DESIGN OF PLANT TO PRODUCE 100,000 TONNES OF TETRACHLOROETHYLENE PER DAY

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DEDICATION

The first, the last, the right, the left, the centre, the all known, the creator of the heaven, the earth, the oceans, the seas and every thing they comprised, the giver and taker of life, success and wisdom, Almighty Allah. You are the King of kings. I bow before Thee and I dedicate this project work unto Thee. And to my brother and sister Oyekanmi Shereeph and Alimat shadiah I wish and pray we meet some day.

CERTIFICATION

This thesis on plant design by group k in which Oyekanmi B.G. has been accessed and certified to conform with the requirement of the chemical engineering department in the school of engineering and engineering technology in the federal university of technology Mnna for the award of bachelor of chemical engineering.

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Date 11/12/07

Oyekanmi B.G.

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To Allah who promised to take no other gratitude or compensation from me than alamdu *li*'Lah, His messenger, Muhammad (SAW). I acknowledge my late dad my mum Elhaj and Elhaja Muh'Mustaphar. To the accolade lover, the one I qualify as the priceless gem, Oyekanmi G.B. Omolere. May Allah the almighty give you all the joy and comfort you desire under my umbrella. My appreciation also goes to my cousin sister, Oyekanmi Naimat and her love and to my brother and sister Abdul Majeed and Latifah.

ABSTRACT

The important of tetrachloroethene used in dry cleaning, metal decreasing, solvent xtraction, chemical intermediate and pharmaceutical industries can not be over mphasized. It is against this background that the design of a plant to produce 100,000 onnes per day of tetrachloroethene from chlorination of di-chloroethane has been ndertaken. Material and energy balance for the process was carried out. Waste from the lant; HCl, TCE are raw materials for other process industries. The project capital nvestment was estimated to be 10.937 million dollars, the return back investment was 6.17%, payback period of 3.4 years, hence these project was concluded to be conomically viable.

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CHAPTER ONE

1.0 INTRODUCTION

Tetrachloroethene, commonly known as perchloroethylene – PCE, or tetrachloroethene is a commercially important chlorinated hydrocarbon solvent and chemical intermediate. It is used as a day clearing and textile – processing solvent, and for vapour degreasing in metal clearing operations.

Tetrachloroethene is a colourless liquid with ethereal odour; it is slightly soluble in water, soluble in alcohol, ether and oils. It decomposes slowly in the presence of moisture to produce trichloroacetic and hydrochloric acids which may corrode metal containers. It may react violently or explosively with certain alkali metals, sodium hydroxide and aluminum.

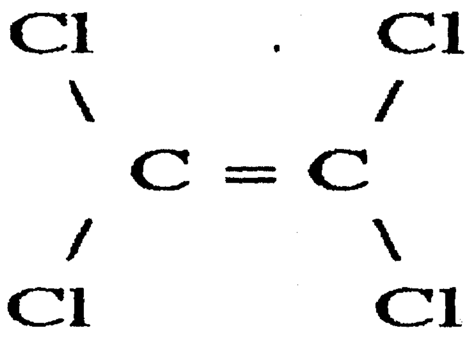
Chlorinated hydercabon solvent such as tetrachloroethen undergo rapid environmental degradation. Tetrachloroethen is not persistent in surface waters due to its water insolubility and because it easily evaporates. It is removed from soil by evaporation to the atmosphere and by leaching action of water. It is non flammable (Orica Botany, 2000).

Like many chlorinates hydrocarbons, tetrachloroethen is a central nervous system depressant, it cause dizziness, headache, sleepiness, confusion, nausea, difficulty in speaking and walking.

Animal studies have shown that, long term exposure to PCE is connected to kidney, liver damage, cancer, unconsciousness and death when its vapour is inhaled in closed, poorly ventilated areas. It causes skin irritation (Wikipedia) PCE is used as antihelmintic agent (IARC 1995, ATSOR 1997).

Michael Faraday first synthesized tetrachloroethene in 1821 by heating hexachloro etha[illegible] until it decomposed into tetrachloroethene and chlorine. (Wikipedia). Tetrachloroethene was first commercially produced in the United States in 1925 via a four-step process using acetylene and chlorine as raw materials. (IARC, 1979). By 1975, only one US plant was using this process because of the high cost of acetylene. Currently, the majority of tetrachloroethene produced in the United State are made by one of the two processor; direct chlorination of certain hydrocarbons or oxychlorination. The first process involves the reaction of chlorine with hydrocarbon such as methane, ethane, propane, or propylene. A chlorinated derivative of hydrocarbon may also be used. The reaction forms a crude product which can be purified to yield a market able grade of tetrachloroethene. This is easier and more economical than acetylene process.

The structure of tetrachloroethylene is illustrated below:



1.1 Raw Materials Used

The raw materials used for manufacture of tetrachloroethene are;

(1) Chlorine gas which can be obtained as a by-product of caustic soda manufactured by electrolysis of brine.

(2) 1,2-Dichloroethane – ethylene dichloride (DCE) which can be obtained via chlorination of thane to form 1,2-dichloroethan. It can be got in large quantity from petrochemical industries.

(3) Hydrochloric acid

(4) Power – The source of power is mainly electricity and steam for heating reactors and distillation columns.

The major equipment used in the plant and their principal use are:

(1) Reactor – Plug flow reactor for reacting chlorine and dichloroethane to form tetrachloroethene, HCl, and trichloroethene.

(2) Quench Tank – The quench tank is a form of reactor more rum away reaction, can be stopped or curtailed.

(3) Separator – The separator is a form of tubular vessel where separation of gracious component can be separated from liquid component by temperature difference. It is mostly used where the boiling point of components/or desired product is far higher than the by-product.

(4) Distillation column – The distillation column is used in separating components with narrow temperature difference.

1.2 Justification

This design work titled "Plant design to produce 100,000 tones of tetrachloroethene per day is essential because of numerous uses of the product.

Tetrachloroethene is the major solvent used in the dry clearing industry because of two important properties. Tetrachloroethene is non-flammable and can be used without fire risk.

Tetrachloroethene can be distilled easily and economically because of its low specific heat. Its low latent heat of vapourization facilities removal of the solvent from garments.

It is used for vapour degreasing of metal articles for use in engineering and automobile applications. The relatively high boiling point of tetrachloroethene enables efficient removal of high melting point waxes and grease.

Tetrachloroethene has high solvent power and thus used for extraction of vegetable, animal and fish oils, and for degreasing bones, worl and leather.

Tetrachloroethene has traditionally been used as a major raw material for the manufacture of the chloro-fluorocarbon R113 (1,1,2-trichloro – 1,2,2-trifluoroethene). R113 has enjoyed wide spread application as a clearing solvent in a variety of industries, particularly where very high clearing standards are required, such as the electronics avitronics, space and defence industries. Since its recognition as an ozone deflecting substances, the manufacture and use of R113 has been controlled under montreal protocol. There has consequently been significant decline in its use and subsequently, demand for tetrachloroethene.

Tetrachloroethene is also used as an insulating fluid and cooling has in electrical transformers, in paint removers printing inks, industries, formulations, paper coatings and leather treatments, in aerosed formulations such as water repellant, automotive cleaners, silicone lubricants, and spot removers, as an extractant for pharmacenticals and as an anthelmiatic agent (IARC 1995, ATSOR 1997).

1.3 Design Philosophy

The task facing process designer at all levels in analyzing, synthesizing and optimizing chemical process system, developing new high performance chemical enterprises, intensisying and optimizing existing chemical complexes, must be tackled on the basis of a precisely formulated objective function. The objective function should be chosen and the condition for its optimization should be assured in the light of the advanced technological principles underlying the development of chemical process system. These include rational use of raw materials and energy, use of bigger items and units, reduction of production wastes, control of objectionable emission and effluents from chemical processing, establishment of inw waste or wasteless manufacturers, environmentally friendly manufacturing etc. When principles are properly adhered to, these principles will enable the designer to come up with a processing unit chich shows optimal performance, both technically and economically.

1.4 Problem Statement

Design of a plant to produce 100,000 tonnes per day of tetrachloroethene by chlorination of 1,2-dichloroethane at 200^0C and 131.0 Kpa.

1.5 Math Cad Software Packages

Math CAD can perform, document, and share all calculations and design work. Math CAD's visual format and scratch pad interface integrate standard mathematical notation, text, and graphs in a single worksheet, thus, making math CAD ideal for knowledge capture, calculation runes, and engineering collaboration. Math CAD allows the design and documentation of engineering work with unit-aware calculations.

Math CAD's open application architecture combined with its support of .NET and its native XML format make it easy to integrate math CAD into other engineering applications.

The Math CAD Calculation Management Suite is the only enterprise – wide solution for managing engineering design and attributes. The files produced and readily publishable into a variety of formats; XML, HTML, PDF, and RTF, and with the use of Math CAD application server, the engineer can publish live maths on the web using existing Math CAD worksheet. For the aforementioned reasons, math CAD will be the choice of the software package for this design work.

CHAPTER TWO

2.0 LITERATURE REVIEW

Tetrachloroethene, also known industrially as perchloroethylene (PCE), is a good solvent used to clean machinery, electronic parts, and clothing. It and trichloroethene (TCE) are suspected carcinogens and some of the most abundant environmental pollutants of groundwater in the United States. In some groundwater, they undergo reductive dechlorination catalyzed by anaerobic bacteria that yields vinyl chloride, a potent human carcinogen. Removal by dumping or air stripping is now largely disallowed and this has focused efforts on biological methods of PCE and TCE remediation in soil and water.

Tetrachloroethylene is not known to occur naturally. Man-made tetrachloroethylene can occur in air over rural and urban sites, in sea-, surface-, ground-, and drinking-water, and in various foodstuffs. The highest levels of tetrachloroethylene in air are found in factories and dry-cleaning establishments. Most tetrachloroethylene is released into the ambient air where it is degraded by sunlight to form products such as hydrogen chloride, trichloroacetic acid, and carbon dioxide. Tetrachloroethylene rapidly evaporates from surface water, and little degradation takes place in water. The compound is persistent in groundwater, which is reason for concern considering the increasing incidence of contamination of groundwater through industrial spillage and waste dumps. Most people can smell tetrachloroethylene when it is present in the air at a concentration of 1 part per million (1 ppm), although some can smell it at even lower levels

2.1 Process Description

1,2-dichloroethane (ethylene dichloride - DCE) chlorination process.

The major products of the 1,2-dichloroethane chlorination process are tetrachloroethene (per chloroethylene – PCE or tetrachloroethylene) and trichloroethene (trichloroethylene - TCE) hydrogen chloride (HCl) is produced as a by-product. The direct chlorination process involves the reactions of DCE with chlorine to a crude product from which marketable – grade PCE and TCE are derived following distillation and purification. The

DCE/chlorine ratio determine which product (PCE or TCE) will be produced in greater quantity. The following chemical equation characterizes the DCE chlorination process.

$$\mathrm{ClCH_2CH_2} + \mathrm{3Cl_2} \xrightarrow[\mathrm{131Kpa}]{200^0} \mathrm{HCl} + \mathrm{Cl2CCCl_2} + \mathrm{0.555Cl2CCHCl}$$

DCE Chlorine PCE TCE

Basic operations that are used in the production of tetrachloroethene by DCE chlorination are shown on the flow diagram in chapter 5.

Alternative Processes

(i) Production from ethylene via 1,2 – dichloroethane by heating dichloro ethane and chlorine to 400^{0}C in the presence of a mixture of potassium chloride and aluminum chloride or activated carbon. Trichloroethene is a major by-product of the reaction.

(ii) Production by chlorination and pyrolysis of propylene at 600^{0}C in a nickel tabular reaction. Tetra chloromethane (Halon 14) is a major byproduct. Tetra chloromethane was listed among the chemical, causing zone layer depletion by Montreal protocol. It has been legislated by USA EPA that no domestic plant should make use of this process because of the tetra chloromethane byproduct and no plant using this process should be commissioned and the existing plants are to be phased out.

(iii)Production by dichloroethane oxochlorination process by the reaction of dichloroethane, chlorine, hydrochloric acid and oxygen at 430^{0}C in the presence of cuper I chloride (CuCl). The major byproduct, are trichloroethene and water.

(iv)Production from tetra chloromethane (carbon tetrachloride) by heating tetra chloromethane at 800 – 900^{0}C chlorine gas is a major by-product.

Chlorination of DCE at 200^{0}C and 131Kpa to produce tetrachloroethene and trichloroethene as a more economical process and also environment friendly.

Catalyst is not used, which means cost of catalyst and catalyst regeneration after fouling has been avoided.

- ✓ The reaction takes place at a lower temperature of 200⁰C. Temperature of 200⁰C is more economical to raise compared to 430⁰C – 600⁰C required for other processes.
- ✓ The byproduct are marketable and environment friendly unlike tetra chloromethane which causes ozone layer depletion.
- ✓ Use of separator as against decanters, caustic washer, and dehydrators, makes the process more economical.

