DESIGN OF A PLANT TO PRODUCE FOUR HUNDRED THOUSAND POUNDS PER YEAR OF PHTHALIC ANHYDRIDE VIA VAPOUR PHASE OXIDATION OF O- XYLENE

BY

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2001/ 11542EH

DEPARTMENT OF CHEMICAL

ENGINEERING

FEDERAL UNIVERSITY OF TECHNOLOGY,

MINNA, NIGERIA

NOVEMBER, 2007

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A DESIGN PROJECT SUBMITTED TO THE DEPARTMENT OF
CHEMICAL ENGINEERING, SCHOOL OF ENGINEERING AND
ENGINEERING TECHNOLOGY, FEDERAL UNIVERSITY OF
TECHNOLOGY, MINNA, NIGER STATE, NIGERIA.
IN PARTIAL FULFILMENT OF THE REQUIREMENT FOR THE
AWARD OF BACHELOR OF ENGINEERING (B.ENG) DEGREE IN
CHEMICAL ENGINEERING

NOVEMBER, 2007

DECLARATION

I hereby declare that this project work was carried out by me under the supervision of Engr.M.U. Garba and Engr. Habib Uthman of the Department of Chemical Engineering. This project is a record of my own personal research work and all the information from the published work of others is duly acknowledged by way of reference.

CERTIFICATION

This is to certify that this research project titled " Design of a plant to produce four hundred thousand pound per year of phthalic anhydride via vapour phase oxidation of o-xylene'' was carried out by **IGBAOFO LINUS .I.** and submitted to the Department of Chemical Engineering, School of Engineering and Engineering Technology, Federal University of Technology, Minna, Niger state, in partial fulfillment of the requirement for the award of Bachelor of Engineering (B.Eng.) Degree in Chemical Engineering.

11/12/2007

Engr. M.U. Garba **Date**

Dr. M.O. Edoga **Date**
(HEAD OF DEPARTMENT)

EXTERNAL EXAMINER **Date**

DEDICATION

This design work is dedicated to God Almighty who has been the source of my strength and inspiration in this journey of life.

ACKNOWLEDGEMENT

All praise to God Almighty who has been the source of my inspiration and strength in this journey of life.

My special gratitude goes to my diligent supervisors, Engr. M.U. Garba and Engr. U. Habibu, without whom this work would not be complete.

My sincere appreciation goes to the Dean of the School of Engineering and Engineering Technology, Prof. (Engr) J.O Odigure, for the special role he played in making this work a reality and the entire efforts of all lecturers of chemical engineering department.

ABSTRACT

This project work was carried out to design a plant that has the capacity to produce 400,000 pound/ year of phthalic anhydride. The technology chosen for the process is the vapor phase oxidation of ortho-xylene using vanadium V oxide catalyst. The cost analysis carried out after the design predicts a total investment requirement of ₦260, 200,000 per year an annual profit after tax (PAT) of ₦6, 860, 000 per year and a pay back period of 13 years for the proposed plant.

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CHAPTER ONE

1.0 INTRODUCTION

Phthalic anhydride is a white crystalline solid which is the first in the series of cyclic anhydride. In the molten state, it is white liquid which resembles water. Although it's normal boiling point is 280°C and its normal boiling point is 131 °C. The vapour has a strong tendency to exist at temperatures below the boiling point and to sublime. It is toxic at low levels (2 ppm), a severe skin irritant and can form explosive mixture with air at concentrations 1.7 to 10.5%.

Orthoxylene is now the the primary feed material, having replaced naphthalene in the 1970s. A fixed bed catalytic oxidation process using air is preferred by most current manufacturers. The principal use is for the production of plastics from vinyl chloride Phthalate esters, which function as plasticizers, are derived from Phthalic anhydride. Phthalic anhydride has another major use in the production of polyester resins and other minor uses in the **production** of alkyd resins used in paints and lacquers, certain dyes (anthraquinone, phthalein, rhodamine, phthalocyanine, fluorescein, and xanthene dyes), insect repellents, and urethane polyester polyols. It has also been used as a rubber scorch inhibitor and retarder.

The production of Phthalic anhydride consists of two main steps:

i. Catalytic oxidation of orthoxyle using oxygen in air.

ii. Purification of the reaction products to obtain Phthalic anhydride.

Aims and Objectives

The aim of the project is to design a plant that would have the capacity to produce 400,000lb/ year of phthalic anhydride from controlled catalytic oxidation of o- xylene at a minimum cost of equipment design and all that it entails for optimization and efficient performance of the plant

1.2 Methodology and scope of work

The design of the plant is a mathematical work which can be done with the aid of scientific calculator but this is rather tasking. With advancements in technology, computer software applications have developed in order to achieve efficiency with respect to time and accuracy.

MathCAD is used for carrying out calculations, the AutoCAD is used for drawing the flow diagrams.

CHAPTER TWO

2.0 LITERATURE SURVEY

2.1 Raw Materials

The principal raw material used in the production of Phthalic anhydride are ortho-xylene and oxygen.

2.1.1 Ortho-xylene

Xylenes and ethyl benzenes are C_8 benzene homologues with the molecular formula C8 H10. The three-xylene isomers are ortho-xylene (o-xylene), meta-xylene (m-xylene) and para-xylene (p-xylene,), which differ in the positions of the two-methyl groups on the benzene ring. The term mixed xylenes' describes a mixture of ethyl benzene and the three xylenes isomers. Mixed xylenes are largely derived from petroleum.

Ethyl benzene is always present, except in the small amount of xylenes produced by toluene disproportionation. Ethyl benzene is diluents, which can accumulate in the recycle processing schemes, and hence has a strong impact on the separation of the individual xylene isomers.

The demand for gasoline far surpasses that for petrochemicals. Gasoline contains 24% aromatic material. Thus, the demand for mixed xylenes for petrochemicals use is strongly influenced by the demand for gasoline. By-product credits have a decisive impact on the production economics of the individual isomers. Xylene serve as an indicator of the nation's petrochemical prowess since its close link to petrochemical production ensures that its supply is intertwined with the production of other chemicals. However, it is not as important as many other products of the chemical industry. Therefore, the main problems faced by market analysts looking at the xylenes business are projecting the future growth in this field. Virgin xylenes are available in plenty and are in most cases directly processed to give pure forms of the isomers. However, the xylene separations are complicated by the fact that the physical and the chemical properties of the isomers are similar. This necessitates the use of other expensive procedures and the use of distillation columns to separated in the petrochemical refinery. The C8 aromatic cut is sent through many processing stages to finally obtain individual isomers of high purity. The Indian scenario for xylenes reveals an expanding market, with the leading petrochemical companies like reliance industries running xylene separation plants.

Production of p- xylene and o- xylene is mainly a separation of the above isomers from a C_8 cut from various sources of virgin xylene, i.e. petroleum sources, which includes catalytic reformate or pyrolysis gasoline and a minor chunk as a coke oven by-product. The other source is toluene disproportionation. Toluene disproportionation is defined as the process in which two moles of toluene are converted to one mole of benzene and one mole of xylenes (the ratio however can be altered). Xylenes obtained by this method are more expensive than by the conventional routes but have significant feedstock advantages when recovering o-and p- xylene isomers.

2.1.2 Physical properties

Because of their similar structure, the three xylenes and the isomeric ethyl benzene exhibit similar properties. The distillation characteristics of the C8 aromatic compounds are of considerable importance.

O-xylene is more readily separated from m-xylene because of a 5°C difference in boiling point. The difference in freezing point between the p-xylene and other C8 aromatic compounds is utilized for p-xylene separation. The critical compression ratios are 14.2, 13.6, and 9.6 for p-xylene, m-xylene and o-xylene respectively. The research octane values are 113, 116.4, 117.5 and 107.4 for Ethyl benzene, p-xylene, m-xylene and o-xylene respectively.

The physical properties of these compounds are summarized as follows:

Table 2.1: Physical Properties of Xylene

Molecular weight	106.167	106.167	106.167	106.167
Density @ 25°C, g/cm^3	0.8610	0.8642	0.8802	0.8671
Boiling point °C	138.37	139.12	144.41	136.19
Freezing point °C	13.263	-47.872	-25.182	-94.975
Refractive	1.4958	1.4971	1.5054	1.4959

2.1.2 Chemical Properties

Reactions involving the position of the alkyl substituents: These reactions include isomerization, disproportionation and dealkylation. Acids catalyze the interconversion of the three-xylene isomers. Xylenes isomerize to near equilibrium levels in a hydrogen fluoride – boron trifluoride system with low boron trifluoride concentrations. Isomerization at lower temperatures produces more p-xylene and o-xylene.

2.2 Phthalic Anydride

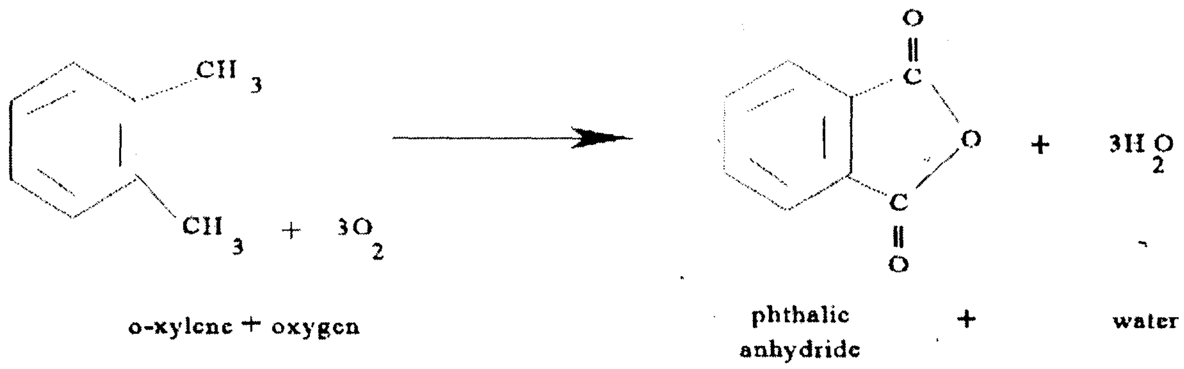
Phthalic anhydride (PAN) production in the United States in 1972 was 0.9 billion pounds per year; this total is estimated to increase to 2.2 billion pounds per year by 1985. Of the current production, 50 percent is used for plasticizers, 25 percent for alkyd resins, 20 percent for unsaturated polyester resins, and 5 percent for miscellaneous and exports. PAN is produced by catalytic oxidation of either orthoxylene or naphthalene. Since naphthalene is a higher-priced feedstock and has a lower feed utilization (about 1.0 lbPAN/lb o-xylene versus 0.97 lb PAN/lb naphthalene), future production growth is predicted to utilize o-xylene. Because emission factors are intended for future as well as present application, this report will focus mainly on PAN production utilizing o-xylene as the main feedstock.

