquifer injection:

$$OperatingCost = \frac{\$0.0000912}{\left(\frac{kg}{hr}\right)(mile)} ZQ_{\mathrm{CO_2}} = \frac{\$0.0000912}{\left(\frac{kg}{hr}\right)(feet)}(3100 feet)\left(410{,}810\frac{kg}{hr}\right) = \$116{,}000$$

Functions are taken from Group 8, sequestering of CO_2.