2.2 Physico-chemical Properties

Tetrachloroethylene is a volatile, non-flammable, colourless liquid. Most people can smell it at 1 part of perc per million parts of air (ppm), which is equivalent to about 6.78 mg of perc per m^3 of air. Tetrachloroethylene is slightly soluble in water and is miscible with most organic solvents. Chemical Abstract Society (CAS) number is 127-18-4. The summary of its relevant physico-chemical properties is presented in the table below:

Table2. 1: Physical and Chemical Properties of Tetrachloroethylene

PROPERTY	CHARACTERISTIC
Chemical formula	C_2Cl_4
Physical state	Liquid (at room temperature)
Colour	Colourless
Molecular Weight	165.83
Density at 20°C	1.6227g/mL
Melting point	-19°C
Boiling point	121°C
Odour	Ethereal

2.3 Methods of exposure

People are exposed to Tetrachloroethylene in air, water, and food. Exposure can also occur when Tetrachloroethylene or material containing it (for example, soil) gets on the skin. For most people, almost all exposure is from it in air.

Tetrachloroethylene gets into outdoor and indoor air by evaporation from industrial or dry-cleaning operations and from areas where chemical wastes are stored or disposed. Groundwater near these areas may become contaminated if PCE is improperly dumped or leaks into the ground People may be exposed if they drink the contaminated water. They may also be exposed if PCE evaporates from contaminated drinking water into indoor air during cooking and washing. PCE may evaporate from contaminated groundwater and soil and into the indoor air of buildings above the contaminated area. PCE also may evaporate from dry-cleaned clothes and into indoor air or may get into indoor air after PERC-products, such as spot removers, are used. Indoor air PCE levels may get high if its-products are used in poorly ventilated areas.

2.3.1 Long-Term Exposure – Numerous studies of dry-cleaning workers indicate that long-term exposure (9 to 20 years, for example) to workplace air levels averaging about 50,000 mcg/m$_3$ to 80,000 mcg/m$_3$ reduces scores on behavioral tests and causes biochemical changes in blood and urine. The effects were mild and hard to detect. How long these effects would last if exposure ended is not known.

2.3.2 Long-Term Exposure – Numerous studies of dry-cleaning workers indicate that longterm exposure (9 to 20 years, for example) to workplace air levels averaging about 50,000 mcg/m$_3$ to 80,000 mcg/m$_3$ reduces scores on behavioral tests and causes biochemical changes in blood and urine. The effects were mild and hard to detect. How long these effects would last if exposure ended is not known (NYDOH, 2003).

2.4 Disposal of used tetrachloroethylene

Base on International Register of Potentially Toxic Chemicals (IRPTC), Contaminated tetrachloroethylene can be regenerated by distillation. The residue may be treated further by steam distillation. The remaining waste should be incinerated after mixing with a combustible fuel. Assure complete combustion to prevent the formation of phosgene. An acid scrubber is necessary to remove the haloacids produced. The haloacids may be recovered from waste gases and reused. Recent Federal regulations prohibit land disposal of various chlorinated solvent materials that may contain tetrachloroethylene. Any solid waste containing tetrachloroethylene must be listed as a hazardous waste unless the waste is shown not to endanger the health of humans or the environment (EPA 1985b, 1988). Destruction and removal efficiency of tetrachloroethylene that is designated as a principal organic hazardous constituent must be 99.99%. Discharge of PCE into U.S. waters requires a permit (WHO,1987). Before implementing land disposal of waste residue, environmental regulatory agencies should be consulted for recent guidance on acceptable disposal practice (HSDB, 1996).

2.5 Main Hazards for Man

Tetrachloroethylene vapour irritates the skin, eyes, and respiratory tract and affects the central nervous system. The liquid also irritates the skin and eyes. The compound may be toxic for the human embryo at high concentrations.

2.5.1 Health effect

In high concentrations in air, particularly in closed, poorly ventilated areas, single exposures to tetrachloroethylene can cause central nervous system (CNS) effects leading to dizziness, headache, sleepiness, confusion, nausea, difficulty in speaking and walking, and possibly unconsciousness and death. As might be expected, these symptoms occur almost entirely in work (or hobby) environments. The potential long-term health effects that might occur in humans from breathing lower levels of tetrachloroethylene than those that produce CNS effects or from ingesting very low levels of the chemical found in some water supplies have not been identified. The effects of exposing infants to tetrachloroethylene through breast milk are unknown

Animal studies, conducted with amounts much higher than typical environmental levels, have shown that tetrachloroethylene can cause liver and kidney damage, liver and kidney cancers, and leukemia (cancer of the tissues that form the white blood cells). Developmental effects in fetuses have been observed but only at tetrachloroethylene exposure levels that also produce toxicity in the maternal animal.

The U.S. Department of Health and Human Services has determined that tetrachloroethylene may reasonably be anticipated to be a carcinogen. Based on evidence from animal studies, tetrachloroethylene is thought to be capable of causing cancer in humans. It should be emphasized, however, that currently available information is not sufficient to determine whether tetrachloroethylene causes cancer in humans.

Short-term exposures to air containing more than 100 ppm of tetrachloroethylene have produced harmful effects in both humans and animals, and more prolonged exposures to approximately 9 ppm caused harmful liver effects in mice. It should be pointed out that some of the highest environmental levels of tetrachloroethylene ever recorded (at waste disposal sites, for example) were still 150 times smaller than the concentrations shown to produce symptoms of toxicity in animals after repeated exposure. Drinking (or eating) the equivalent of approximately 60 to 80 mg (less than a spoonful) of undiluted tetrachloroethylene per kg of body weight (1 kg = 2.2 pounds) has produced effects similar to drinking alcohol. Tetrachloroethylene was used in the past as a medicine to eliminate worms in humans, but safer and more effective drugs are now available. More prolonged exposures in animals have produced harm to the liver at doses of approximately 100 mg/kg/day. These levels of exposure are more than 1,000 times higher than would be expected even if humans ingested the most contaminated drinking water ever reported.

Cancer--From data in animals, EPA has estimated that if people breathe air containing 1 ppm tetrachloroethylene all day every day for 70 years, there would be an added risk of 66 additional cases of cancer in a population of 10,000 people (or 65,500 additional cases in a population of 10,000,000) over the number of cases that would be observed in a population not exposed to tetrachloroethylene. If people consume 1.0 mg tetrachloroethylene/kg/day in food and water every day for 70 years, there would be at the most a risk of 510 additional cases of cancer in a population of 10,000, or 510,000 additional cases in a population of 10,000,000. It should be noted that these risk values are plausible upper-limit estimates. Actual risk levels are unlikely to be higher and may be lower (ATSDR, 1990)

2.6 Testing for Tetrachloroethylene

One method of testing for tetrachloroethylene exposure is to measure the amount of the chemical in the breath, much the same way breath-alcohol measurements are used to determine the amount of alcohol in the blood.

Because it is stored in the body's fat and slowly released into the bloodstream, tetrachloroethylene can be detected in the breath for weeks following a heavy exposure.

Tetrachloroethylene and trichloroacetic acid (TCA), a breakdown product of tetrachloroethylene, can be detected in the blood. These tests are relatively simple to perform. These tests are not available at most doctors' offices, but can be performed at laboratories with the necessary equipment. Because exposure to other chemicals can produce the same breakdown products in the urine and blood, the tests for breakdown products cannot determine if one has been exposed to tetrachloroethylene or the other chemicals.

2.7 Genotoxicity and Carcinogenicity

It appears that the mutagenic activities of perc in *in vivo* rodent tests are due to the activities of its glutathione conjugates. Glutathione conjugation is of less importance as a metabolic process in humans than in rodents. It is therefore expected that perc may induce only minimal genotoxic effects in humans at low doses (ATSDR, 1995).

The evidence for increases of cancer incidence of any type in human epidemiological studies is inconsistent for perc. Important species difference exists, implicating that humans may be relatively less sensitive to the cancer-causing effects of perc than rodents. The carcinogenic effect of perc is probably due to the metabolite TCA. This metabolite is of minor importance in humans but is much more important in mice. Furthermore, mice and rats respond to TCA by hepatocellular peroxisome induction, while humans are relatively insensitive to this compound and other peroxisome proliferators. Peroxisome proliferation is believed to induce cancer, although the exact mechanism of this induction is not yet known.

There is no consensus in the scientific and regulatory community regarding the likelihood of perc as a carcinogen in humans. Because this issue could have a significant impact on the assessment of its toxicity, it will be discussed below in some detail.
Based on relatively weak evidence of carcinogenicity in humans but good evidence of carcinogenicity in rodents, International Agency for Research on Cancer (IARC, 1995) has classified perc as *probably carcinogenic to humans* ("2A" carcinogen). The most recent IRIS update (US EPA, 1992) has not included the US EPA's weight-of-evidence classification of perc with reference to its carcinogenicity.

However, ATSDR (1995) reported US EPA's official position regarding perc being on the continuum between group B2 (probable human carcinogen, sufficient evidence from animals studies but inadequate evidence or no data from epidemiological studies) and group C (possible human carcinogen, limited evidence for carcinogenicity in animals, inadequate human carcinogenicity data). In 1986, USEPA proposed to classify perc as a probable human carcinogen (*B2*), which was not supported by the Science Advisory Board of USEPA (ATSDR, 1995). While California Environmental Protection Agency (Cal EPA, 1991) supported the classification of perc as a *probable human carcinogen*, Health Canada (CEPA, 1993) considered perc as *possibly carcinogenic to humans* (Group III) in 1993, but revised its classification to Group IV (unlikely to be carcinogenic to humans) in 1996 (Health Canada, 1996a). The European Union, on the other hand, considered perc not classifiable as to carcinogenicity, but is of concern to humans owing to possible carcinogenic effects (Beck, 2000). Germany also considered perc to have suspected carcinogenic potential (Beck, 2000).

Health Canada's position is well supported by ATSDR's (1995) discussion on the subject. In essence, there is a general agreement that the human data are by themselves insufficient to definitively identify perc as a carcinogen. There is also a good agreement on the toxicity and carcinogenicity of perc in rodents. The key area of contention for perc relates to whether rodent data can be directly applied to humans. (CEPA 1993) argued that there were sufficient differences in the metabolism of perc in rodents versus humans (see earlier paragraphs in the section for discussion of these differences) that it was unlikely that perc induces cancer effects in humans by the same mechanism as in rodents. World Health Organization (WHO, 1996) also concluded that there was limitation in epidemiological evidence and in our understanding of the mechanism of tumour induction in animals for perc. As a result, (WHO,1996) chose to assess perc related health risk based on toxic endpoints other than cancer. The rationale for evaluating perc toxicity based on its non-cancer endpoints is compelling and it is recommended that perc not be treated as a human carcinogen for the purpose of evaluating health risk due to perc exposure.

2.8 Regulations

The government has made recommendations to limit the exposure of the general public to tetrachloroethylene in drinking water and the exposure of workers to tetrachloroethylene in the work place.

The Environmental Protection Agency (EPA) has developed the following health advisories to describe concentrations of tetrachloroethylene in drinking water at which no adverse effects are anticipated to occur: 2.0 milligrams per liter of water (mg/L) for short-term exposure of children, 1.4 mg/L for longer term exposure of children, and 5.0 mg/L for long-term exposure of adults. In addition, a drinking water equivalent level (DWEL) of 0.5 mg/L has been established.

The Occupational Safety and Health Administration (OSHA) has a legally enforceable exposure limit of 25 ppm tetrachloroethylene in air for an 8-hour workday, 40-hour workweek based on noncancer health considerations. The National Institute for Occupational Safety and Health (NIOSH) has classified tetrachloroethylene as a potential occupational carcinogen and recommends that workplace exposure be limited to the lowest possible level.

2.9 Trichloroethylene

This is one of the major by-products from the production of tetrachloroethylene. Trichloroethylene is a chlorinated hydrocarbon commonly used as an industrial solvent. It is a clear non-flammable liquid with a sweet smell. Trichloroethylene is an effective solvent for a variety of organic materials. When it was first widely produced in the 1920s, its major use was to extract vegetable oils from plant materials such as soy, coconut, and palm. Other uses in the food industry included coffee decaffeination and the preparation of flavoring extracts from hops and spices. It was also used as a dry cleaning solvent, although tetrachloroethylene (also known as perchloroethylene) surpassed it in this role in the 1950s. Typically, trichloroethylene and tetrachloroethylene are collected together and then separated by distillation.

2.10 Environmental fate of tetrachloroethylene

Environmental fate of tetrachloroethylene has been reviewed extensively by Agency for Toxic Substances and Diseases Registry (ATSDR, 1994; CEPA, 1993). Only a brief summary will be provided below.

Monitoring data have demonstrated that tetrachloroethylene is present in the atmosphere world-wide and at locations far removed from anthropogenic emission sources. This chemical is highly volatile and wet deposition will be quickly reversed by volatilisation. It also rapidly volatilises from dry soil surfaces. It has a long half-life in the air.