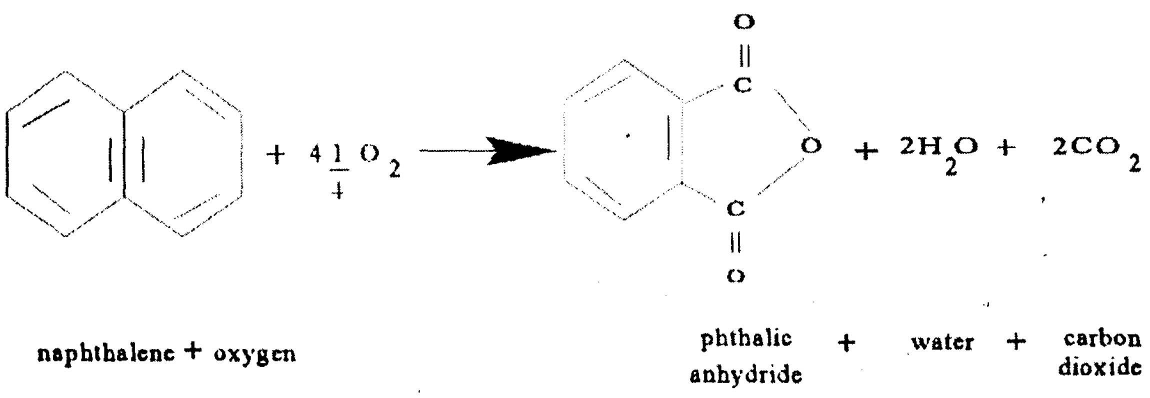
The processes for producing PAN by o-xylene or naphthalene are the same except for reactors, catalyst handling, and recovery facilities required for fluid bed reactors.

compressed, and mixed with vaporized o-xylene and fed into the fixed-bed tubular reactors. The reactors contain the catalyst, vanadium pentoxide on silical gel supported on potassium sulphate, and are operated at 650 to 725°F (340 to 385°C). Small amounts of sulfur dioxide are added to the reactor feed to maintain catalyst activity. Exothermic heat is removed by a molten salt bath circulated around the reactor tubes and transferred to a steam generation system.

Naphthalene-based feedstock is made up of vaporized naphthalene and compressed air. It is transferred to the fluidized bed reactor and oxidized in the presence of a catalyst, vanadium pentoxide, at 650 to 725 °F (340 to 385°C). Cooling tubes located in the catalyst bed remove the exothermic heat, which is used to produce high-pressure steam. The reactor effluent consists of PAN vapors, entrained catalyst, and various byproducts and non reactant gas. The catalyst is removed by filtering and returned to the reactor.

The chemical reactions for air oxidation of o-xylene and naphthalene are as follows.





The reactor effluent containing crude PAN plus products from side reactions and excess oxygen passes to a series of switch condensers where the crude PAN cools and crystallizes. The condensers are alternately cooled and then heated, allowing PAN crystals to form and then melt from the condenser tube fins.

The crude liquid is transferred to a pretreatment section in which phthalic acid is dehydrated to anhydride. Water, maleic anhydride, and benzoic acid are partially evaporated. The liquid then goes to a vacuum distillation section where pure PAN (99.8 wt. percent pure) is recovered. The product can be stored and shipped either as a liquid or a solid (in which case it is dried, flaked, and packaged in multi-wall paper bags). Tanks for holding liquid PAN are kept at 300 °F (150°C) and blanketed with dry nitrogen to prevent the entry of oxygen (fire) or water vapor (hydrolysis to phthalic acid).

Maleic anhydride is currently the only byproduct being recovered. Figure 2.1 and Figure 2.2 show the process flow for air oxidation of o-xylene and naphthalene, respectively.

Emissions and Controls

Emissions from o-xylene and naphthalene storage are small and presently are not controlled.

The major contributor of emissions is the reactor and condenser effluent which is vented from the condenser unit. Particulate, sulfur oxides (for o-xylene-based production), and carbon monoxide make up the missions, with carbon monoxide comprising over half the total. The most efficient (96 percent) system of control is the combined usage of a water scrubber and thermal incinerator. A thermal incinerator alone is approximately 95 percent efficient in combustion of pollutants for o-xylene-based production, and 80 percent efficient for naphthalene-based production. Thermal incinerators with steam generation show the same efficiencies as thermal incinerators alone. Scrubbers have 99 percent efficiency in collecting particulates, but are practically ineffective in reducing carbon monoxide emissions. In naphthalene-based production, cyclones can be used to control catalyst dust emissions with 90 to 98 percent efficiency.

Pretreatment and distillation emissions—particulates and hydrocarbons—are normally processed through the water scrubber and/or incinerator used for the main process stream (reactor and condenser) or scrubbers alone, with the same efficiency percentages applying.

Product storage in the liquid phase results in small amounts of gaseous emissions. These gas streams can either be sent to the main process vent gas control devices or first processed through sublimation boxes or devices used to recover escaped PAN. Flaking and bagging emissions are negligible, but can be sentto a cyclone for recovery of PAN dust. Exhaust from the cyclone presents no problem.

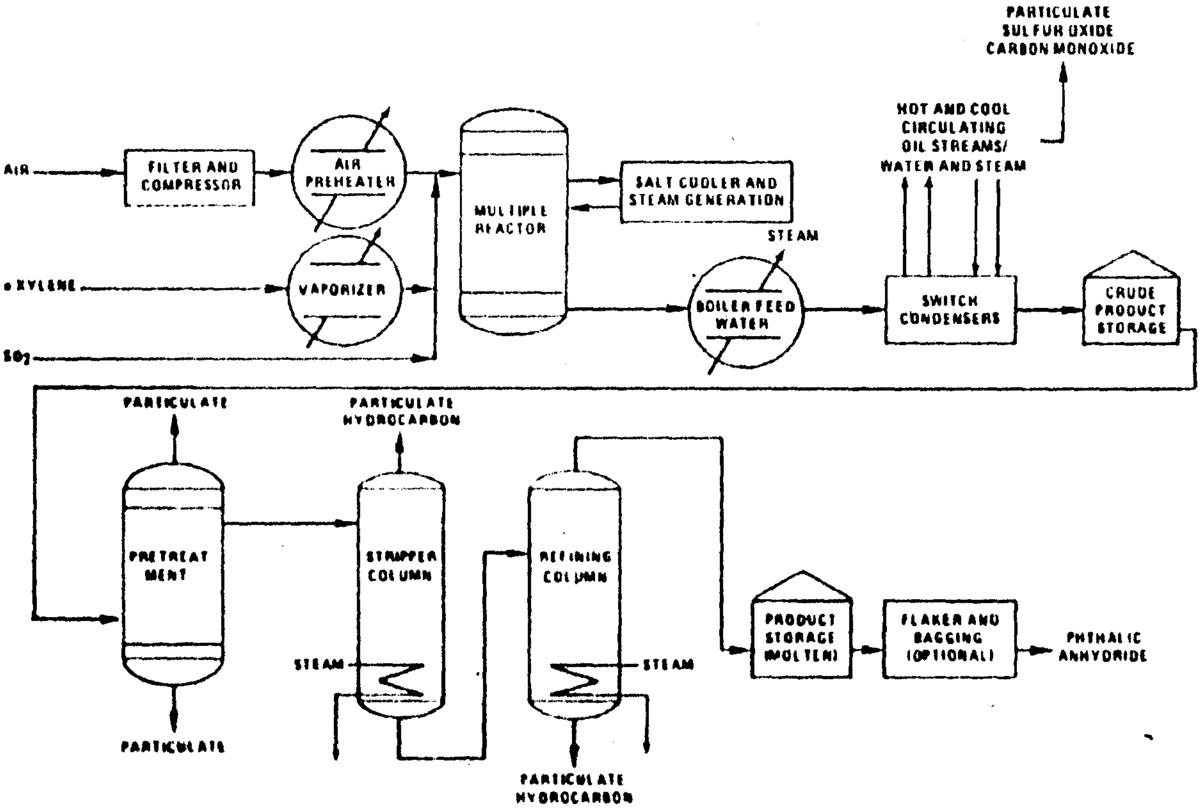


Figure 2.1: Flow diagram for Phthalic anhydride using o-xylene as basic feedstock.