Tetrachloroethylene partitions rapidly to the atmosphere from surface water and evaporation is the major route of removal of tetrachloroethylene from water. The half-life of evaporation from surface water is several hours. The half-life for volatilisation from the soil ranges from several days to several weeks. The mobility in soil depends greatly on the organic content. In sandy soil, the mobility is high. In fine soil rich in organic matter, the mobility is low due to adsorption on particles rich with organic matter.

Tetrachloroethylene does not bioaccumulate and biomagnification in the aquatic food chain does not appear to be important. Bioaccumulation in plants may be indicated by the presence of tetrachloroethylene in fruits and vegetables but it is unclear whether accumulation takes place during growth or at some point after harvesting

The most important means of degrading tetrachloroethylene in the atmosphere is its reaction with photochemically produced hydroxyl radicals. The half-life for this process is within months. The degradation products of this reaction include phosgene, chloroacetylchlorides, formic acid, carbon monoxide, carbon tetrachloride, and hydrochloric acid.

Tetrachloroethylene does not readily transform in water. There are large variations in the estimates for its half-life of abiotic transformation in water, but it probably ranges from several months to several years.

Biodegradation is probably somewhat faster, but even this process proceeds slowly. Since neither biodegradation nor hydrolysis occurs at a rapid rate, tetrachloroethylene present in surface waters can be expected to volatilise into the atmosphere or sink and thus be removed from contact with the surface.

Volatilisation will therefore not be a viable process for this fraction of tetrachloroethylene, which may instead be rapidly transported into groundwater by leaching through fissures rather than matrix pores. The sinking of tetrachloroethylene into groundwater also makes clean up difficult.

Biodegradation of tetrachloroethylene in soil appears to occur only under specific conditions, and then only to a limited degree. The main proximal metabolite is trichloroethylene and the ultimate metabolite is vinyl chloride under anaerobic conditions.

2.10.1 Environmental Concentrations

Predicted Environmental Concentrations (PECs) have been calculated for specific sites involved in the production of tetrachloroethylene and its use as an intermediate. For other uses a combination of specific information and default values has been used. Calculations were performed using the Technical Guidance document.

CHAPTER THREE

3.0 MATERIAL BALANCE

$BASIS = 100\frac{kmol}{hr}$ of Dichloroethlene

$i := 1..6$

Balance Around DCE Pump

$Species_i :=$	$Mole\_1_i :=$	$Mwt_i :=$
DCE	100	98.96
CL_2	0	70.91
TCE	0	131.39
PCE	0	165.83
HCL	0	36.46
H2O	0	18.02

Pump Mass inlet

$Mass\_Pump\_in_i := Mole\_1_i \cdot Mwt_i \cdot \delta$

$Species_i :=$	$Mass\_Pump\_in_i$ $\frac{kg}{s}$
DCE	2.749
CL_2	0
TCE	0
PCE	0
HCL	0
H2O	0

$Mass\_Pump\_out_i := Mass\_Pump\_in_i$

$Species_i :=$	$Mass\_Pump\_out_i$ $\frac{kg}{s}$
DCE	2.749
CL_2	0
TCE	0
PCE	0
HCL	0
H2O	0

$$\text{Pump\_input} := \sum_i \text{Mass\_Pump\_in}_i$$

$$\text{Pump\_input} = 2.749 \frac{kg}{s}$$

$$\text{Pump\_output} := \sum_i \text{Mass\_Pump\_out}_i$$

$$\text{Pump\_output} = 2.749 \frac{kg}{s}$$

MASS BALANCE AROUND PREHEATER

PREHEATER INPUT

$$\text{Mass\_Preheater\_input}_i := \text{Mass\_Pump\_out}_i$$

$\text{Species}_i :=$	$\text{Mass\_Preheater\_input}_i$ ($\frac{kg}{s}$)
DCE	2.749
CL_2	0
TCE	0
PCE	0
HCL	0
H2O	0

PREHEATER OUTPUT

$$\text{Mass\_Preheater\_output}_i := \text{Mass\_Preheater\_input}_i$$

$\text{Species}_i :=$	$\text{Mass\_Preheater\_output}_i$ ($\frac{kg}{s}$)
DCE	2.749
CL_2	0
TCE	0
PCE	0
HCL	0
H2O	0

MASS BALANCE AROUND CHLORINE COMPRESSOR

$\text{Species}_i :=$

DCE
CL_2
TCE
PCE
HCL
H2O

$\text{CHL\_MOLE\_IN}_i :=$

0
300
0
0
0
0

$$\text{Comp\_Mass\_in}_i := \text{CHL\_MOLE\_IN}_i \cdot \text{Mwt}_i \cdot \delta$$

$\text{Species}_i :=$

DCE
CL_2
TCE
PCE
HCL
H2O

$\text{Comp\_Mass\_in}_i =$ $\frac{kg}{s}$

	0
0	0
1	5.909
2	0
3	0
4	0
5	0

COMPRESSOR OUTPUT

$$\text{Comp\_Mass\_out}_i := \text{Comp\_Mass\_in}_i$$

$\text{Species}_i :=$

DCE
CL_2
TCE
PCE
HCL
H2O

Comp_Mass_out_i $\frac{kg}{s}$

0
5.909
0
0
0
0

$$\text{Compressor\_Input} := \sum_i \text{Comp\_Mass\_in}_i$$

$$\text{Compressor\_Input} = 5.909 \frac{kg}{s}$$

$$\text{Compressor\_Output} := \sum_i \text{Comp\_Mass\_out}_i$$

$$\text{Compressor\_Output} = 5.909\frac{kg}{s}$$

3.5 BALANCE AROUN THE REACTOR

REACTOR INPUT

$\text{RCT\_input\_1}_i := \text{Comp\_Mass\_out}_i$

$\text{RCT\_input\_2}_i := \text{Mass\_Preheater\_output}_i$

$\text{Species}_i :=$	RCT_input_1_i $\frac{kg}{s}$	RCT_input_2_i $\frac{kg}{s}$
DCE	0	2.749
CL_2	5.909	0
TCE	0	0
PCE	0	0
HCL	0	0
H2O	0	0

$$\text{TOTAL\_REACTOR\_INPUT} := \sum_i \left(\text{RCT\_input\_1}_i + \text{RCT\_input\_2}_i\right)$$

$$\text{TOTAL\_REACTOR\_INPUT} = 8.658\frac{kg}{s}$$

REACTOR OUTPUT STREAM

$\text{Species}_i :=$	$\text{RCT\_Fraction\_out}_i :=$
DCE	0.0032
CL_2	0.0068
TCE	0.2316
PCE	0.5267
HCL	0.2316
H2O	0.0

$$\text{TOTAL\_FRACTION} := \sum_{i} \text{RCT\_Fraction\_out}_{i}$$

$$\text{TOTAL\_FRACTION} = 1$$

$$\text{RCT\_Mass\_Out}_{i} := \text{RCT\_Fraction\_out}_{i} \cdot M$$

$\text{Species}_{i} :=$	RCT_Mass_Out_{i} ($\frac{kg}{s}$)
DCE	0.028
CL_2	0.059
TCE	2.005
PCE	4.56
HCL	2.005
H2O	0

$$\sum_{i} \text{RCT\_Mass\_Out}_{i} = 8.657 \frac{kg}{s}$$

MATERIAL BALANCE AROUND QUENCHING TANK

INPUT

$$\text{QCH\_TANK\_INPUT\_1}_{i} := \text{RCT\_Mass\_Out}_{i}$$

$$\text{QCH\_TANK\_INPUT\_2}_{i} := \text{HCl\_IN}_{i} \cdot \frac{kg}{hr}$$

$\text{Species}_{i} :=$	$\text{QCH\_TANK\_INPUT\_1}_{i}$ ($\frac{kg}{s}$)	$\text{QCH\_TANK\_INPUT\_2}_{i}$ ($\frac{kg}{s}$)
DCE	0.028	0
CL_2	0.059	0
TCE	2.005	0
PCE	4.56	0
HCL	2.005	0.101
H2O	0	0

$$\mathrm{TANK\_INPUT} := \sum_{i} \left(\mathrm{QCH\_TANK\_INPUT\_1}_{i} + \mathrm{QCH\_TANK\_INPUT\_2}_{i} \right)$$

$$\mathrm{TANK\_INPUT} = 8.759 \frac{kg}{s}$$

QUENCHING TANK OUTPUT

$$\mathrm{QCH\_TANK\_OUTPUT}_{i} := \mathrm{QCH\_TANK\_INPUT\_1}_{i} + \mathrm{QCH\_TANK\_INPUT\_2}_{i}$$

$\mathrm{Species}_{i} :=$	$\mathrm{QCH\_TANK\_OUTPUT}_{i}$ ($\frac{kg}{s}$)
DCE	0.028
CL_2	0.059
TCE	2.005
PCE	4.56
HCL	2.107
H2O	0

$$\mathrm{TOTAL\_TANK\_OUTPUT} := \sum_{i} \mathrm{QCH\_TANK\_OUTPUT}_{i}$$

$$\mathrm{TOTAL\_TANK\_OUTPUT} = 8.759 \frac{kg}{s}$$

3.7 MATERIAL BALANCE AROUND SEPARATOR

$$\mathrm{SEPARATOR\_INPUT}_{i} := \mathrm{QCH\_TANK\_OUTPUT}_{i}$$

$\mathrm{Species}_{i} :=$	$\mathrm{SEPARATOR\_INPUT}_{i}$ ($\frac{kg}{s}$)
DCE	0.028
CL_2	0.059
TCE	2.005
PCE	4.56
HCL	2.107
H2O	0

$$\mathrm{TOTAL\_SEPARATOR\_INPUT} := \sum_{i} \mathrm{SEPARATOR\_INPUT}_{i}$$

$$\mathrm{TOTAL\_SEPARATOR\_INPUT} = 8.759 \frac{\mathrm{kg}}{\mathrm{s}}$$

SEPARATOR OUTPUT

$\mathrm{Species}_i :=$	$\mathrm{SPTR\_OUTPUT\_FRACTION\_1}_i :=$	$\mathrm{SPTR\_OUTPUT\_FRACTION\_2}_i :=$
DCE	0.00265	0.004
CL_2	0.0006	0.0188
TCE	0.2658	0.1555
PCE	0.7254	0.1124
HCL	0.0054	0.7092
H2O	0.0	0.0

$$\sum_{i} \mathrm{SPTR\_OUTPUT\_FRACTION\_1}_{i} = 1$$

$$\sum_{i} \mathrm{SPTR\_OUTPUT\_FRACTION\_2}_{i} = 1$$

OUTPUT

$$\mathrm{HCL\_STREAM}_{i} := \mathrm{SPTR\_OUTPUT\_FRACTION\_2}_{i} \cdot 21000 \frac{\mathrm{kg}}{\mathrm{hr}}$$

$$\mathrm{PCE\_TCE\_STREAM}_{i} := \mathrm{SPTR\_OUTPUT\_FRACTION\_1}_{i} \cdot 10530 \frac{\mathrm{kg}}{\mathrm{hr}}$$

$\mathrm{Species}_i :=$	$\mathrm{HCL\_STREAM}_i$ ($\frac{\mathrm{kg}}{\mathrm{s}}$)	$\mathrm{PCE\_TCE\_STREAM}_i$ ($\frac{\mathrm{kg}}{\mathrm{s}}$)
DCE	0.023	7.751?10-3
CL_2	0.11	1.755?10-3
TCE	0.907	0.777
PCE	0.656	2.122
HCL	4.137	0.016
H2O	0	0

$$\text{SEPARATOR\_OUTPUT} := \sum_{i} \left(\text{HCL\_STREAM}_i + \text{PCE\_TCE\_STREAM}_i\right)$$

$$\text{SEPARATOR\_OUTPUT} = 8.76\,\frac{kg}{s}$$

3.8 MATERIAL BALANCE AROUND THE DISTILLATION COLUMN

$$\text{COLUMN\_INPUT\_STREAM}_i := \text{PCE\_TCE\_STREAM}_i$$

$\text{Species}_i :=$

DCE
CL_2
TCE
PCE
HCL
H2O

PCE_TCE_STREAM_i

$7.751\cdot10^{-3}$	$\frac{kg}{s}$
$1.755\cdot10^{-3}$	
0.777	
2.122	
0.016	
0	

COLUMN OUTPUT

OVERALL BALANCE

$F = D + B \qquad ...1$

COMPONENT BALANCE OF PCE

$0.7264\cdot F = 0.04\cdot D + 0.98\cdot B \qquad ...2$

$F := \text{SEPARATOR\_OUTPUT}$

FROM EQN 1

$D = F - B \qquad ...3$

PUT EQN 3 INTO EQN 2

$0.7264\cdot F = 0.04\cdot(F - B) + 0.98\cdot B$

$B := .73021276595744680851F$

$$B = 6.395\frac{kg}{s}$$

$$D := F - B$$

$$D = 2.363\frac{kg}{s}$$

$\mathrm{Species}_i :=$	$\mathrm{TOP\_PROD}_i :=$	$\mathrm{BOTTOM\_PROD}_i :=$
DCE	0.001	0
CL_2	0.004	0
TCE	0.935	.02
PCE	.04	.98
HCL	.02	0
H2O	0	0

FLOWRATE

$$\mathrm{TCE\_STRM}_i := D \cdot \mathrm{TOP\_PROD}_i$$

$$\mathrm{PCE\_STRM}_i := B \cdot \mathrm{BOTTOM\_PROD}_i$$

$\mathrm{Species}_i :=$	$\mathrm{TCE\_STRM}_i =$ ($\frac{kg}{s}$)	$\mathrm{PCE\_STRM}_i =$ ($\frac{kg}{s}$)
DCE	$2.363 \cdot 10^{-3}$	0
CL_2	$9.45 \cdot 10^{-3}$	0
TCE	2.209	0.128
PCE	0.095	6.267
HCL	0.047	0
H2O	0	0

CHAPTER FOUR

4.0 ENERGY BALANCE

4.1 ENERGY BALANCE AROUND PUMP

INLET ENERGY = INLET MASS * INLET ENTHALPHY

$\text{Species}_i :=$

Species_i	Mass_Pump_in_i $\frac{kg}{s}$	$\text{Pump\_inlet\_enthalpy}_i$ $\frac{m^2}{s^2}$
DCE	2.749	1.623?106
CL_2	0	0
TCE	0	0
PCE	0	0
HCL	0	0
H2O	0	0

Inlet Energy

$$\text{pump\_inlet\_energy}_i := \text{Pump\_inlet\_enthalpy}_i \cdot \text{Mass\_Pump\_in}_i$$

$\text{Species}_i :=$

Species_i	$\text{pump\_inlet\_energy}_i$ W
DCE	4.461?106
CL_2	0
TCE	0
PCE	0
HCL	0
H2O	0

at_25 °C

Outlet Energy

$$pump\_outlet\_energy_i := pump\_inlet\_energy_i$$

Species$_i$:=	pump_outlet_energy$_i$
DCE	4.461?106 W
CL_2	0
TCE	0
PCE	0
HCL	0
H2O	0

at_25 °C

4.2 ENERGY BALANCE AROUND PREHEATER

INLET ENERGY = INLET MASS * INLET ENTHALPY

at_25 °C

Species$_i$:=	Mass_Preheater_input$_i$	Preheater_inlet_enthalpy$_i$
DCE	2.749 $\frac{kg}{s}$	1.623?106 $\frac{m^2}{s^2}$
CL_2	0	0
TCE	0	0
PCE	0	0
HCL	0	0
H2O	0	0

Inlet Energy

$$preheater\_inlet\_energy_i := Preheater\_inlet\_enthalpy_i \cdot Mass\_Preheater\_input_i$$

Species$_i$:=	preheater_inlet_energy$_i$
DCE	4.461?106 W
CL_2	0
TCE	0
PCE	0
HCL	0
H2O	0

$$PREHEATER\_ENERGY\_INLET := \sum_i preheater\_inlet\_energy_i$$

$\text{PREHEATER\_ENERGY\_INLET} = 4.461 \times 10^{6}\ \text{W}$

PREHEATER OUTLET ENERGY AT 25°C

$\text{Species}_i :=$	$\text{Mass\_Preheater\_output}_i$ $\frac{kg}{s}$	$\text{preheater\_outlet\_enthalpy}_i$ $\frac{m^2}{s^2}$
DCE	2.749	1.28?106
CL_2	0	0
TCE	0	0
PCE	0	0
HCL	0	0
H2O	0	0

outlet energy

$$\text{preheater\_outlet\_energy}_i := \text{preheater\_outlet\_enthalpy}_i \cdot \text{Mass\_Preheater\_output}_i$$

$\text{Species}_i :=$	$\text{preheater\_outlet\_energy}_i$ W
DCE	3.518?106
CL_2	0
TCE	0
PCE	0
HCL	0
H2O	0

$$\text{ENERGY\_OUTPUT} := \sum_i \text{preheater\_outlet\_energy}_i$$

$\text{ENERGY\_OUTPUT} = 3.518 \times 10^{6}\ \text{W}$

ENERGY BALANCE EQUATION

$Q_{in} + Q\_PRE\_HT_{rqd\_1} = Q_{out}$

$Q_{in} = PREHEATER\_ENERGY\_INLI$

$Q_{out} = ENERGY\_OUTPU$

$Q\_PRE\_HT_{rqd\_1} := Q_{out} - Q_{in}$

$Q\_PRE\_HT_{rqd\_1} = 9.431 \times 10^{5}\ W$

4.4 ENERGY BALANCE AROUND THE REACTOR

$Q\_RCT\_IN\_1_i := Comp\_Mass\_out_i \cdot 5628.6 \frac{J}{kg}$

$Q\_RCT\_IN\_2_i := preheater\_outlet\_energy_i$

HCl @ 40°C

EDC@

$Species_i :=$	$Q\_RCT\_IN\_1_i =$ (W)	$Q\_RCT\_IN\_2_i =$ (W)
DCE	0	3.518?106
CL_2	3.326?104	0
TCE	0	0
PCE	0	0
HCL	0	0
H2O	0	0

OUTPUT ΔH @ 200°C

$Species_i :=$	$RCT\_Mass\_Out_i$ ($\frac{kg}{s}$)	$\Delta H\_RCT\_OUT_i =$ ($\frac{m^2}{s^2}$)
DCE	0.028	1.157?106
CL_2	0.059	8.597?104
TCE	2.005	7.36?104
PCE	4.56	3.457?104
HCL	2.005	2.392?106
H2O	0	1.305?107

$Q\_RCT\_OUT_i := RCT\_Mass\_Out_i \cdot \Delta H\_RCT\_OUT_i$

$Species_i :=$

DCE
CL_2
TCE
PCE
HCL
H2O

$Q\_RCT\_OUT_i =$

3.206?104	W
5.062?103	
1.476?105	
1.576?105	
4.796?106	
0	

ENERGY BALANCE EQUATION

$$Q\_RCT\_OUT_i = \sum_i \left[\left(Q\_RCT\_IN\_1_i + Q\_RCT\_IN\_2_i \right) + Q_{add} \right]$$

$$Q_{add} := \sum_i Q\_RCT\_OUT_i - \sum_i \left(Q\_RCT\_IN\_1_i + Q\_RCT\_IN\_2_i \right)$$

$$Q_{add} = 1.587 \times 10^6 \, W$$

4.5 ENERGY BALANCE AROUND QUENCHING TANK

INPUT

$Q\_IN\_QCH\_TK\_1_i := Q\_RCT\_OUT_i$

$Q\_IN\_QCH\_TK\_2_i := QCH\_TANK\_INPUT\_2_i \cdot -2530.4\varepsilon \cdot \frac{J}{kg}$

$Species_i :=$

DCE
CL_2
TCE
PCE
HCL
H2O

$Q\_IN\_QCH\_TK\_1_i$

3.206?104	W
5.062?103	
1.476?105	
1.576?105	
4.796?106	
0	

$Q\_IN\_QCH\_TK\_2_i$

0	W
0	
0	
0	
-2.563?105	
0	

OUTPUT @ 195°C

$Species_i :=$	$\Delta H\_QCH\_TK\_OUT_i$
DCE	1.162?106
CL_2	8.343?104
TCE	6.989?104
PCE	3.123?104
HCL	2.396?106
H2O	1.306?107

$\frac{m^2}{s^2}$

$$Q\_OUT\_QCH\_TK_i := \Delta H\_QCH\_TK\_OUT_i \cdot QCH\_TANK\_OUTPUT_i$$

$Species_i :=$	$Q\_OUT\_QCH\_TK_i$
DCE	3.22?104
CL_2	4.912?103
TCE	1.401?105
PCE	1.424?105
HCL	5.047?106
H2O	0

W

$$Q\_QCH\_TK\_LOSS := \sum_i \left(Q\_IN\_QCH\_TK\_1_i + Q\_IN\_QCH\_TK\_2_i\right) - \sum_i Q\_OUT\_QCH\_TK_i$$

$$Q\_QCH\_TK\_LOSS = -4.845 \times 10^5 \, W$$

This is the amount of heat loss from reactor product to chlorine quenching stream

Energy Balance Around the Separator

Separator_Input_Energy = Queching_Tank_Output_Energy

$\text{Species}_i :=$

DCE
Cl_2
TCE
PCE
HCL
H2O

$\text{Q\_SPTR\_IN}_i =$

3.22·104	W
4.912·103	
1.401·105	
1.424·105	
5.047·106	
0	

$$\text{Q\_SPRT\_IN} := \sum_i \text{Q\_SPTR\_IN}_i$$

$\text{Q\_SPRT\_IN} = 5.367\times 10^6\ \text{W}$

SEPARATOR OUTPUT ENERGY

AT 40 deg

OUTPUT ENTHALPY

$\text{Species}_i :=$

DCE
Cl_2
TCE
PCE
HCL
H2O

$\Delta\text{H\_SPRT\_OUT}_i =$

-1.605·106	$\frac{m^2}{s^2}$
6.097·103	
7.182·104	
-2.938·105	
-2.522·106	
4.522·104	

OUTPUT ENERGY

STREAM ONE OUTPUT

$\text{Q\_SPRT\_1}_i := \text{PCE\_TCE\_STREAM}_i \cdot \Delta\text{H\_SPRT\_OUT}_i$

$\text{Q\_SPRT\_2}_i := \text{HCL\_STREAM}_i \cdot \Delta\text{H\_SPRT\_OUT}_i$

$\text{Species}_i :=$

DCE
CL_2
TCE
PCE
HCL
H2O

$\text{Q\_SPRT\_1}_i =$

$-1.244\cdot 10^{4}$	W
10.7	
$5.583\cdot 10^{4}$	
$-6.234\cdot 10^{5}$	
$-3.984\cdot 10^{4}$	
0	

$$\text{Q\_SPRT\_OUT} := \sum_i \left(\text{Q\_SPRT\_1}_i + \text{Q\_SPRT\_2}_i\right)$$

$$\text{Q\_SPRT\_OUT} = -1.122\times 10^{7}\ \text{W}$$

HEAT EQUATION

$$\text{Q\_REMOVED} := \text{Q\_SPRT\_OUT} + \text{Q\_SPRT\_IN}$$

$$\text{Q\_REMOVED} = -5.851\times 10^{6}\ \text{W}$$

CHAPTER FIVE

5.0 FLOW SHEET

The flow sheet below shows the movement of the raw material the process line, till the final product is formed alongside the major and minor by-products. The basic operations that may be used in the production of PCE and TCE, are shown in the flow sheet shown below.

The EDC stream is subjected to heating by passage through a heater and this is emptied into the chlorinating reactor, alongside chlorine stream which is also passed into the chlorinating reactor. Both vapours are thus fed into the chlorinating reactor. Chlorination is carried out at a high temperature of about 200,°C, slightly above the atmospheric pressure, without the use of a catalyst.

The product stream from the chlorinating chamber, TCE/PCE/HCl consists of a mixture of chlorinated hydrocarbons and HCl, Hydrogen chloride stream. The product mixture is then passed into a quench tank to reduce the temperature of the product fluid .The quenched product mixture emerges from the quench tank, LV stream and moves into the product separator to separate HCl stream from its mixture with the chlorinated hydrocarbons, PROD stream, which proceed into the distillation column where both PCE stream and TCE stream, these then proceeds into storage tanks.

The HCl i.e. Hydrogen chloride is also sent to a storage tank, to be put to other uses. The above described flow sheet is diagrammatically represented below.

Figure 5.1: Flow sheet of the process

CHAPTER SIX

6.0 EQUIPMENT DESIGN

6.1 DESIGN OF PREHEATER

Mass flowrate of Ethylene DiChloride $M_{EDC} := 9896\frac{kg}{hr}$

Density of Ethylene Dichloride $\rho_{EDC} := 1182.56\frac{kg}{m^3}$

Volumetric flowrate of Ethylene DiChloride $\upsilon_{EDC} := \frac{M_{EDC}}{\rho_{EDC}}$

$\upsilon_{EDC} = 2.325\times 10^{-3}\frac{m^3}{s}$

$Q\_PRE\_HT_{rqd\_1} = 9.431\times 10^{5}\ W$ Energy required in the preheater calcualed from energy balance around the preheater.