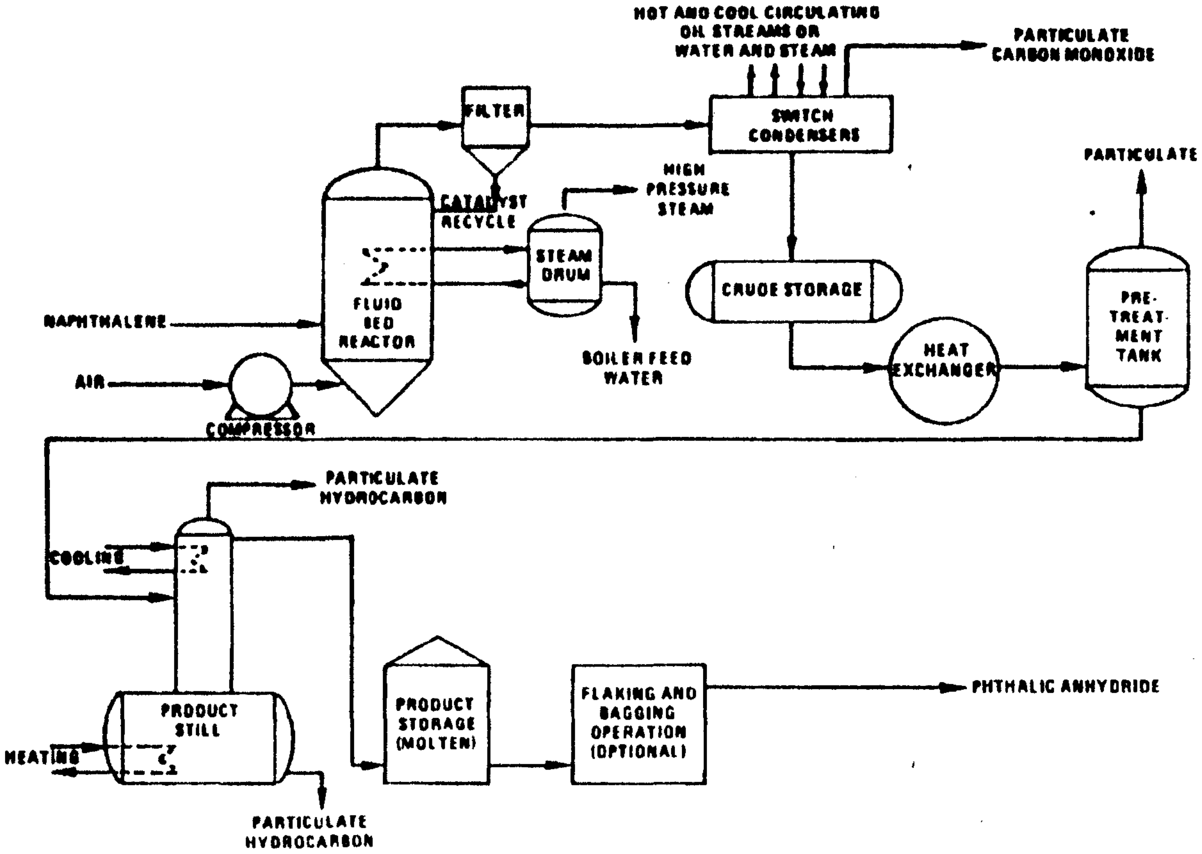


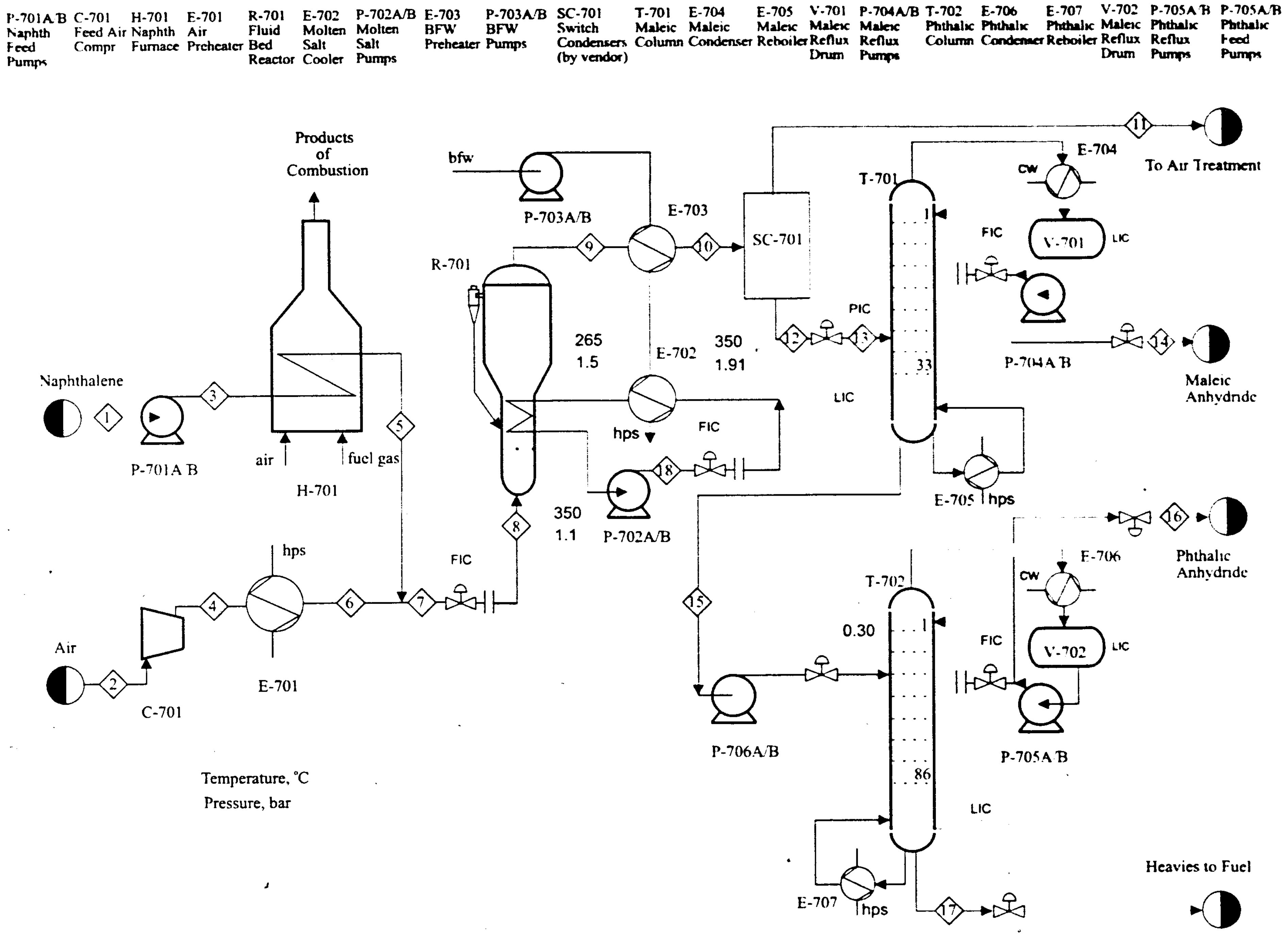
Figure 2.2: Flow diagram for Phthalic anhydride using naphthalene as basic feedstock.

2.3 Technology of Production

Phthalic Anhydride can be produced from orthoxylene and naphthalene. The technology based on the use of the two raw materials are discussed under this section

2.3.1 Production of Phthalic anhydride from Naphthalene

Figure 2.3 produces phthalic anhydride from naphthalene. The feeds are essentially pure naphthalene and excess air. These are pressurized, heated and vaporized (naphthalene) and reacted in a fluidized bed with a vanadium oxide on silica gel catalyst. The reactions are:


P-701A/B Naphth Feed Pumps
C-701 Feed Air Compr
H-701 Naphth Furnace
E-701 Air Preheater
R-701 Fluid Bed Reactor
E-702 Molten Salt Cooler
P-702A/B Molten Salt Pumps
E-703 BFW Preheater
P-703A/B BFW Pumps
SC-701 Switch Condensers (by vendor)
T-701 Maleic Column
E-704 Maleic Condenser
E-705 Maleic Reboiler
V-701 Maleic Reflux Drum
P-704A/B Maleic Reflux Pumps
T-702 Phthalic Column
E-706 Phthalic Condenser
E-707 Phthalic Reboiler
V-702 Maleic Reflux Drum
P-705A/B Phthalic Reflux Pumps
P-705A/B Phthalic Feed Pumps
Products of Combustion
bfw
P-703A/B
E-703
R-701
SC-701
T-701
E-704
cw
FIC
V-701
LIC
To Air Treatment
Naphthalene
P-701A/B
air
fuel gas
H-701
265
1.5
E-702
350
1.91
PIC
LIC
hps
FIC
P-702A/B
350
1.1
P-704A/B
Maleic Anhydride
E-705
hps
Phthalic Anhydride
hps
E-701
Air
C-701
FIC
T-702
E-706
cw
0.30
FIC
V-702
LIC
P-706A/B
P-705A/B
LIC
E-707
hps
Heavies to Fuel
1
33
1
86
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
Temperature, °C
Pressure, bar

$$\underset{\text{naphthalene}}{C_{10}H_8} + \tfrac{9}{2}O_2 \rightarrow \underset{\substack{\text{phthalic}\\ \text{anhydride}}}{C_8H_4O_3} + 2H_2O + 2CO_2$$

$$C_{10}H_8 + 6O_2 \rightarrow \underset{\text{maleic anhydride}}{2C_4H_2O_3} + 2H_2O + 2CO_2$$

$$C_{10}H_8 + \tfrac{3}{2}O_2 \rightarrow \underset{\text{naphthoquinone}}{C_{10}H_6O_2} + H_2O$$

Additionally, the complete and incomplete combustion reactions of naphthalene also occur. The large exothermic heat of reaction is removed by molten salt circulated through coils in the reactor. The molten salt is used to produce high-pressure steam. Total conversion of naphthalene is very close to 100%. The reaction products proceed to a set of devices known as switch condensers. These are described in detail later. Design and operation of these devices is provided under contract by Condenser. They guarantee us that their condensers can operate at any capacity and provide the same separation as in current operation, as long as the pressure and the composition of the condensable portion of Stream 10 remain constant. The net result of the switch condensers is that essentially all of the light gases and water leave as vapor, with small amounts of maleic and phthalic anhydrides, and that the remaining anhydrides and naphthoquinone leave as liquid. The liquid pressure is then reduced to vacuum for distillation. The first column removes maleic anhydride impurity overhead, and the second column removes the phthalic anhydride product overhead.

Organic waste is burned for its fuel value. The dirty air, Stream 11, must be treated. The anhydrides are scrubbed using water, which is then sent to the on-site wastewater treatment facility.

2.3.2 Production of Phthalic anhydride from O-xylene

The raw materials are air and o-xylene. The o-xylene feed, which contains 5 wt% inert impurities is vaporized in unit V-701. Air, which may be assumed to contain only O_2

and N_2, is mixed with recycle, if there is any recycle, and heated. The hot air and vaporized o-xylene are mixed and sent to a packed bed reactor. The contents of Stream 7 must be below the LFL of o-xylene, which is 1 mole%. In this reactor, essentially 100% of the o-xylene is reacted. Most goes to form phthalic anhydride, but some complete and incomplete combustion of o-xylene occurs, some maleic anhydride is formed, and a heavy impurity is also formed. The selectivities are given later. The reactor effluent enters a complex series of devices known as switch condensers. The net result is that all light gases and water leave in Stream 9, with small amounts of both anhydrides, and the phthalic anhydride, maleic anhydride, inerts, and heavy impurity leave in Stream 10. The "dirty air" in Stream 9 must be treated before it can be vented, and this is an additional expense. It is also possible to recycle some of the "dirty air." Any "dirty air" not recycled must be sent to a scrubber, in which the anhydrides are scrubbed into water. The water is then sent to an on-site waste water treatment plant, and an operating charge is assessed. The contents of Stream 10 are sent to a series of two distillation columns which produce liquid waste (Streams 13 and 16) which is burned for fuel. No economic credit is allowed. The product in Stream 15 must be 99.9% phthalic anhydride. This process must produce 75,000 metric tons/year of phthalic anhydride.

2.3.1.1 Process details

- **Feed Streams**

Stream 1: air, consisting of 79% N_2 and 21% O_2 - free

Stream 2: o-xylene with 5 wt % inert impurity

2.3.1.2 Equipment

Compressor (C-701): increases pressure of air feed from 1 atm to 3 atm

Vaporizer (E-701): vaporizes o-xylene feed which is already above 3 atm

Fired Heater (H-701): heats air to reaction temperature

Reactor (R-701): the following reactions occur:

$$\underset{o-xylene}{C_8H_{10}} + 3O_2 \rightarrow \underset{\substack{phthalic\\anhydride}}{C_8H_4O_3} + 3H_2O$$

$$C_8H_{10} + 7.5O_2 \rightarrow \underset{\textit{maleic anhydride}}{C_4H_2O_3} + 4H_2O + 4CO_2$$

The selectivity for the phthalic anhydride reaction is 70%, for the complete combustion of o-xylene is 15%, for the incomplete combustion of o-xylene is 5%, for maleic anhydride is 9%, and for the heavy impurity is 1%. The heavy impurity consumes a negligible amount of oxygen and produces a negligible amount of light gases.