$Q\_PRE\_HT_{rqd\_1} = I\cdot V\cdot t$

Where I = Current Flowing

V = Voltage

t = time of preheating

IV = Power Rating of the heating coil (Watt)

Using a standard heating coil of 5000W

therefore,

$$\tau = \frac{Q\_PRE\_HT_{rqd\_1}}{HR_{coil}}$$

$HR_{coil} = \text{Heating\_Rate\_of\_Coil}$

$HR_{coil} := 3200W$

$\tau = 294.732s$

Volume ,V = volumetric flowrate * time

$V_{EDC} := \upsilon_{EDC} \cdot \tau$

$V_{EDC} = 685.113L$

6.1.2 PREHEATER DIMENSIONING

$\phi := 1.5$ Volume consolidation factor

$V_{Prehter} := V_{EDC} \cdot \phi$

$V_{Prehter} = 1.028 \times 10^{3} L$

$V_{Prehter} = \pi \cdot R^{2} \cdot L$ $\qquad L = 1.2D_{preher}$ $\qquad D_{prehter} = \frac{R}{2}$

$$V_{Prehter} = 1.2 \cdot \frac{\pi \cdot D_{prehter}^{3}}{4}$$

$$D_{prehter} := \begin{bmatrix} \frac{1}{3 \cdot \pi} \cdot 90^{\frac{1}{3}} \cdot \left(V_{Prehter} \cdot \pi^{2}\right)^{\frac{1}{3}} \\ \frac{-1}{6 \cdot \pi} \cdot 90^{\frac{1}{3}} \cdot \left(V_{Prehter} \cdot \pi^{2}\right)^{\frac{1}{3}} + \frac{1}{6} \cdot i \cdot \frac{3^{\frac{1}{2}}}{\pi} \cdot 90^{\frac{1}{3}} \cdot \left(V_{Prehter} \cdot \pi^{2}\right)^{\frac{1}{3}} \\ \frac{-1}{6 \cdot \pi} \cdot 90^{\frac{1}{3}} \cdot \left(V_{Prehter} \cdot \pi^{2}\right)^{\frac{1}{3}} - \frac{1}{6} \cdot i \cdot \frac{3^{\frac{1}{2}}}{\pi} \cdot 90^{\frac{1}{3}} \cdot \left(V_{Prehter} \cdot \pi^{2}\right)^{\frac{1}{3}} \end{bmatrix}$$

$$D_{prehter} = \begin{pmatrix} 1.029 \\ -0.515 + 0.891i \\ -0.515 - 0.891i \end{pmatrix} m$$

Diameter of preheater = 1.029m

$$L_{prehter} := 1.2D_{prehter}$$

$$L_{prehter} = \begin{pmatrix} 1.235 \\ -0.618 + 1.07i \\ -0.618 - 1.07i \end{pmatrix} m$$

Lenght of preheater is 1.235m

6.2 DESIGN OF REACTOR

6.2.1 Calculating Volume of Reactor

$$V_{PDT} = F_{A0} \cdot \int_{0}^{XA} \frac{1}{-r_A} \, dXA$$

V_{PDT} = VOLUME_OF_PRODUCTS_FORME

V_{RCT} = VOLUME_OF_REACTOI

F_{A0} = MOLAR_FLOW_RATI

XA = DEGREE_OF_CONVERSIO

$-r_A$ = RATEE_QUATION $\quad -r_A = k \cdot C_A$

$$C_A = C_{A0} \cdot \left(\frac{1 - XA}{1 + E_A \cdot XA}\right)$$

$V_F := 4 + 1$

$V_I := 1 + 3$

$E_A := \frac{V_F - V_I}{V_F}$ Volume Correction Factor

$X_A := 99\%$

$\upsilon_{Cl} := 13.62\frac{m^3}{hr}$

$\upsilon_{RCT} := \upsilon_{EDC} + \upsilon_{Cl}$ Total Volumetric Flowrate

$F_{EDC} := 100\frac{mol}{hr}$

$F_{Cl} := 300\frac{mol}{hr}$

$F_{A0} := F_{EDC} + F_C$ Total Molar Flowrate

$C_{A0} := \frac{F_{A0}}{\upsilon_{RCT}}$ Combined Inlet Concentraton

$$C_A^2 = C_{A0}^2 \cdot \left(\frac{1 - X_A}{1 + E_A \cdot X_A}\right)^2$$

$C_A = 0.152\frac{mol}{m^3}$

$k := 0.921\frac{m^3}{mol \cdot s}$ From Wilkipedia Encyclopedia

$$V_{PDT} = F_{A0} \cdot \int_{0}^{X_A} \frac{1}{k \cdot {C_A}^2} \, dX_A$$

$$V_{PDT} = 5.18 \times 10^3 \, L$$

6.2.2 Reactor Dimensioning

$$V_{RCT} := 1.12 \cdot V_{PDT}$$

$$V_{RCT} = 5.801 \times 10^3 \, L$$

$$V_{RCT} = \pi \cdot {R_{RCT}}^2 \cdot L_{RCT}$$

$$L_{RCT} = 12 D_{RCT}$$

$$D_{RCT} = \frac{R_{RCT}}{2}$$

$$V_{RCT} = 12 \cdot \frac{\pi \cdot {D_{RCT}}^3}{4}$$

$$D_{RCT} := \begin{bmatrix} \frac{1}{3 \cdot \pi} \cdot 9^{\frac{1}{3}} \cdot \left(V_{RCT} \cdot \pi^2\right)^{\frac{1}{3}} \\ \frac{-1}{6 \cdot \pi} \cdot 9^{\frac{1}{3}} \cdot \left(V_{RCT} \cdot \pi^2\right)^{\frac{1}{3}} + \frac{1}{6} \cdot i \cdot \frac{3^{\frac{1}{2}}}{\pi} \cdot 9^{\frac{1}{3}} \cdot \left(V_{RCT} \cdot \pi^2\right)^{\frac{1}{3}} \\ \frac{-1}{6 \cdot \pi} \cdot 9^{\frac{1}{3}} \cdot \left(V_{RCT} \cdot \pi^2\right)^{\frac{1}{3}} - \frac{1}{6} \cdot i \cdot \frac{3^{\frac{1}{2}}}{\pi} \cdot 9^{\frac{1}{3}} \cdot \left(V_{RCT} \cdot \pi^2\right)^{\frac{1}{3}} \end{bmatrix}$$

$$D_{RCT} = \begin{pmatrix} 0.851 \\ -0.425 + 0.737i \\ -0.425 - 0.737i \end{pmatrix} m$$

$$L_{RCT} = \begin{pmatrix} 10.208 \\ -5.104 + 8.84i \\ -5.104 - 8.84i \end{pmatrix} m$$

ACUTUAL LENGHT = 10.0147m

ACTUAL DIAMETER = 0.846m

6.3 DESIGN OF QUENCHING TANK

$$\upsilon_{pdt} := 23.54 \frac{m^3}{hr}$$

$$\upsilon_{HCL} := 0.9083 \frac{m^3}{hr}$$

$$\upsilon_{Total} := \upsilon_{HCL} + \upsilon_{pdt}$$

$$\upsilon_{Total} = 6.791 \times 10^{-3} \frac{m^3}{s}$$

Quenching time, λ

$\lambda := 1.88min$ From Wilkipedia Encyclopedia

$$V_{rt} := \upsilon_{Total} \cdot \lambda$$

$$V_{rt} = 766.047L$$

$V_{QCH\_TK} := \Psi \cdot V_{rl}$ $\Psi := 1.32$ From Perry Handbook

Ψ Foaming and Pulsation Factor

$V_{QCH\_TK} = 1.011 \times 10^{3}\,L$

$$V_{QCH\_TK} = \frac{\pi \cdot D_{QCH\_TK}^{\;3}}{4}$$

6.3.1 Dimensioning of Quenching Tank

$$D_{QCH\_TK} := \begin{bmatrix} \frac{1}{\pi} \cdot 4^{\frac{1}{3}} \cdot \left(V_{QCH\_TK} \cdot \pi^{2}\right)^{\frac{1}{3}} \\ \frac{-1}{2 \cdot \pi} \cdot 4^{\frac{1}{3}} \cdot \left(V_{QCH\_TK} \cdot \pi^{2}\right)^{\frac{1}{3}} + \frac{1}{2} \cdot i \cdot \frac{3^{\frac{1}{2}}}{\pi} \cdot 4^{\frac{1}{3}} \cdot \left(V_{QCH\_TK} \cdot \pi^{2}\right)^{\frac{1}{3}} \\ \frac{-1}{2 \cdot \pi} \cdot 4^{\frac{1}{3}} \cdot \left(V_{QCH\_TK} \cdot \pi^{2}\right)^{\frac{1}{3}} - \frac{1}{2} \cdot i \cdot \frac{3^{\frac{1}{2}}}{\pi} \cdot 4^{\frac{1}{3}} \cdot \left(V_{QCH\_TK} \cdot \pi^{2}\right)^{\frac{1}{3}} \end{bmatrix}$$

$$D_{QCH\_TK} = \begin{pmatrix} 1.088 \\ -0.544 + 0.942i \\ -0.544 - 0.942i \end{pmatrix} m$$

$$l_{QCH\_TK} := 1.5 \cdot D_{QCH\_TK}$$

$$L_{QCH\_TK} = \begin{pmatrix} 1.632 \\ -0.816 + 1.413i \\ -0.816 - 1.413i \end{pmatrix} m$$

Quenching Tank Diameter = 1.088m

Quenching Tank Height = 1.632m

6.4 DESIGN OF DISTILLATION COLUMN

OVERALL BALANCE

$F = D + B$ ...1

COMPONENT BALANCE OF PCE

$0.7264 \cdot F = 0.04 \cdot D + 0.98 \cdot B$

$F := SEPARATOR\_OUTPUT$

FROM EQN 1

$D = F - B$ ...3

PUT EQN 3 INTO EQN 2

$0.7264 \cdot F = 0.04 \cdot (F - B) + 0.98 \cdot B$

$B := .73021276595744680851F$

$B = 6.395 \frac{kg}{s}$

$D := F - B$

$D = 2.363 \frac{kg}{s}$

$V_n = L_n + D$ ...4

$R = \frac{L_n}{D}$ ...5

Choosing Economic Reflux of 1.7

$L_n := R \cdot D$

$L_n = 4.016 \frac{kg}{s}$

CALCULATION OF NUMBER OF TRAYS USING FUG METHOD

(FENSKE-UNDERWOOD-GILLAND)

$X_{A.d} := 0.93$ $X_{A.s} := 0.0$

$X_{B.d} := 0.0$ $X_{B.s} := 0.9$

$\alpha_{av} := 2.1$

$$N_T := \frac{\log\left(\frac{D \cdot X_{A.d}}{B \cdot X_{B.d}} \cdot \frac{B \cdot X_{B.s}}{D \cdot X_{A.s}}\right)}{\log\left(\alpha_{av}\right)}$$

$N_T = 9.376$

ACTUAL NUMBER OF TRAYS IS 10

Column Height calculation

$\text{Tray\_space} := .55\text{m}$

$\text{Column\_height} := N_T \cdot \text{Tray\_space}$

$\text{Column\_height} = 5.157\text{m}$

Column Energy Requirement

Energy Removed in the Condenser

$\Delta H_c := -351500\frac{J}{kg}$

$Q_c := D \cdot \Delta H_c$

$Q_c = -8.305 \times 10^5\,W$

Energy Supplied to the Reboiler

$\Delta H_r := 181340\frac{J}{kg}$

$Q_r := B \cdot \Delta H_r$

$Q_r = 1.16 \times 10^6\,W$

CHAPTER SEVEN

7.0 Material Selection

The materials used for this plant design is nickel/ nickel alloy

As nickel is relatively expensive material costing about 150 pounds/kg the high nickel alloys are only used where there distinctive properties are essential. Cost can be educed by using them as linings. The two main attributes that can be developed in nickel alloys are resistance to corrosion and high temperature strength. Whilst all the nickel alloys have both of these properties to some degree most of them have been developed for use in applications which utilize one of these properties to annul greater extent than the other. Nickel alloys can be divided into two based on their properties as:

1) Alloys for medium and low temperature corrosion resistant application.
2) Alloys for high temperature conditions where creep resistance is of main importance. Two other classes of nickel alloys which may be of interest in chemical engineering are those in which electrical and thermal expansion properties are important.

7.1 Nickel/ Copper Alloy

Probably the first nickel alloy to be developed was by Monel(trademark of international Nickel), which has a composition of 66% nickel 33% copper; it has been given the ASTM designation of alloy 400. This alloy has good mechanical properties up to 500oC, it is easy to fabricate and available in all rough forms and as castings. K-500 is a modified version of this alloy which can be thermally hardened by heat treatment and so its suitable for items requiring strength as well as corrosion resistance. Example shafting or ware resistance example cutter blades. Alloy 400 is more expensive thab stainless steel and so is choosen for conditions where its following attributes are important.

First immunity to stress corrosion cracking and pitting in solutions containing chlorides and caustic alkalis. For example most tubes and shell evaporators for caustic soda plants are now made of alloy 400 tube and plate because of frequent stress corrosion cracking of stainless steel items. It is also suitable for equipment handle dry halogen gases and chlorinated hydro-carbons. Secondly resistance to reducing conditions. In this respect alloy 400 is complementary to stainless steel which is best chosen for oxidizing conditions.