Switch Condensers (SC-701): These are a complex set of condensers. Phthalic anhydride is first desublimated and then melted. There are three condensers, one in the desublimation mode, one in the melting mode, and one in stand-by mode.

Distillation Column (T-701): Here, 99% of the phthalic anhydride and all of the heavy impurity goes to stream 14. All of the inert and enough of the maleic anhydride to allow stream 15 to satisfy its purity requirement go to Stream 13.

Distillation Column (T-702): Here, 99.9% of the phthalic anhydride, and any remaining maleic anhydride go to stream 15, and all of the heavy impurity goes to stream 16.

2.3.1.3 Economic Analysis

When evaluating alternative cases, the following relationship should be used:

EAOC = -(product value - feed cost - other operating costs - capital cost annuity)

EAOC is an equivalent operating cost. A negative EAOC means there is a profit. It is desirable to minimize the EAOC; i.e., a large negative EAOC is very desirable.

Phthalic anhydride is valued at \$0.77/kg, and o-xylene costs \$0.30/kg. The capital cost annuity is an annual cost associated with plant construction (kind of like mortgage payments), and may be assumed to be $\$1.2 \times 10^6$/yr. The other operating costs are for compression and for waste treatment.

Compression costs are:

CHAPTER THREE

3.0 MATERIAL BALANCE

Definition: Species indices in the order O-xylene, Oxygen, Phthalic anhydrde, Water, Nitrogen, Carbondioxide, Maleic anhydride, Heavy impurities.

Stream initializtion:

$s := 0..7$ $j := 1..23$ kmol := 1000mo

Mass flow rate (Amount) of a component s in a stream j is:

$n_{s,j} := 0\cdot\frac{kg}{hr}$

Total Mass flow rate (Total Amount) of a stream j is:

$N_j := 0\cdot\frac{kg}{hr}$

Mass composition of a stream s in a stream j is:

$x_{s,j} := 0$

Molar flow rate of a component s in a stream j is:

$z_{s,j} := 0\cdot\frac{kmol}{hr}$

Total Molar flow rate of a stream j is:

$Z_j := 0\frac{kmol}{hr}$

Molar composition of a stream s in a stream j is:

$y_{s,j} := 0$

Scale-up Factor:

$Input_j := 0\cdot\frac{kg}{hr}$ $\lambda_s := 0\cdot\frac{kJ}{kmol}$ $kJ \equiv 1000J$

Plant Attainment:

From literature (Sinnot, 2005), the plant attainment is between 90-95%

Plant_Attainment ≡ 0.904

Plant Working days: $annum \equiv 365\cdot day\cdot Plant\_Attainment$

$$\$/h = 0.007m\left[\left(\frac{P_{out}}{P_{in}}\right)^{0.3} - 1\right]$$

Air treatment is accomplished by absorption of the organic matter into water, with the light gases vented to the atmosphere. The water is then sent to a waste water treatment plant. The cost is based upon the amount of organic matter (phthalic and maleic anhydrides) in stream 11. The cost is: $\$500/1000kg$ organic matter annum = 330.07day

Basis:

Production Rate of :

$$PR := 400000\,\frac{lb}{annum} \qquad PR = 22.904\,\frac{kg}{hr}$$

Molecular Weight of Phthalic anhydrde:

$$M_{wPanhydride} := 148\,\frac{kg}{kmol}$$

Amount of Phthalic anhydrde in kmol:

$$Panhydride_{kmol} := \frac{PR}{M_{wPanhydride}}$$

$$Panhydride_{kmol} = 0.155\,\frac{kmol}{hr}$$

REACTION 1: (MAIN REACTION)

The stoichiometry reaction for the production of Phthalic anhydrde is as follows:

$$\underset{o-xylene}{C_8H_{10}} + 3O_2 \rightarrow \underset{phthalic\ anhydride}{C_8H_4O_3} + 3H_2O$$

Based on stoichiometric reaction, amount of Phthalic anhydrde in kmol/hr is:

$$Oxylene_{kmol} := Panhydride_{kmo}$$

$$Oxylene_{kmol} = 0.155\,\frac{kmol}{hr}$$

Molecular Weight of O-xylene:

$$M_{wOxylene} := 106\,\frac{kg}{kmol}$$

Amount of O-xylene in kg/hr is:

$$Oxylene_{kg} := Oxylene_{kmol} \cdot M_{wOxylene}$$

$\text{Oxylene}_{kg} = 16.404\,\frac{kg}{hr}$

Assumption:

Purity of the O-xylene is 60%

$\text{Oxylene\_Purity} := 60\%$

Amount of the oil feedstock is:

$\text{Oxylene\_Feedstock} := \frac{\text{Oxylene}_{kg}}{\text{Oxylene\_Purity}}$

$\text{Oxylene\_Feedstock} = 27.34\,\frac{kg}{hr}$

Amount of unreacted O-xylene in reaction 1 is:

$\text{Rxn1Un}_{\text{Oxylene}} := \text{Oxylene\_Feedstock} - \text{Oxylene}_{kg}$

$\text{Rxn1Un}_{\text{Oxylene}} = 10.936\,\frac{kg}{hr}$

Based on stoichiometric reaction, amount of oxygen in kmol/hr is:

$\text{Oxygen}_{kmol} := 3\cdot\text{Oxylene}_{kmo}$

$\text{Oxygen}_{kmol} = 0.464\,\frac{kmol}{hr}$

Molecular Weight of Oxygen:

$M_{\text{wOxygen}} := 32\cdot\frac{kg}{kmol}$

Amount of oxygen in kg/hr is:

$\text{Oxygen}_{kg} := M_{\text{wOxygen}}\cdot\text{Oxygen}_{kmo}$

$\text{Oxygen}_{kg} = 14.857\,\frac{kg}{hr}$

From Literature (Sinnot, 2005), the % molar composition of air is 21% oxygen and 79% nitrogen.

Amount of nitrogen charged to the reactor in kmol/hr:

$\mathrm{Air_{kmol}} := \dfrac{\mathrm{Oxygen_{kmol}}}{0.21}$ $\qquad$ $\mathrm{Air_{kmol}} = 0.614\,\dfrac{\mathrm{mol}}{\mathrm{s}}$

$\mathrm{Nitrogen_{kmol}} := \mathrm{Air_{kmol}} - \mathrm{Oxygen_{kmo}}$ $\qquad$ $\mathrm{Nitrogen_{kmol}} = 1.747\,\dfrac{\mathrm{kmol}}{\mathrm{hr}}$

Molecular Weight of Nitrogen:

$\mathrm{M_{wNitrogen}} := 28\cdot\dfrac{\mathrm{kg}}{\mathrm{kmol}}$

Amount of nitrogen in kg/hr:

$\mathrm{Nitrogen_{kg}} := \mathrm{M_{wNitrogen}}\cdot\mathrm{Nitrogen_{kmol}}$

$\mathrm{Nitrogen_{kg}} = 48.903\,\dfrac{\mathrm{kg}}{\mathrm{hr}}$

Based on stoichiometric reaction, amount of water in kmol/hr is:

$\mathrm{Water_{kmol}} := 3\cdot\mathrm{Oxylene_{kmo}}$

$\mathrm{Water_{kmol}} = 0.464\,\dfrac{\mathrm{kmol}}{\mathrm{hr}}$

Molecular Weight of water:

$\mathrm{M_{wWater}} := 18\cdot\dfrac{\mathrm{kg}}{\mathrm{kmol}}$

Amount of water in kg/hr is:

$\mathrm{Water_{kg}} := \mathrm{M_{wWater}}\cdot\mathrm{Water_{kmo}}$

$\mathrm{Water_{kg}} = 8.357\,\dfrac{\mathrm{kg}}{\mathrm{hr}}$

Reaction 1: Summary

Amount of Reacted O-xylene:

$Rxn1_{Oxylene} := Oxylene_{kg}$

$Rxn1_{Oxylene} = 16.404 \frac{kg}{hr}$

Amount of unreacted O-xylene in reaction 1:

$Rxn1_{unreacted\_Oxylene} := Rxn1Un_{Oxylene}$

$Rxn1_{unreacted\_Oxylene} = 10.936 \frac{kg}{hr}$

Amount of Reacted Oxygen in reaction 1:

$Rxn1_{Oxygen} := Oxygen_{kg}$

$Rxn1_{Oxygen} = 14.857 \frac{kg}{hr}$

Amount of Phthalic anhydride product of reaction 1:

$Rxn1_{phthalic\_anhydride} := PR$

$Rxn1_{phthalic\_anhydride} = 22.904 \frac{kg}{hr}$

Amount of water product of reaction 1:

$Rxn1_{water} := Water_{kg}$

$Rxn1_{water} = 8.357 \frac{kg}{hr}$

Molecular Weight of Maleic anhydride:

$M_{wMaleic\_Anhydride} := 98 \cdot \frac{kg}{kmol}$

Molecular carbon dioxide:

$M_{wCarbon\_dioxide} := 44 \cdot \frac{kg}{kmol}$

REACTION 2: (SIDE REACTION)

The stoichiometry reaction for the production of Maleic anhydrde is as follows:

$$C_8H_{10} + 7.5O_2 \rightarrow C_4H_2O_3 + 4H_2O + 4CO_2$$

maleic anhydride

Literature Information:

2. Literature (Aita, 2007) states that 80% of unconverted O-xylene is react with oxygen to form

maleic anhydride as by product

$\%\_of\_Oxylene\_in\_Rxn2 := 80\%$

Amount O-xylene that reacted in reaction 2 is:

$$Rxn2\_Oxylene_{kg} := \%\_of\_Oxylene\_in\_Rxn2 \cdot Rxn1_{unreacted\ Oxylene}$$

$$Rxn2\_Oxylene_{kg} = 8.749 \frac{kg}{hr}$$

Amount O-xylene in kmol/hr is:

$$Rxn2\_Oxylene_{kmol} := \frac{Rxn2\_Oxylene_{kg}}{M_{wOxylene}}$$

$$Rxn2\_Oxylene_{kmol} = 0.083 \frac{kmol}{hr}$$

Based on stoichiometric reaction, amount of oxygen in kmol/hr is:

$$Rxn2\_Oxygen_{kmol} := \frac{15}{2} \cdot Rxn2\_Oxylene_{kmo}$$

$$Rxn2\_Oxygen_{kmol} = 0.619 \frac{kmol}{hr}$$

Amount of oxygen in kg/hr is:

$$Rxn2\_Oxygen_{kg} := M_{wOxygen} \cdot Rxn2\_Oxygen_{kmo}$$

$$\text{Rxn2\_Oxygen}_{kg} = 19.809\frac{kg}{hr}$$

From Literature (Sinnot, 2005), the % molar composition of air is 21% oxygen and 79% nitrogen.