CHAPTER EIGHT

8.0 SAFETY AND QUALITY CONTROL

In designing a plant, safety is one of the major criteria for the selection of the best alternative along with economic viability. This is because of the value placed on the operating personnel and equipments involved.

Operating conditions and equipments in operation are usually dangerous and could lead to a serious injury or major damage to the plant as well as disability to the personnel or even loss of life.

Safety becomes even more pertinent when the materials being handled are hazardous. This is the case in the design of the Tetrachloroethylene plant. The plant should be sited far away from the public to avoid environmental pollution to the host community. For this design, the hazards and some of the actions that could lead to these hazards are identified and safety measures are then recommended to fit into the plant design.

8.1 Safety

8.1.1 Hazards in Tetrachloroethylene plant

A hazard is generally defined as the presence of a material or condition that has the potential of causing loss or harm (Odigure, 1998). Prevention reduces the likelihood of the hazard occurring, whereas protection lessens that chance of the consequences from happening and mitigation makes less severe, given that a deviation occurs.

To identify the hazards present in the tetrachloroethylene plant, material and equipment inventory were carried out.

8.1.1.1 Inventory

The types of the inventories present in the process plant are material and equipment inventories.

8.1.1.1.1 Material Inventory

Regarding the material inventory, the followings are present:

i. Hydrochloric acid.

ii. Trichloroethylene.

iii. Tetrachloroethylene.

iv. Chlorine.

v. 1,2-dichloroethene.

8.1.1.2 Equipment Inventory

In this case, the followings are present:

i. Reactors, which house the actual chemical reaction in which endothermic reactions take place.

ii. Product separators, which handles the separations of PCE and TCE

iii. Quench tank, in which HCl was used to quench reaction in order to avoid run away reaction.

iv. Distillation column in which the separation of PCE and TCE occur.

8.1.2 Identification of Hazards

Having carried out the material and equipment inventories, the following hazards were identified as the ones present in the formaldehyde plant designed.

8.1.2.1 Explosion

This is a sudden release of energy as a pressure or blast wave. It usually occurs on ignition of vapour cloud and also by a pressure building that leads to the sudden release from a vessel.

8.1.2.2 Fire

This is the result of the combustion of material in air. The material to be combusted forms a mixture, which would then burn when ignited. There three components that are necessary for combustion, namely; combustible material, heat and air. As such, safety measures must be put in place to prevent reactions of tetrachloroethylene and trichloroethylene with hydroxides of alkaline metals. Also the temperature of the reactor should be controlled not to exceed the flash point of the materials.

8.1.2.3 Poisoning

Poisoning is related to the toxicity of the material being handled. This phenomenon (poisoning) affects the personnel safety. It normally occurs in two forms; first, its existence as a safety hazard and, second, as a health hazard. Tetrachloroethylene is normally present at low levels, usually less than 0.06 ppm (parts per million), in both outdoor and indoor air. When present in the air at levels at or above 0.1 ppm, acute health effects can occur including watery eyes; burning sensations in the eyes, nose and throat; nausea; coughing; chest tightness; wheezing; skin rashes; and other irritating effects.

8.1.3 Safety Measures

This is the need for safety measure because of the possibility of process becoming instable. The chemical process industries always have searched for ways to operate safely and efficiently to prevent unnecessary plant shut down, schedule delay, hazard or to event that can cause any environmental implication. Outlined below are the general safety measures to be adopted in the formaldehyde plant.

i. All materials of construction should be well selected on the basis of corrosion resistance and structural strength. This is to avoid the collapse of any equipment or structure.

ii. All pipelines carrying flammable materials must be installed with flame traps.

iii. Relief valves should be installed along all lines carrying gases and vapours.

iv. Automatic controllers should be installed to control temperature, pressure and flow rates at various points of the process.

v. Competent staff should be assigned for carrying out qualitative maintenance work in the plant.

vi. Signs and placards warnings of hazardous materials should be placed over in the strategic places of the plant.

vii. Foam fire extinguishers should be easily accessible and ready at all times for operation in case of fire accidents.

viii. Plant should be laid in such that the storage facilities are placed away from the plant, all electrical installation are earthed and insulated and, in addition, kept away from the processing unit, and exit and escape route are provided and labelled well, should there be any emergency.

8.1.4 Strategies for Safer Process Design

There are four major strategies for safer process design:

1. Minimizing the size of process equipment.
2. Substituting a less hazardous substance or process step.
3. Moderate storage or processing conditions.
4. Simplifying process and plant design.

8.1.5 Safety Decisions via Risk Mapping

Risk is defined as a combination of the likelihood of occurrence and severity of impact from unexpected loss incidents (Odigure, 1998). Risk represents potential expenditure or liabilities, but is not generally included in a budget or financial forecast. A probability exists that an expenditure or liability will actually be incurred within each period. Thus, the expense will be zero if the incident does not occur. Since decisions are generally made on an economic basis, it follows that risks must also be converted to monetary values (Odigure, 1998). Risk avoidance can result in increased productivity that translates directly to the corporate bottom line.

Developing an understanding of risk requires addressing three questions:

1. What is the hazard?
2. What are the possible undesired outcomes?
3. How likely are these to occur?

Having adequate knowledge about the hazards and the safe limits of certain key parameters such as the ignition temperature and explosion concentration is very important in risk mapping.

8.2 Quality Control

Quality simply means "fitness for use". But, according to the International Standard Organisation (ISO), quality is defined as the totality of the characteristics of an entity that bear on its ability to satisfy stated and intended needs. It is more costly to exceed a specification than to meet it. Therefore, there is the need to get quality goal or target for effective quality control.

Maintaining product quality in accordance with acceptable standard has been a major role for industrial instrumentation since its inception decades ago. With the ever-increasing interest in speeding up production, one becomes aware of the fact that rejectable as well as acceptable products can be produced at high rates.

8.2.1 Quality Assurance

Quality assurance is defined by ISO as all the planned and systematic activities implemented within the quality system and demonstration is needed to provide adequate confidence on entity will fulfil requirement for quality.

8.2.1.1 Principles of Quality Assurance

The principles of quality assurance include the following:

i. Management involvements and objective (management) involvement is very essential to ensure quality.

ii. Programming and planning.

iii. Application of quality control principles.

iv. Design and specification control.

v. Purchasing control and vendor appraisal.

vi. Production control.

vii. Marketing and service quality functions.

viii. Proper documentation.

ix. Non-conformance control.

x. Remedial action.

xi. Defect and failure analysis.

8.2.1.2 Quality Management

Quality management involves all activities of the overall management functions that determine the quality policy, objective and responsibilities and implement then by means, such as quality planning control assurance and improvement within the quality system. Responsibility of quality lies at all level of all. To successfully implement quality management, the organisation structure, procedure process and resources are requisite.

9.2 Instrumentation and Control Objectives

The key objectives adhered to in the specification of the instrumentation and control schemes are:

1. Safe plant operation
    - i. To keep the process variables within known safe operations limits.
    - ii. To defect dangerous situations as they develop and to provide alarms and automatic shut – down systems
    - iii. To provide interlocks and alarms to prevent dangerous operation procedures
2. Production rate. To achieve the desired product output
3. Product quality. To maintain the product composition within the specific quality standards
4. Cost. They operate at the lowest production cost, but not to the detriment of the product quality.

In the plant design some of the variables needed to be monitored and controlled are, the flow rate, temperature, pressure and composition.

- i. Flow rates/feed ratio control: a feed ratio controller is applied between the methane stream and the oxygen stream with the aim of maintaining a complete conversion of methane to the desired products. This is necessary to avoid excess oxygen being built up in the reactor.
- ii. Temperature control reaction: temperature is controlled by regulating the flow rate of the reaction into it. This can also be controlled by heat transfer. The reaction is exothermic. It produces heat, which tends to raise reaction temperature thereby increasing reaction rate and producing more heat. This positive feedback is countered by negative feedback in the cooling system, which removes more heat as reactor temperature rises.

The temperature controller, which in turn operates the coolant value, to counter the rise or drop in temperature in the sector.

iii. Pressure control: pressure sensing is quite straightforward with the aid of pneumatic instrumentation such as Bourdon gauge, diaphragms and bellows. These sensors measure absolute pressure and pressure differences between two levels. Therefore, pressure control is achieved by manipulating the airflow rate in the compressor to avoid deviation from set point.

iv. Composition control: first requirement here is to establish proper stoichiometry of the reactants in propositions needed to satisfy the reaction chemistry and also the desired output product. This is achieved by setting input flow rates in ratio to one another, or a composition measurement (analyzer) can be used to trim the ratios to the right proportion

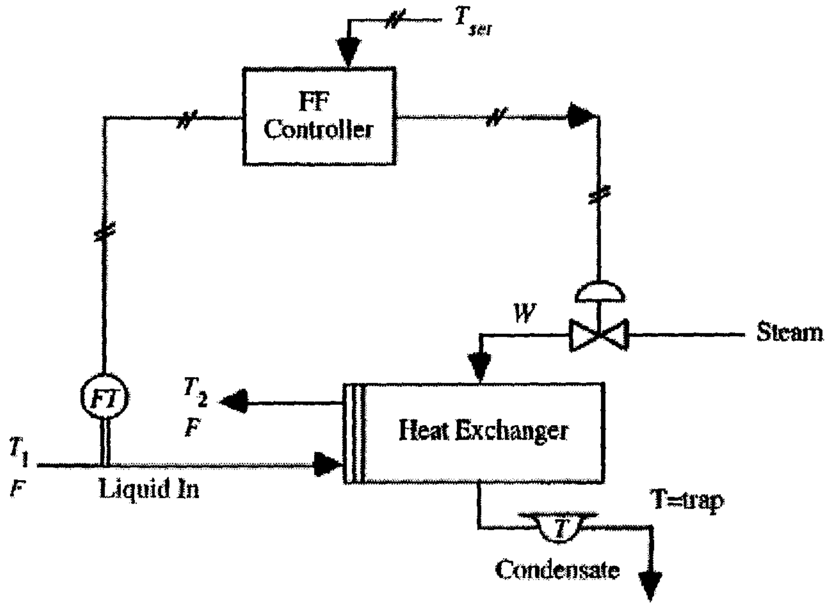


Fig. 9.1: Feed-forward control of a heat exchanger.

CHAPTER TWELVE

12.0 SITE FOR PLANT LOCATION

The location of the Tetrachloroethylene plant can have a crucial effect on the profitability of the Tetrachloroethylene production project and the scope for future expansion. Many factors must be considered when selecting a suitable site, and a review of the principal factors will be given in this chapter of this design project for the production of Tetrachloroethylene. The principal factors to be considered are:

i. Location, with respect to the marketing area.
ii. Raw materials supply.
iii. Transport facilities.
iv. Availability of labour.
v. Availability of utilities.
vi. Availability of suitable land.
vii. Environmental impact and effluent disposal.
viii. Local community considerations.
ix. Climate.
x. Political and strategic considerations.

12.1 Factors Considered for Site and Plant Location

The factors considered for site and plant location are as described thus.

12.1.1 Location, With Respect To the Marketing Area

For a material produced in bulk quantities such as the Tetrachloroethylene where the cost of the product per tonne is relatively low and the cost of transport is a significant fraction of the sales price, the plant should be located close to the primary market. This consideration will be less important for low volume production, high-priced products; such as pharmaceuticals.

12.1.2 Raw Materials

The availability and price of suitable raw materials will often determine the site location. Plants producing bulk chemical as the Tetrachloroethylene plant are best located close to the source of the major raw materials (which is 1,2-dichloroethene); where this is also close to the marketing area.

12.1.3 Transport

The transport of materials and products to and from the plant will be an overriding consideration for site selection.

If practicable, a site should be selected that is close to at least tow major forms of transport: road, rail, waterway (canal or river), or a sea port. Road transport is being increasingly used, and is suitable for local distribution from a central warehouse. Rail transport will be cheaper for the long-distance transport of bulk chemicals.

Air transport is convenient and efficient for the movement of personnel and essential equipment and supplies, and the proximity of the site to a major airport should be considered.

12.1.4 Availability of Labour

Labour will be needed for construction of the plant and its operation. Skilled construction workers will usually be brought in from outside the site area, but there should be an adequate pool of unskilled labour available locally; and labour suitable for training to operate the plant. Skilled tradesmen will be needed for plant maintenance. Local trade union customs and restrictive practices will have to be considered when assessing the availability and suitability of the local labour for recruitment and training.

12.1.5 Utilities (Services)

Chemical processes invariably require large quantities of water for cooling and general process use, and the plant must be located near a source of water of suitable quality. Process water may be drawn from a river, from wells, or purchased from a local authority.

At some sites, the cooling water required can be taken from a river or lake, or from the sea; at other locations cooling towers will be needed. Electrical power will be needed at all sites. Electrochemical processes that require large quantities of power; need to be located close to a cheap source of power.

A competitively priced fuel must be available on site for steam and power generation.