Amount of nitrogen charged to the reactor with oxygen that reacted in reaction 2 in kmol/hr:

$$\text{Rxn2\_Air}_{kmol} := \frac{\text{Rxn2\_Oxygen}_{kmol}}{0.21} \qquad \text{Rxn2\_Air}_{kmol} = 0.819\frac{mol}{s}$$

$$\text{Rxn2\_Nitrogen}_{kmol} := \text{Rxn2\_Air}_{kmol} - \text{Rxn2\_Oxygen}_{kmo} \qquad \text{Nitrogen}_{kmol} = 1.747\frac{kmol}{hr}$$

Amount of nitrogen in kg/hr:

$$\text{Rxn2\_Nitrogen}_{kg} := M_{wNitrogen}\cdot\text{Rxn2\_Nitrogen}_{kmo}$$

$$\text{Rxn2\_Nitrogen}_{kg} = 65.204\frac{kg}{hr}$$

Based on stoichiometric reaction 2, amount of maleic anhydride in kmol/hr is:

$$\text{Rxn2\_Maleic\_Anhydride}_{kmol} := \text{Rxn2\_Oxylene}_{kmo}$$

$$\text{Rxn2\_Maleic\_Anhydride}_{kmol} = 0.083\frac{kmol}{hr}$$

Amount of maleic anhydride in kg/hr is:

$$\text{Rxn2\_Maleic\_Anhydride}_{kg} := M_{wMaleic\_Anhydride}\cdot\text{Rxn2\_Maleic\_Anhydride}_{kmo}$$

$$\text{Rxn2\_Maleic\_Anhydride}_{kg} = 8.089\frac{kg}{hr}$$

Based on stoichiometric reaction 2, amount of water formed in reaction 2 in kmol/hr is:

$$\text{Rxn2\_Water}_{kmol} := 4\cdot\text{Rxn2\_Oxylene}_{kmo}$$

$$\text{Rxn2\_Water}_{kmol} = 0.33\frac{kmol}{hr}$$

Amount of water in kg/hr is:

$$\text{Rxn2\_Water}_{\text{kg}} := M_{\text{wWater}} \cdot \text{Rxn2\_Water}_{\text{kmo}}$$

$$\text{Rxn2\_Water}_{\text{kg}} = 5.943 \frac{\text{kg}}{\text{hr}}$$

Based on stoichiometric reaction 2, amount of carbon dioxide in kmol/hr is:

$$\text{Rxn2\_Carbon\_dioxide}_{\text{kmol}} := 4 \cdot \text{Rxn2\_Oxylene}_{\text{kmo}}$$

$$\text{Rxn2\_Carbon\_dioxide}_{\text{kmol}} = 0.33 \frac{\text{kmol}}{\text{hr}}$$

Amount of water in kg/hr is:

$$\text{Rxn2\_Carbon\_dioxide}_{\text{kg}} := M_{\text{wCarbon\_dioxide}} \cdot \text{Rxn2\_Carbon\_dioxide}_{\text{kmo}}$$

$$\text{Rxn2\_Carbon\_dioxide}_{\text{kg}} = 14.526 \frac{\text{kg}}{\text{hr}}$$

Amount of unreacted O-xylene leaving the reactor is

$$\text{Rxn2}_{\text{unreacted\_Oxylene}} := (1 - \text{\%\_of\_Oxylene\_in\_Rxn2}) \cdot \text{Rxn1}_{\text{unreacted\_Oxylene}}$$

$$\text{Rxn2}_{\text{unreacted\_Oxylene}} = 2.187 \frac{\text{kg}}{\text{hr}}$$

Reaction 2: Summary

Amount of reaction 2 reacted O-xylene:

$$\text{Rxn2\_Oxylene}_{\text{kg}} = 8.749 \frac{\text{kg}}{\text{hr}}$$

Amount of reaction 2 unreacted O-xylene:

$$\text{Rxn2}_{\text{unreacted\_Oxylene}} = 2.187 \frac{\text{kg}}{\text{hr}}$$

Amount of Reacted Oxygen in reaction 2:

$$\text{Rxn2\_Oxygen}_{\text{kg}} = 19.809 \frac{\text{kg}}{\text{hr}}$$

Amount of Reacted nitrogen charged with air in reaction 2:

$$\text{Rxn2\_Nitrogen}_{kg} = 65.204\frac{kg}{hr}$$

Amount of Phthalic anhydride product of reaction 1:

$$\text{Rxn2\_Maleic\_Anhydride}_{kg} = 8.089\frac{kg}{hr}$$

Amount of Phthalic anhydride product of reaction 1:

$$\text{Rxn2\_Maleic\_Anhydride}_{kg} = 8.089\frac{kg}{hr}$$

Amount of water product of reaction 2:

$$\text{Rxn2\_Water}_{kg} = 5.943\frac{kg}{hr}$$

Amount of carbon dioxide product of reaction 2:

$$\text{Rxn2\_Carbon\_dioxide}_{kg} = 14.526\frac{kg}{hr}$$

Reaction 1 Balance:

$$\text{Rxn1}_{Oxygen} + \text{Rxn1}_{Oxylene} = 8.684\times 10^{-3}\frac{kg}{s}$$

$$\text{Rxn1}_{phthalic\_anhydride} + \text{Rxn1}_{water} = 8.684\times 10^{-3}\frac{kg}{s}$$

Reaction 2 Balance:

$$\text{Rxn2\_Oxygen}_{kg} + \text{Rxn2\_Oxylene}_{kg} = 7.933\times 10^{-3}\frac{kg}{s}$$

$$\text{Rxn2\_Maleic\_Anhydride}_{kg} + \text{Rxn2\_Water}_{kg} + \text{Rxn2\_Carbon\_dioxide}_{kg} = 7.933\times 10^{-3}\frac{kg}{s}$$

General Reaction Balance

$$\text{Rxn1}_{Oxygen} + \text{Rxn1}_{Oxylene} + \left(\text{Rxn2\_Oxygen}_{kg} + \text{Rxn2\_Oxylene}_{kg}\right) = 0.017\frac{kg}{s}$$

$$\text{Rxn1}_{phthalic\_anhydride} + \text{Rxn1}_{water} + \left(\text{Rxn2\_Maleic\_Anhydride}_{kg} + \text{Rxn2\_Water}_{kg}\right) \ldots = 0.017\frac{kg}{s}$$
$$+ \text{Rxn2\_Carbon\_dioxide}_{kg}$$

$$\text{Consumed}_{Oxygen} := \text{Rxn1}_{Oxygen} + \text{Rxn2\_Oxylene}_{kg}$$

$Water_{Total} := Rxn1_{water} + Rxn2\_Water_{kg}$

$Water_{Total} = 14.299 \frac{kg}{hr}$

$Consumed_{Oxylene} := Rxn1_{Oxylene} + Rxn2\_Oxylene_{kg}$

$Entering_{Oxygen} := Rxn1_{Oxylene} + Rxn2\_Oxylene_{kg}$

$Leaving_{Nitrogen} := Rxn2\_Nitrogen_{kg} + Nitrogen_{kg}$

$Entering_{Nitrogen} := Rxn2\_Nitrogen_{kg} + Nitrogen_{kg}$

$Unreacted_{Oxylene} := Rxn2_{unreacted\_Oxylene}$

$Unreacted_{Oxylene} = 6.076 \times 10^{-4} \frac{kg}{s}$

$Rxn1_{Oxygen} + Oxylene\_Feedstock + \left(Rxn2\_Oxygen_{kg}\right) + \left(Rxn2\_Nitrogen_{kg} + Nitrogen_{kg}\right) = 0.049 \frac{kg}{s}$

$$\begin{aligned} & Rxn1_{phthalic\_anhydride} + Rxn1_{water} + \left(Rxn2\_Maleic\_Anhydride_{kg} + Rxn2\_Water_{kg}\right) \ldots = 0.049 \frac{kg}{s} \\ & + Rxn2\_Carbon\_dioxide_{kg} + Unreacted_{Oxylene} + \left(Rxn2\_Nitrogen_{kg} + Nitrogen_{kg}\right) \end{aligned}$$

Heavy metals present in O-xylene is 0.01%.

$\%_{HM} := 0.01\%$

$Heavy\_Metals_{kg} := \%_{HM} \cdot Oxylene\_Feedstock$

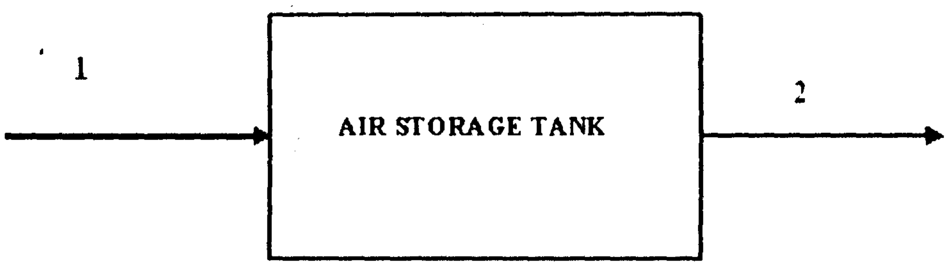
$Heavy\_Metals_{kg} = 2.734 \times 10^{-3} \cdot \frac{kg}{hr}$

1. Air Storage Tank

Air Tank Assumptions

1. 100% material recovery

2.



Stream 1 (Feed to Air Storage Tank):

Oxygen in stream 1 is:

$n_{1,1} := \mathrm{Rxn1}_{Oxygen} + \mathrm{Rxn2\ Oxygen}_{kg}$

$n_{1,1} = 34.665\frac{kg}{hr}$

Nitrogen in stream 1 is:

$n_{6,1} := \mathrm{Leaving}_{Nitrogen}$

$n_{6,1} = 114.107\frac{kg}{hr}$

Total amount of stream 1

$N_1 := \sum_s n_{s,1}$

$N_1 = 148.772\frac{kg}{hr}$

$N_1 = 148.772\frac{kg}{hr}$

Stream 2 (Feed to the mixer):

Oxygen in stream 2 is:

$n_{1,2} := n_{1,1}$

$n_{1,2} = 34.665 \frac{kg}{hr}$

Nitrogen in stream 2 is:

$n_{6,2} := n_{6,1}$

$n_{6,2} = 114.107 \frac{kg}{hr}$

Total amount of stream 2

$N_2 := \sum_s n_{s,2}$

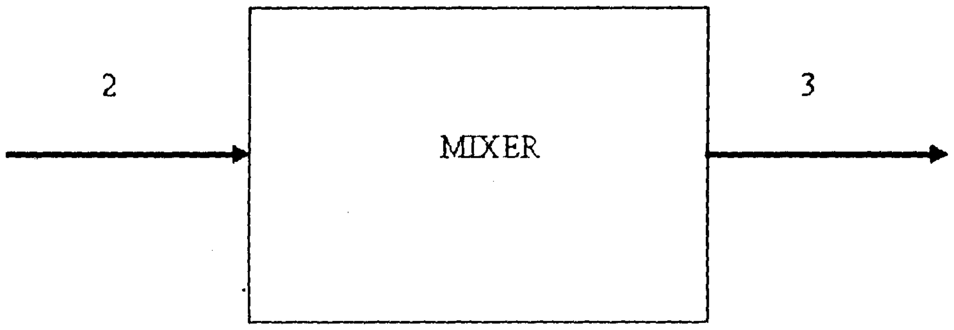
$N_2 = 148.772 \frac{kg}{hr}$

2.Mixer(mix-100)

Mixer Assumptions

1. 100% material recovery

2.