The word "utilities" is now generally used for the ancillary services needed in the operation of any production process. These services will normally be supplied from a central facility; and will include:

a. **Electricity:** - power required for electrochemical processes, motors, lightings, and general use.

b. **Steam for process heating:** - The steams required for the process are generated in the Tube boilers using most economic fuel.

c. **Cooling water:** - Natural and forced draft cooling towers are generally used to provide the cooling water required on site.

d. **Water for general use:** - The water required for the general purpose will be taken from local water supplies like rivers, lakes and seas. Because of this reason all the plants located on the banks of river.

e. **Demineralised water:** - Demineralised water, from which all the minerals have been removed by ion-exchange is used where pure water is needed for the process use, in boiler feed water.

f. **Refrigeration:** - Refrigeration is needed for the processes, which require temperatures below that are provided by the cooling water.

g. **Compressed air:** - In an ethylene oxide plant compressed air is one of the raw materials. It is also needed for pneumatic controllers etc.

h. **Effluent disposal facilities:** - facilities must be provided for the effective disposal of the effluent without any public nuisance.

12.1.6 Environmental Impact, and Effluent Disposal

All industrial processes produce waste products, and full consideration must be given to the difficulties and coat of their disposal. The disposal of toxic and harmful effluents will be covered by local regulations, and the appropriate authorities must be consulted during the initial site survey to determine the standards that must be met.

12.1.7 Local Community Considerations

The proposed plant must be fit in with and be acceptable to the local community. Full consideration must be given to the safe location of the plant so that it does not impose a significant additional risk to the community.

On a new site, the local community must be able to provide adequate facilities for the plant personnel: schools, banks, housing, and recreational and cultural facilities.

12.1.8 Availability of Suitable Land (Site Considerations)

Sufficient suitable land should be available for the proposed plant and for future expansion. The land should be ideally flat, well drained and have suitable load bearing capacity. A full site evaluation should be made to determine the need for pining or other special foundations. It should also be available at low cost.

12.1.9 Climate

Adverse climatic conditions at a site will increase costs. Abnormally low temperatures will require the provision of additional insulation & special heating for equipment & pipe runs. Stronger structures will be needed at locations subject to high winds or earthquakes.

12.1.10 Political and Strategic Consideration

Capital grants, tax concessions and other incentives provided by governments to direct new investment to preferred locations, such as areas of high un-employment should be the overriding considerations in the site selection.

12.2 Selection of Site

Careful consideration of the factors for the site selection outlined above reveals that the best site for this project.

12.3 Justification of The Selected Site

The selection has been based on some requirements, which the site was able to meet among the factors for the site selection discussed above. The justifications for the selected site are as follows:

12.3.1 Availability of Raw Materials

The major raw materials in the production of PCE are Cl_2, and dichloroethylene . DCE is obtained in large quantity from petrochemical industries, while Cl_2 which is a by-product of electrolysis of brine in the production of caustic soda is also available in large quantity. In addition, considering the situations in the country. So, siting the Tetrachloroethylene plant close the source of the raw material is of great importance

12.3.2 Nearness to Marketing Area

Since Tetrachloroethylene is used mainly in the dry-cleaning industry, siting its plant close to the place of primary marketing area, that is, solvent utilising industries, will be very ideal.

12.3.3 Transport

Regarding the transport facilities, closeness to seaport, railway and or trunk-A road or close to a major airport. So, the good and many means of transportation present in the area will ensure effective transportation of the raw materials, products and even the skilled experts at low cost.

12.3.4 Availability of Labour

It is important that the site is located in a place where all kinds of labour force are available.

12.3.5 Climate

The absence of adverse climatic conditions such as too low temperature or too high wind loads or earthquakes is important to make a good site for the Tetrachloroethylene plant.

12.3.6 Utilities

Since the silver process of Tetrachloroethylene production requires large quantities of services such as steam for the distillation columns, quench tanks, e.t.c; cooling water for the condensers and other services, it is important that the Tetrachloroethylene plant should be sited in a place where there is abundance of water. Further, the readily available gas powered electricity generation plant.

12.4 Plant Layout

The economic construction and operation of a process unit will depend on how well the plant equipment specified on the process flow sheet and laid out. The principal factors to be considered are:

a. Economic consideration: construction and operation cost.
b. The process requirement
c. Convenience of operation
d. Convenience of maintenance
e. Safety
f. Future expansion
g. Modular construction

12.4.1 Costs

The cost of construction can be minimized by adopting a layout that gives shortest run of connecting pipes between equipment, and adopting the least amount of nickel/copper alloy work. However, this will not necessarily be the best arrangement for operation and maintenance.

12.4.2 Process Requirement

All the required equipments have to be placed properly within process. Even the installation of the auxiliaries should be done in such a way that it will occupy the least space.

12.4.3 Operation

Equipment that needs to have frequent operation should be located convenient to the control room. Valves, sample points, and instruments should be located at convenient position and height. Sufficient working space and headroom must be provided to allow easy access to equipment.

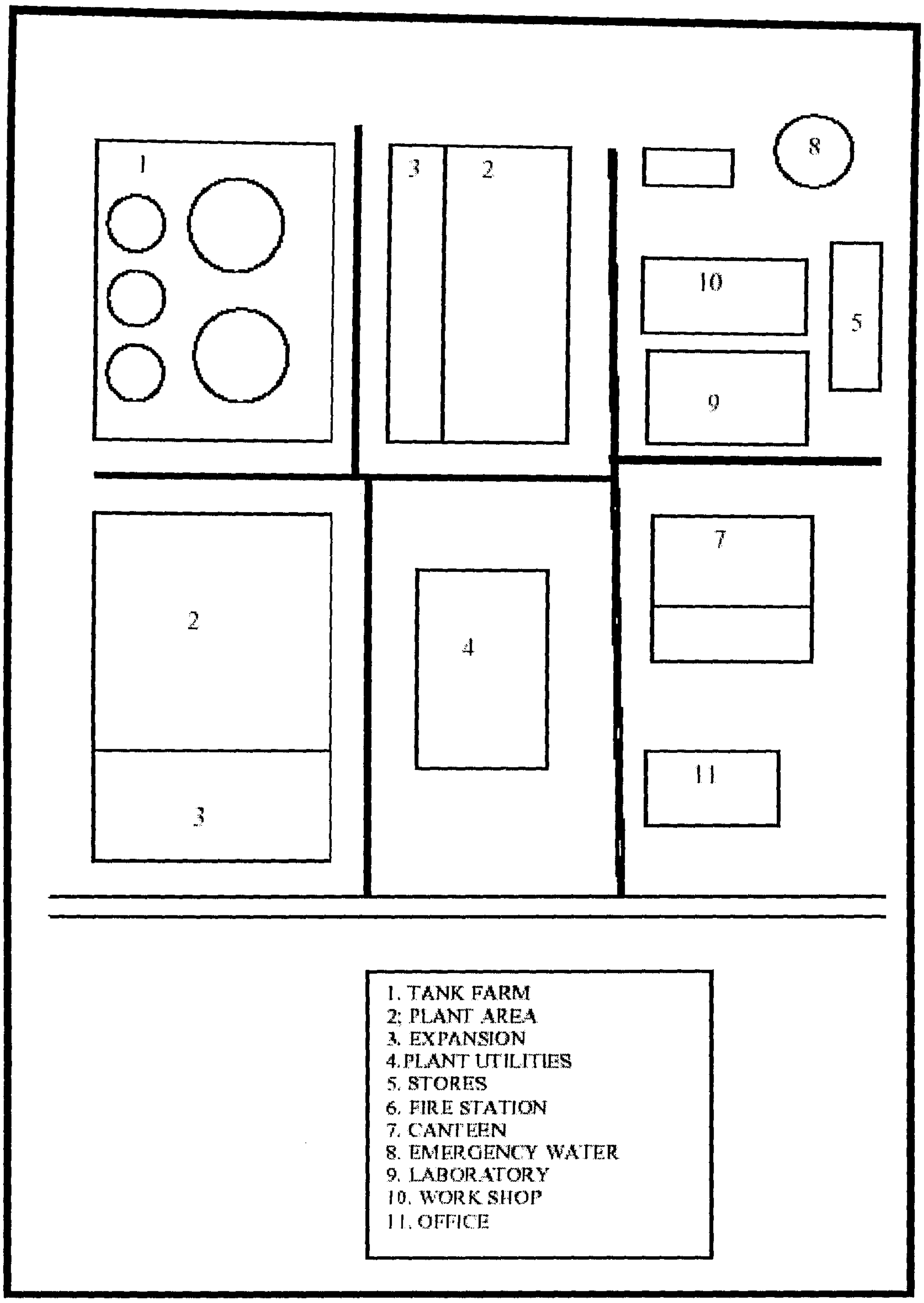


Fig. 12.1: The Tetrachloroethylene plant layout

12.4.4 Maintenance

Distillation towers need to be sited so that the tube bundles can be easily withdrawn for cleaning and tube replacement. Vessels that require frequent replacement of catalyst or packing should be located on the outside of buildings. Equipment that requires dismantling for maintenance, such as compressors and large pumps, should be placed under cover.

12.4.5 Safety

Blast walls may be needed to isolate potentially hazardous equipment, and confine the effects of an explosion. At least two escape routes for operator must be provided from each level in the process building.

12.4.6 Plant Expansion

Equipment should be located so that it can be conveniently tied in with any future expansion of the process. Space should be left on pipe alleys for future needs, service pipes over-sized to allow for future requirements.

12.4.7 Modular Construction

In recent years, there has been a move to assemble sections of the plant at the manufacturer site. These modules will include the equipment, nickel/copper alloy, piping and instrumentation. The modules then transported to the plant site, by road or sea.

CHAPTER THIRTEEN

13.0 ECONOMIC ANALYSIS

13.1 Introduction

For any industrial plant to be put into operation, huge sum of money must have been invested in it to purchase and install the necessary machinery and equipment. Land and service facilities must be obtained and the plant must be erected complete with the piping, controls, and service. In addition to all these cost, it is necessary to have money available for the payment of expenses involved in plant operation.

The capital requires to have the necessary manufacturing and plant facilities is called the fixed capital investment. That which is necessary for operation of the plant is termed the working capital. The sum of the fixed investment and the working capital is the total capital equipment (TCI).

13.2 Accuracy and Purpose of Capital Cost Estimates

The accuracy of an estimate depends on the amount of design detail available: the accuracy of the cost data available; and the time spend on preparing the estimate. In the early stages of a project only an appropriate estimate will be required, and justified, by the amount of information by then developed.

13.3 Fixed and Working Capital

13.3.1 Fixed Capital

Fixed capital is the total cost of the plant ready for start-up. It is the cost paid to the contractors.

It includes the cost of:

1. Design, and other engineering and construction supervision.
2. All items of equipment and their installation.
3. All piping, instrumentation and control systems.
4. Buildings and structures.
5. Auxiliary facilities, such as utilities, land and civil engineering work.

It is a once-only cost that is not recovered at the end of the project life, other than the scrap value.

13.3.2 Working Capital

Working capital is the additional investments needed, over and above the fixed capital, to start the plant and operate it to the point when income is earned.

It includes the cost of:

1. Start-up.
2. Initial catalyst charges.
3. Raw materials and intermediates in the process.
4. Finished product inventories.
5. Funds to cover outstanding accounts from customers.

Most of the working capital is recovered at the end of the project. The total investment needed for a project is the sum of the fixed and working capital.

Working capital can vary from as low as 5 per cent of the fixed capital for a simple, single-product, process with little or no finished product storage; to s high as 30 per cent for a process producing a diverse range of product grades for a sophisticated market, such a synthetic fibres.

13.3 Operating Costs

An estimate of the operating costs, the cost of producing the product, is needed to judge the viability of a project, and to make choices between alternative processing possible schemes. These costs can be estimated from the flow-sheet, which gives the raw material and service requirements, and the capital cost estimate.

The cost of producing a chemical product will include the items listed below. They are divided into two groups.

1. Fixed operating costs: costs that do not vary with production rate. These are the bills that have to be paid whatever the quantity produced.

2. Variable operating costs: costs that ate dependent on the amount of product produced.

13.3.1 Fixed Operating Costs

1. Maintenance (labour and materials).
2. Operating labour.
3. Laboratory costs.
4. Supervision.
5. Plant overheads.
6. Capital charges.
7. Rates (and any other local taxed).
8. Insurance.
9. License fees and royally payments.

13.3.2 Variable Operating Costs

1. Raw materials.
2. Miscellaneous operating materials.
3. Utilities (services).
4. Shipping and packaging.

The costs listed above are the direct costs of producing the product at the plant site. In addition to these costs the site will have to carry its share of the company's general operating expenses. These will include:

1. General overheads.
2. Research and development costs.
3. Sales of expense.
4. Reserves.

13.4 Computer-Aided Algorithm for Costing

Most large manufacturing and contracting organisations use computer programs to aid in the preparation of cost estimates and in process evaluation. Many have developed their own programs, using cost data available from company records to ensure that the estimates are reliable.