Stream 3 (Feed to the compressor):

Oxygen in stream 3 is:

$n_{1,3} := n_{1,2}$

$n_{1,3} = 34.665 \frac{kg}{hr}$

Nitrogen in stream 3 is:

$n_{6,3} := n_{6,2}$

$n_{6,3} = 114.107 \frac{kg}{hr}$

Total amount of stream 2

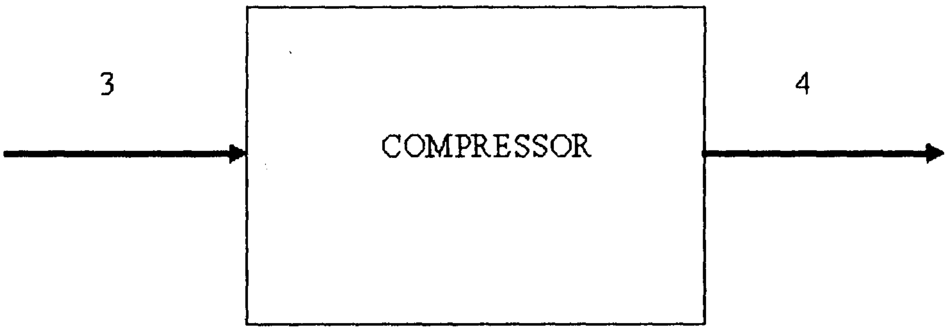
$N_3 := \sum_s n_{s,3}$

$N_3 = 148.772 \frac{kg}{hr}$

. 3 Compressor (K-100)

Compressor Assumptions

1. 100% material recovery



Stream 4 (Feed to Furnace):

Oxygen in stream 4 is:

$n_{1,4} := n_{1,3}$

$n_{1,4} = 34.665\frac{kg}{hr}$

Nitrogen in stream 4 is:

$n_{6,4} := n_{6,3}$

$n_{6,4} = 114.107\frac{kg}{hr}$

Total amount of stream 4

$$N_4 := \sum_s n_{s,4}$$

$N_4 = 148.772\frac{kg}{hr}$

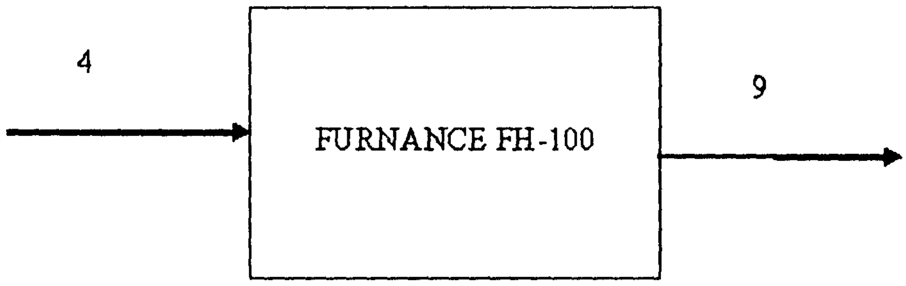
$N_4 = 148.772\frac{kg}{hr}$

4. Furnace (FH-100)

Furnace Assumptions

1. 100% material recovery

2.



Stream 9 (Furnace outlet):

Oxygen in stream 9 is:

$$n_{1,9} := n_{1,4}$$

$$n_{1,9} = 34.665\frac{kg}{hr}$$

Nitrogen in stream 9 is:

$$n_{6,9} := n_{6,4}$$

$$n_{6,9} = 114.107\frac{kg}{hr}$$

Total amount of stream 9

$$N_9 := \sum_s n_{s,9}$$

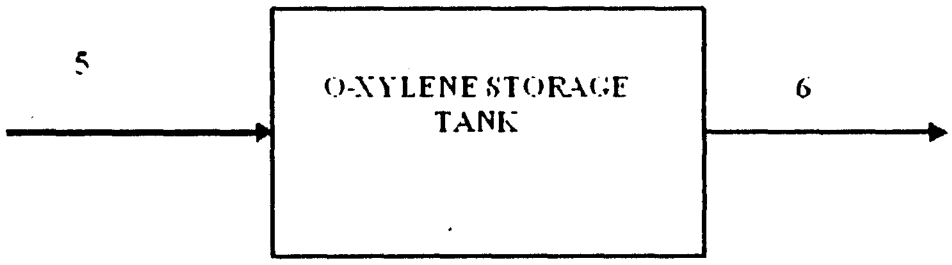
$$N_9 = 148.772\frac{kg}{hr}$$

5. O-xylene Storage Tank

O-xylene Storage Tank Assumptions

1. 100% material recovery

2.



Stream 5 (Feed to O-xylene Storage Tank)

O-xylene in stream 5 is:

$$n_{0,5} := \text{Oxylene\_Feedstock}$$

$n_{0,5} = 27.34\frac{kg}{hr}$

Heavy metals in stream 5 is:

$n_{7,5} := Heavy\_Metals_{kg}$

$n_{7,5} = 2.734\times 10^{-3}\cdot\frac{kg}{hr}$

Total amount of stream 5

$N_5 := \sum_s n_{s,5}$

$N_5 = 27.343\frac{kg}{hr}$

Stream 6 (Feed to the pump):

O-xylene in stream 6 is:

$n_{0,6} := n_{0,5}$

$n_{0,6} = 27.34\frac{kg}{hr}$

Heavy metals in stream 6 is:

$n_{7,6} := n_{7,5}$

$n_{7,6} = 2.734\times 10^{-3}\cdot\frac{kg}{hr}$

Total amount of stream 6

$N_6 := \sum_s n_{s,6}$

$N_6 = 27.343\frac{kg}{hr}$

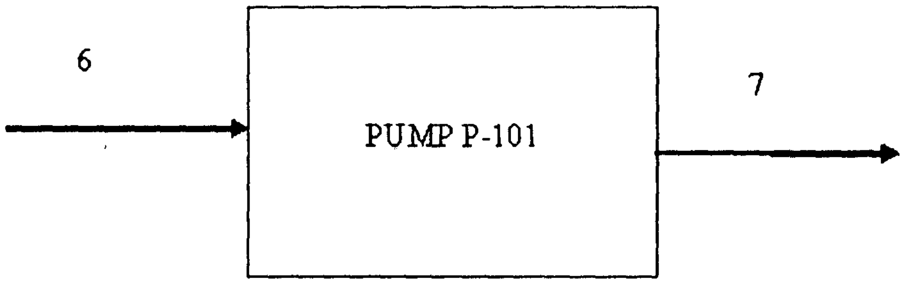
$N_6 = 27.343\frac{kg}{hr}$

6. Pump 101

Pump 101 Assumptions

1. 100% material recovery

2.



Stream 7 (Pump outlet)

O-xylene in stream 7 is:

$n_{0,7} := n_{0,6}$

$n_{0,7} = 27.34\frac{kg}{hr}$

Heavy metals in stream 7 is:

$n_{7,7} := n_{7,6}$

$n_{7,7} = 2.734\times 10^{-3}\cdot\frac{kg}{hr}$

Total amount of stream 7

$N_7 := \sum_{s} n_{s,7}$

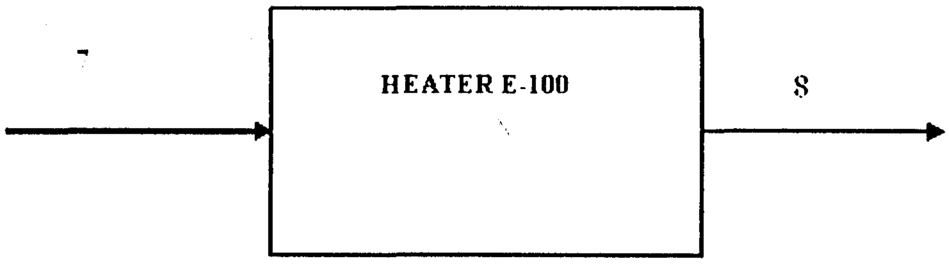
$N_7 = 27.343 \frac{kg}{hr}$

7. Heater(E-100)

Heater(E-100) Assumptions

1. 100% material recovery

2.



Stream 8 (Heater outlet)

O-xylene in stream 8 is:

$n_{0,8} := n_{0,7}$

$n_{0,8} = 27.34 \frac{kg}{hr}$

Heavy metals in stream 8 is:

$n_{7,8} := n_{7,7}$

$n_{7,8} = 2.734 \times 10^{-3} \cdot \frac{kg}{hr}$

Total amount of stream 8

$N_8 := \sum_s n_{s,8}$

$N_8 = 27.343 \frac{kg}{hr}$

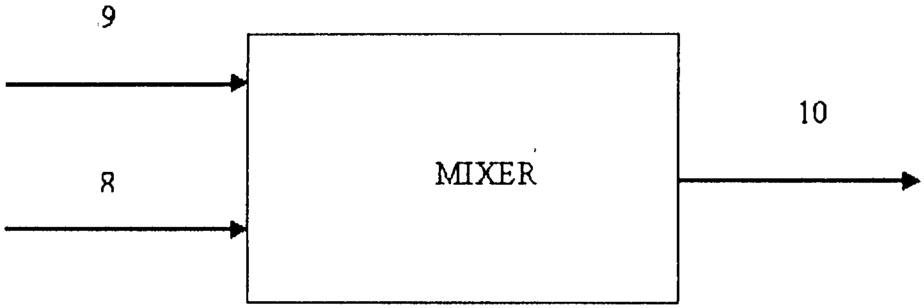
$N_8 = 27.343 \frac{kg}{hr}$

8. Mixer (Mix-101)

Mixer (Mix-101) Assumptions

1. 100% material recovery

2.



Stream 10 (Mixer Product)

Oxygen in stream 10 is:

$n_{1,10} := n_{1,9}$

$n_{1,10} = 34.665 \frac{kg}{hr}$

Nitrogen in stream 10 is:

$n_{6,10} := n_{6,9}$

$n_{6,10} = 114.107 \frac{kg}{hr}$

O-xylene in stream 10 is:

$n_{0,10} := n_{0,8}$

$n_{0,10} = 27.34 \frac{kg}{hr}$

$n_{0,10} = 27.34 \frac{kg}{hr}$

Heavy metals in stream 10 is:

$n_{7,10} := n_{7,8}$

$n_{7,10} = 2.734 \times 10^{-3} \cdot \frac{kg}{hr}$

Total amount of stream 10

$N_{10} := \sum_{s} n_{s,10}$

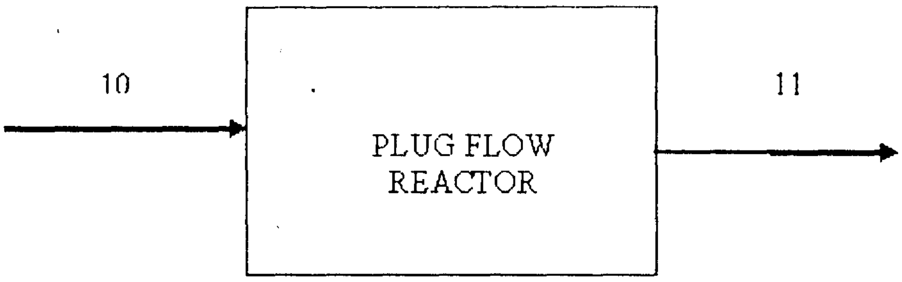
$N_{10} = 176.115 \frac{kg}{hr}$

9. Reactor (PFR-100)

Reactor (PFR-100) Assumptions

1. 100% material recovery

2.



Stream 11 (Reactor Product)

O-Xylene in stream 11 is:

$n_{0,11} := \text{Unreacted}_{\text{Oxylene}}$

$n_{0,11} = 2.187 \frac{kg}{hr}$

Phthalic anhydride in stream 13 is:

$n_{2,11} := Rxn1_{phthalic\_anhydride}$

$n_{2,11} = 22.904\frac{kg}{hr}$

Water in stream 13 is:

$n_{3,11} := Water_{Total}$

$n_{3,11} = 14.299\frac{kg}{hr}$

Maleic Anhydride in stream 11 is:

$n_{4,11} := Rxn2\_Maleic\_Anhydride_{kg}$

$n_{4,11} = 8.089\frac{kg}{hr}$

Carbon dioxide in stream 11 is:

$n_{5,11} := Rxn2\_Carbon\_dioxide_{kg}$

$n_{5,11} = 14.526\frac{kg}{hr}$

Nitrogen in stream 11 is:

$n_{6,11} := n_{6,9}$

$n_{6,11} = 114.107\frac{kg}{hr}$

Heavy metals in stream 11 is:

$$n_{7,11} := n_{7,10}$$

$$n_{7,11} = 2.734\times 10^{-3}\cdot\frac{kg}{hr}$$

Total amount of stream 13

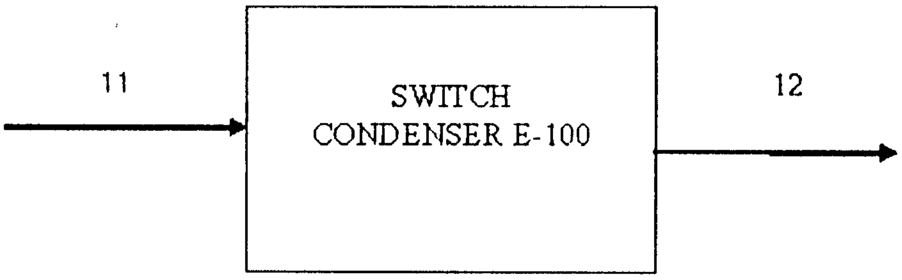
$$N_{11} := \sum_{s} n_{s,11}$$

$$N_{11} = 176.115\frac{kg}{hr}$$

10. Switch Condenser 1 (E-101)

Switch Condenser (E-101) Assumptions

1. 100% material recovery
2.



Stream 12 (Condenser 1 Outlet)

O-Xylene in stream 12 is:

$$n_{0,12} := n_{0,11}$$

$$n_{0,12} = 2.187\frac{kg}{hr}$$

Phthalic anhydride in stream 12 is:

$$n_{2,12} := n_{2,11}$$

$n_{2,12} = 22.904 \frac{kg}{hr}$

Water in stream 12 is:

$n_{3,12} := n_{3,11}$

$n_{3,12} = 14.299 \frac{kg}{hr}$

Maleic Anhydride in stream 12 is:

$n_{4,12} := n_{4,11}$

$n_{4,12} = 8.089 \frac{kg}{hr}$

Carbon dioxide in stream 12 is:

$n_{5,12} := n_{5,11}$

$n_{5,12} = 14.526 \frac{kg}{hr}$

Nitrogen in stream 12 is:

$n_{6,12} := n_{6,11}$

$n_{6,12} = 114.107 \frac{kg}{hr}$

Heavy metals in stream 12 is:

$n_{7,12} := n_{7,11}$

$n_{7,12} = 2.734 \times 10^{-3} \cdot \frac{kg}{hr}$

Total amount of stream 12

$$N_{12} := \sum_{s} n_{s,12}$$

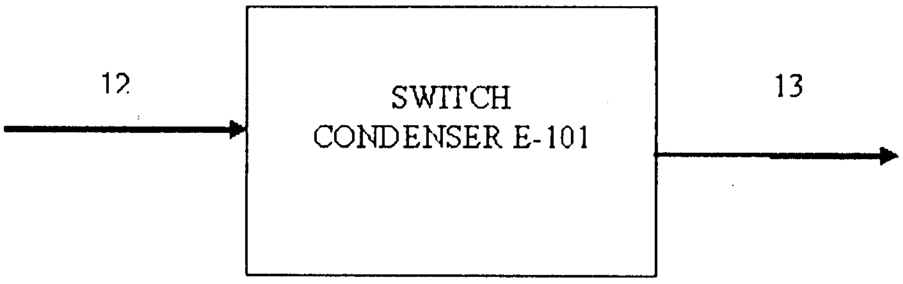
$$N_{12} = 176.115 \frac{kg}{hr}$$

11. Switch Condenser 2 (E-102)

Switch Condenser (E-102) Assumptions

1. 100% material recovery

2.



Stream 13 (Condenser 2 Outlet)

O-Xylene in stream 13 is:

$$n_{0,13} := n_{0,12}$$

$$n_{0,13} = 2.187 \frac{kg}{hr}$$

Phthalic anhydride in stream 13 is:

$$n_{2,13} := n_{2,12}$$

$$n_{2,13} = 22.904 \frac{kg}{hr}$$

Water in stream 13 is:

$$n_{3,13} := n_{3,12}$$

$n_{3,13} = 14.299\frac{kg}{hr}$

Maleic Anhydride in stream 13 is:

$n_{4,13} := n_{4,12}$

$n_{4,13} = 8.089\frac{kg}{hr}$

Carbon dioxide in stream 13 is:

$n_{5,13} := n_{5,12}$

$n_{5,13} = 14.526\frac{kg}{hr}$

Nitrogen in stream 13 is:

$n_{6,13} := n_{6,12}$

$n_{6,13} = 114.107\frac{kg}{hr}$

Heavy metals in stream 13 is:

$n_{7,13} := n_{7,12}$

$n_{7,13} = 2.734\times 10^{-3}\cdot\frac{kg}{hr}$

Total amount of stream 13

$N_{13} := \sum_{s} n_{s,13}$

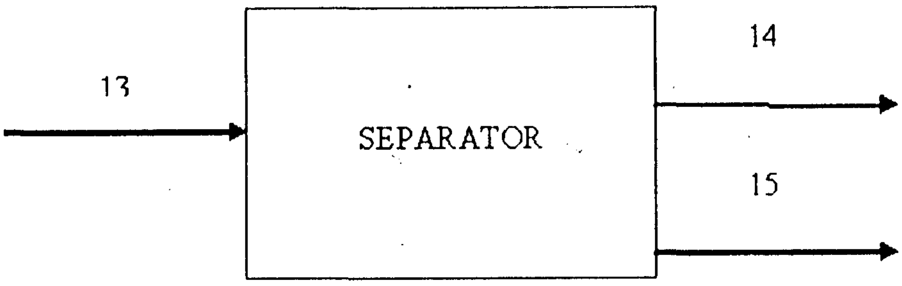
$N_{13} = 176.115\frac{kg}{hr}$

12. Separator V-100

Separator V-100 Assumptions

1. 100% material recovery

2.



Stream 14 (Separator Outlet)

Carbon dioxide in stream 14 is:

$n_{5,14} := n_{5,13}$

$n_{5,14} = 14.526\frac{kg}{hr}$

Nitrogen in stream 14 is:

$n_{6,14} := n_{6,13}$

$n_{6,14} = 114.107\frac{kg}{hr}$

Water in stream 14 is:

$n_{3,14} := 0.01n_{3,13}$

$n_{3,14} = 0.143 \frac{kg}{hr}$

Total amount of stream 14

$N_{14} := \sum_{s} n_{s,14}$

$N_{14} = 128.776 \frac{kg}{hr}$

Stream 15 (Separator Bottom Product)

O-Xylene in stream 15 is:

$n_{0,15} := n_{0,13}$

$n_{0,15} = 2.187 \frac{kg}{hr}$

Phthalic anhydride in stream 15 is:

$n_{2,15} := n_{2,13}$

$n_{2,15} = 22.904 \frac{kg}{hr}$

Maleic Anhydride in stream 15 is:

$n_{4,15} := n_{4,13}$

$n_{4,15} = 8.089 \frac{kg}{hr}$

Heavy metals in stream 15 is:

$n_{7,15} := n_{7,13}$

$n_{7,15} = 2.734\times 10^{-3} \cdot \frac{kg}{hr}$

Water in stream 15 is:

$$n_{3,15} := 0.01 n_{3,13}$$

$$n_{3,15} = 0.143 \frac{kg}{hr}$$

Total amount of stream 15

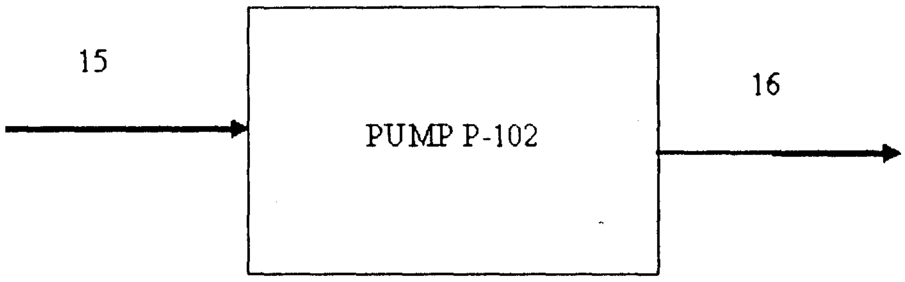
$$N_{15} := \sum_{s} n_{s,15}$$

$$N_{15} = 33.325 \frac{kg}{hr}$$

13. PUMP P-102 ()

PUMP P-102 Assumptions

1. 100% material recovery
2.