Consequently, in order to the cost analysis of this design project, a computer software known as MathCAD will be used to prepare the cost analysis algorithm. In addition, where necessary, Excel package will also be used.

Table 13.1 Costing and Economic Analysis

EXECUTIVE SUMMARY (2006 prices)

****

TOTAL CAPITAL INVESTMENT	5922000	$
CAPITAL INV. CHARGED	5922000	$
OPERATING COST	3361000	$/year
PRODUCTION RATE	5949	kg/hr of TCE
	15050	kg/hr of PCE
UNIT PRODUCTION COST	1.73	$/kg DCE
TOTAL REVENUES	108000	$/year
GROSS MARGIN	17.68	%
RETURN ON INVESTMENT	46.17	%
PAYBACK TIME	3.4	years
NPV (at 7.0 % interest)	30228000	$

****

MAJOR EQUIPMENT SPECIFICATION AND FOB COST (2006 prices)

Quantity/ Stand-by		Description	Unit Cost ($)	Cost ($)
1/0	MX-101	Mixer	0	0
1/0	MX-102	Mixer	0	0
1/0	P-100	PUMP	3000	3000
1/0	MX-104	Mixer	0	0
1/0	MX-105	Mixer	0	0
1/0	R-100	REACTOR	138000	138000
1/0	K-100	COMPRESSOR	7000	7000
1/0	MX-106	Mixer	0	0
1/0	T-101	DISTILLATION	138000	138000

		COLUMN		
1/0	S-101	SEPARATOR	9000	9000
1/0	Q-101	QUENCHING TANK TANK	16000	16000
2/0	F-101	CONDENSER	60000	60000
1/0	A-101	REBOILER	60000	60000
1/0	FSP-101	Flow Splitter	0	0
1/0	FSP-102	Flow Splitter	0	0
1/0	RO-101	PIPING	18000	18000
1/0	D-101	STORAGE TANK	70000	70000
1/0	CR-101	CONTROLLERS	164000	164000
1/0				
		Cost of Unlisted Equipment		171000

****

TOTAL EQUIPMENT PURCHASE COST 854000

****

FIXED CAPITAL ESTIMATE SUMMARY (2006 prices)

****

A. TOTAL PLANT DIRECT COST (TPDC) (physical cost)

1. Equipment Purchase Cost	$	854000
2. Installation		512000
3. Process Piping		299000
4. Instrumentation		342000
5. Insulation		26000
6. Electricals		85000
7. Buildings		384000
8. Yard Improvement		128000

```
 9. Auxiliary Facilities
                                                      342000
                                                  ******************
                                   TPDC =            2972000

B. TOTAL PLANT INDIRECT COST (TPIC)

 10. Engineering
 11. Construction                                     743000
                                                     1040000
                                                  ******************
                                   TPIC =            1783000

C. TOTAL PLANT COST TPC =                            4756000
(TPDC+TPIC)
 12. Contractor's fee                                 238000
 13. Contingency                                      476000
                                                  ******************
                                  (12+13) =           713000

***************************************************************
D. DIRECT FIXED CAPITAL (DFC) TPC+12+13              5469000
***************************************************************



LABOR REQUIREMENT AND COST SUMMARY
********************************************************************
                                Labor
Section                         Hours         Labor Cost
Name                            Per Year      $/year           %
********************************************************************
Main Section                       38016         1574000          100
********************************************************************
TOTAL                              38016         1574000          100
********************************************************************



RAW MATERIALS COST SUMMARY
*****************************************************************************
Raw                             Unit Cost    Annual Amount    Cost
Material                        ($/kg)          (kg)          ($/yr)       %
*****************************************************************************

HCL                                    0        118562.4           0        0
Water                                  0          538.56           0        0
Chlorine                               0        26601.06           0        0
Degreaser                              2            7920       15840    46.87
DCE                                0.005         3591720       17959    53.13
*****************************************************************************

TOTAL                                         3745342.02       34000      100
*****************************************************************************
```

```
**************************************************************************


WASTE TREATMENT / DISPOSAL (2000 prices)

a. SOLID WASTE
**************************************************************************
Stream                                   Unit Cost    Annual Amount      Cost
Name                                     ( $/kg )        ( kg )        ( $/yr )
**************************************************************************
Hazard. Sludge                            1.00E+01        17496.14        175000
**************************************************************************
              a. Subtotal (Solid Waste)                                   175000
**************************************************************************

b. LIQUID WASTE
**************************************************************************
Stream                                   Unit Cost    Annual Amount      Cost
Name                                     ( $/kg )        ( kg )        ( $/yr )
**************************************************************************
Tumbler Sludge                            1.00E-01      1542741.22        154000
**************************************************************************
              b. Subtotal (Liquid Waste)                                  154000
**************************************************************************

c. EMISSIONS
**************************************************************************
  Stream                                 Unit Cost    Annual Amount     Cost
  Name                                    ($/kg)          (kg)          ($/yr)
**************************************************************************
**************************************************************************
              c. Subtotal (Emissions)                                          0


**************************************************************************
WASTE TREATMENT/DISPOSAL TOTAL COST (a+b+c)                               329000
**************************************************************************


UTILITY REQUIREMENTS (2006 prices)
**************************************************************************
```

```
ELECTRICITY
*****************************************************************************
                                                  Annual
Procedure                          Equipment   Amount                Cost
Name                                  Name       ( kWh )            ( $/yr )
*****************************************************************************
P-6                                Reactor                115            67
P-7                                compressor            4556           400
P-12                               Pre-heater          138847         13800
P-16                               Column              152900         15200
P-18                                CR-101                 96           185
Unlisted Equipment                       18532           1853
General Load                             55596           5560
*****************************************************************************
SUBTOTAL                                                               37064


HEAT TRANSFER AGENT :               Steam       (0.2800 $/1000 kg)
*****************************************************************************
                                                  Annual
Procedure                          Equipment   Amount                Cost
Name                                  Name       ( kg )             ( $/yr )
*****************************************************************************
E-101                              Pre-heater         2244563           628
CR-101                             Reactor             244741            69
*****************************************************************************
SUBTOTAL                                                                 697
```

```
ANNUAL OPERATING COST - SUMMARY  (2006 prices)
****************************************************************
Cost Item                          $/Year         %
****************************************************************
Raw Materials                        34000             1.01
Labor-Dependent                    1574000            46.82
Equipment-Dependent                1026000            30.52
Laboratory/QC/QA                    236000             7.02
Consumables                         124000             3.69
Waste Treatment/Disposal            329000             9.79
Utilities                            39000             1.15
Transportation                           0                0
Miscellaneous                            0                0
Advertising and Selling                  0                0
```

```
 Running Royalties                                0              0
 Failed Product Disposal                          0              0
************************************************************
 TOTAL                                      3361000            100
************************************************************



 PROFITABILITY ANALYSIS  (2006 prices)
************************************************************************
 A. DIRECT FIXED CAPITAL                   5469000   $
 B. WORKING CAPITAL                         180000
 C. STARTUP COST                            273000
 D. UP-FRONT R&D                                 0
 E. UP-FRONT ROYALTIES                           0
 F. TOTAL INVESTMENT
(A+B+C+D+E)                                5922000
 G. INVESTMENT CHARGED TO THIS
PROJECT                                    5922000

 H. REVENUE STREAM FLOWRATES
   kg/year of total flow PCE               1942681
   kg/year of total flow TCE                213695

 I. PRODUCTION (UNIT) COST
   $/kg                                       1.73

 J. SELLING/PROCESSING PRICE
   $/MT of total flow PCE                       50
   $/MT of total flow TCE                       50

 K. REVENUES   ($/year)
PCE                                          97000
TCE                                          11000
   --------------                  -----------------
   Total Revenues                           108000

 L. ANNUAL OPERATING COST                  3361000
 M. GROSS PROFIT                           3254000
 N. TAXES (40 %)                                 0
 O. NET PROFIT                             2735000
************************************************************************
   GROSS MARGIN
   RETURN ON INVESTMENT
   PAYBACK TIME (years)                        3.4
************************************************************************
MT = Metric Ton = 1,000 kg


CASH FLOW ANALYSIS (thousand US $)
```

CHAPTER FOURTEEN

14.1 Conclusion

A plant to produce 100,000 tonnes per day of tetrachloroethylene has so been designed. Based on the design, the basic equipment were properly sized and specified after carrying out material and energy balances around each of the units in the overall plant. Safety and effective waste (TCE) disposal measures were considered and thus the plant can be said to be environmentally acceptable. From the economic analysis, the total capital investment for setting up the plant was found to be 10.937 million dollars, the return back on investment was found to be 46.17%. payback period of 3.4 years, with all these, the plant can be said to be economically viable.

14.2 Recommendations To The Industrialist

Based on this design work that has been carried out, the following recommendations are made to the industrialists to be noted during the construction, start-up and operating phases of the work:

i. The safety of workers, equipments and infrastructures should be highly evaluated during the design implementation stage of the design.

ii. The recycle design should be considered without further delay, since it is useful in reducing the level of plant effluent, and it also reduces costs.

iii. Adequate data and technological parameters should be at the possession of the plant operations at all time to forestall any unwanted accident.

iv. Routine turn around plant maintenance should be of paramount importance in the design. An articulate and organised maintenance team should safeguard quick plant shut down and ensure equipment salvage value. This will also take care of schedule, slippage, cost over-run and possible re-work.

v. Personnel should undergo routine training about new work ethic and equipments to improve their knowledge of the plant operation and increase overall plant productivity.
vi. Procurement of raw materials and equipments should be based on strict regulation of specification and maximum quality.
vii. Plant should not be operated above the design specification to avoid abnormal conditions and explosions.
viii. The implementation of this design work must be adequately supervised by the experts.
ix. The plant should be sited close to the source of raw materials.
x. Alternative sources of energy should be available at all times to avoid plant failure and possible sources of failure.
xi. The water and air around the plant should be monitored regularly to ensure compliance with the Environmental Protection Agency Standards.

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APPENDIX

SCALE UP FACTOR

From the bottom stream;

PCE stream

DCE	0
Cl_2	0
TCE	0.128
PCE	6.267
HCl	0
H_2O	0

Total bottom stream = 0.128 + 6.267

= 6.395kg/s

PCE produced per day is given by

6.395 × 24 × 3600 = 552528 kg/s

1 tonne/day = 1,000kg/day

100,000 tonnes/day = 100,000,000 kg/day

Scale up factor = 100,000,000 kg/day / 552528 kg/day

= 180.986

Calculation of Energy Balance

Table A1: Specific Heat Capacity Data

Component	A	B	C	D
1,2-dichloroethane	4.8930	5.518E-2	-3.435E-5	8.094E-9
Chlorine	6.4320	8.082E-3	-9.241E-6	3.695E-9
Hydrochloric acid	7.2350	-1.720E-3	2.976E-6	-9.310E-10
Tetrachloroethene	10.980	5.387E-2	-5.478E-5	2.002E-8
Trichloroethene	7.2070	5.462E-2	-5.324E-5	1.696E-8

$Cp= A + BT + CT^2 + DT^3$ (cal./g mole K) (Sinnot,2001).

In converting from calorie to Joule, a multiplying factor of 4.184 is used (Perry)

For non-reacting component system,

$\Delta Hi = \int cpi\, dT$

$\Delta H = \sum \Delta H$ output - $\sum \Delta H$ input

Energy flow = Molar flow rate * Enthalpy Change

For reacting components system,

$\Delta Hi = \Delta H^0_f + \int cpi\, dT$

Where ΔH^0_f is the enthalpy of formation of individual component at standard reference temperature of 298^0 K

$\Delta H = \Delta H^0_f + \sum \Delta H$ products - $\sum \Delta H$ reactants

Table A3: Standard Enthalpy of Formation Data

Components	ΔH^0_f (l)298.15 K (KJ/mole)	ΔH^0_f (g) 298.15 K (KJ/mole)
DCE	-167.2± 3.5	-132.0 ± 3.5
Chlorine	0	0
HCl	0	-92.3
PCE	-63.9±4.0	-24.2±4.0
TCE	-52.10±3.0	-17.5±3.0

(Journal of Physical Chemistry Reference Data, Vol.31, No.1, 2002)

Calculation of Overall Standard Enthalpy of Formation

$\Delta H^0_{f} = \sum \Delta H^0_{f\,products} - \sum \Delta H^0_{f\,reactants}$

Vapour-liquid Equilibrium for Trichloroethylene/Tetrachloroethylene. P=760mmHg

BP Temp.°C	% by mole, trichloroethylene	
	Liquid	Vapour
117.0	7.5	17.8
115.7	10.0	22.8
112.8	16.2	33.8
110.5	21.7	42.0
109.1	25.0	46.8
106.9	30.8	53.7
105.7	33.6	57.2
103.4	39.4	62.7
101.0	46.2	69.8
100.0	49.3	71.8
98.4	55.0	75.6
96.3	61.4	80.0
94.4	68.5	84.3
93.4	72.3	87.2
92.1	76.9	88.8
89.5	87.5	95.0

GRAPH