Stream 16 (DISTILLATION 1 INLET)

O-Xylene in stream 16 is:

$$n_{0,16} := n_{0,15}$$

$$n_{0,16} = 2.187 \frac{kg}{hr}$$

Phthalic anhydride in stream 16 is:

$n_{2,16} := n_{2,15}$

$n_{2,16} = 22.904 \frac{kg}{hr}$

Water in stream 16 is:

$n_{3,16} := n_{3,15}$

$n_{3,16} = 0.143 \frac{kg}{hr}$

Maleic Anhydride in stream 16 is:

$n_{4,16} := n_{4,15}$

$n_{4,16} = 8.089 \frac{kg}{hr}$

Heavy metals in stream 16 is:

$n_{7,16} := n_{7,15}$

$n_{7,16} = 2.734 \times 10^{-3} \cdot \frac{kg}{hr}$

Total amount of stream 16

$N_{16} := \sum_{s} n_{s,16}$

$N_{16} = 33.325 \frac{kg}{hr}$

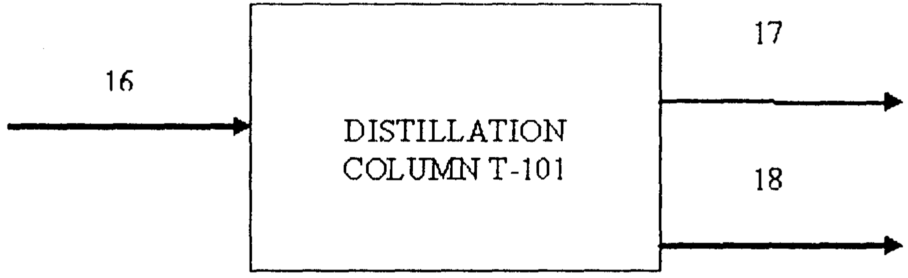
$N_{16} = 33.325 \frac{kg}{hr}$

14. DISTILLATION COLUMN 1 (T-101)

DISTILLATIONAssumptions

1. 100% material recovery

2.



Stream 17 (DISTILLATION OVERHEAD PRODUCT)

O-Xylene in stream 17 is:

$$n_{0,17} := 0.99n_{0,16}$$

$$n_{0,17} = 2.165\frac{kg}{hr}$$

Water in stream 17 is:

$$n_{3,17} := 0.99n_{3,16}$$

$$n_{3,17} = 0.142\frac{kg}{hr}$$

Maleic Anhydride in stream 17 is:

$$n_{4,17} := 0.98n_{4,16}$$

$$n_{4,17} = 7.927\frac{kg}{hr}$$

Total amount of stream 17

$$N_{17} := \sum_{s} n_{s,17}$$

$$N_{17,} = 10.234\frac{kg}{hr}$$

$$N_{17} = 10.234\frac{kg}{hr}$$

Stream 18 (DISTILLATION BOTTOM PRODUCT)

O-Xylene in stream 18 is:

$$n_{0,18} := 0.01n_{0,16}$$

$$n_{0,18} = 0.022\frac{kg}{hr}$$

Water in stream 18 is:

$$n_{3,18} := 0.01n_{3,16}$$

$$n_{3,18} = 1.43\times 10^{-3}\cdot\frac{kg}{hr}$$

Maleic Anhydride in stream 18 is:

$$n_{4,18} := 0.02n_{4,16}$$

$$n_{4,18} = 0.162\frac{kg}{hr}$$

Heavy metals in stream 18 is:

$$n_{7,18} := n_{7,16}$$

$$n_{7,18} = 2.734\times 10^{-3}\cdot\frac{kg}{hr}$$

Phthalic anhydride in stream 18 is:

$$n_{2,18} := n_{2,16}$$

$$n_{2,18} = 22.904\frac{kg}{hr}$$

$$n'_{2,18} = 22.904\frac{kg}{hr}$$

Total amount of stream 18

$$N_{18} := \sum_{s} n_{s,18}$$

$$N_{18} = 23.092\frac{kg}{hr}$$

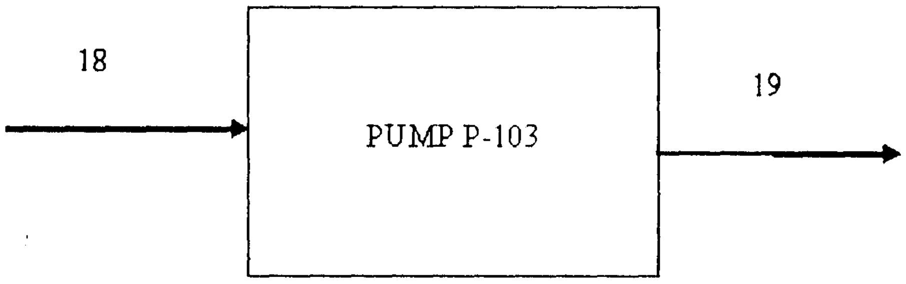
$$N_{18} = 23.092\frac{kg}{hr}$$

15. PUMP P-103

PUMP P-103 Assumptions

1. 100% material recovery

2.



Stream 19 (Pump outlet)

O-Xylene in stream 19 is:

$$n_{0,19} := n_{0,18}$$

$n_{0,19} = 0.022\frac{kg}{hr}$

Water in stream 19 is:

$n_{3,19} := n_{3,18}$

$n_{3,19} = 1.43\times 10^{-3}\cdot\frac{kg}{hr}$

Maleic Anhydride in stream 19 is:

$n_{4,19} := n_{4,18}$

$n_{4,19} = 0.162\frac{kg}{hr}$

Heavy metals in stream 19 is:

$n_{7,19} := n_{7,18}$

$n_{7,19} = 2.734\times 10^{-3}\cdot\frac{kg}{hr}$

Phthalic anhydride in stream 19 is:

$n_{2,19} := n_{2,18}$

$n_{2,19} = 22.904\frac{kg}{hr}$

Total amount of stream 19

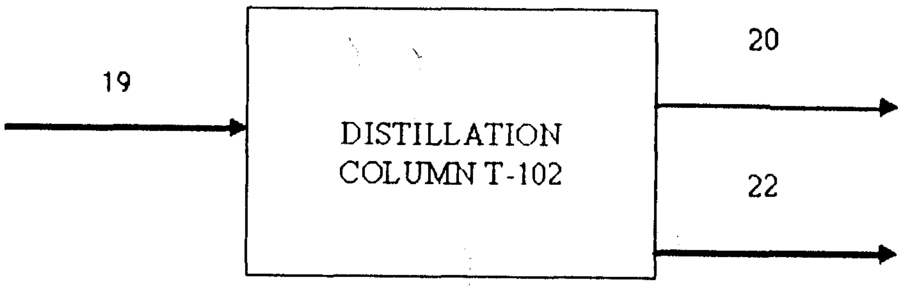
$N_{19} := \sum_{s} n_{s,19}$

$N_{19} = 23.092\frac{kg}{hr}$

16. DISTILLATION COLUMN 2 (T-102)

Distillation 2 Assumptions

1. 100% material recovery
s
2.



Stream 20 (DISTILLATION OVERHEAD PRODUCT)

Phthalic anhydride in stream 20 is:

$$n_{2,20} := 0.99 n_{2,19}$$

$$n_{2,20} = 22.675 \frac{kg}{hr}$$

Heavy metals in stream 20 is:

$$n_{7,20} := 0.001 n_{7,19}$$

$$n_{7,20} = 2.734 \times 10^{-6} \cdot \frac{kg}{hr}$$

O-Xylene in stream 20 is:

$$n_{0,20} := n_{0,19}$$

$$n_{0,20} = 0.022 \frac{kg}{hr}$$

Water in stream 20 is:

$n_{3,20} := n_{3,19}$

$n_{3,20} = 1.43\times 10^{-3}\cdot\frac{kg}{hr}$

Maleic Anhydride in stream 20 is:

$n_{4,20} := n_{4,19}$

$n_{4,20} = 0.162\frac{kg}{hr}$

Total amount of stream 20

$N_{20} := \sum_{s} n_{s,20}$

$N_{20} = 22.86\frac{kg}{hr}$

Stream 21 (DISTILLATION 2 BOTTOM PRODUCT)

Phthalic anhydride in stream 21 is:

$n_{2,21} := 0.01n_{2,19}$

$n_{2,21} = 0.229\frac{kg}{hr}$

Heavy metals in stream 21 is:

$n_{7,21} := 0.999n_{7,19}$

$n_{7,21} = 2.731\times 10^{-3}\cdot\frac{kg}{hr}$

Total amount of stream 21

$$N_{21} := \sum_{s} \left(n_{s,21}\right)$$

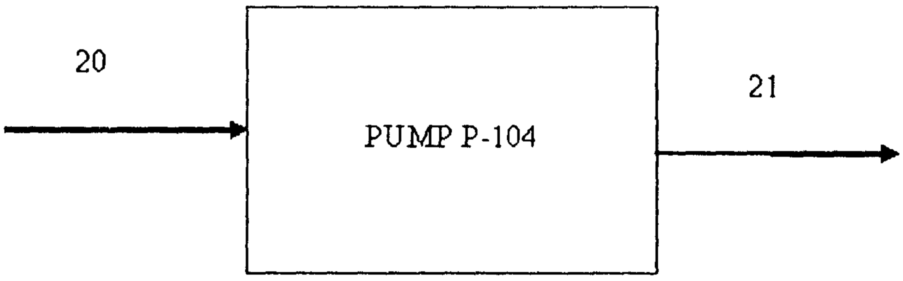
$$N_{21} = 0.232 \frac{kg}{hr}$$

17. PUMP P-104 ()

PUMP P-104 Assumptions

1. 100% material recovery

2.



Stream 22 (Pump P-104 Outlet)

Phthalic anhydride in stream 22 is:

$$n_{2,22} := n_{2,20}$$

$$n_{2,22} = 22.675 \frac{kg}{hr}$$

Heavy metals in stream 22 is:

$$n_{7,22} := n_{2,20}$$

$$n_{7,22} = 22.675 \frac{kg}{hr}$$

O-Xylene in stream 22 is:

$n_{0,22} := n_{0,20}$

$n_{0,22} = 0.022 \cdot \frac{kg}{hr}$

$n_{0,22} = 0.022 \cdot \frac{kg}{hr}$

Water in stream 22 is:

$n_{3,22} := n_{3,20}$

$n_{3,22} = 1.43 \times 10^{-3} \cdot \frac{kg}{hr}$

Maleic Anhydride in stream 22 is:

$n_{4,22} := n_{4,20}$

$n_{4,22} = 0.162 \cdot \frac{kg}{hr}$

Total amount of stream 22

$N_{22} := \sum_{s} n_{s,22}$

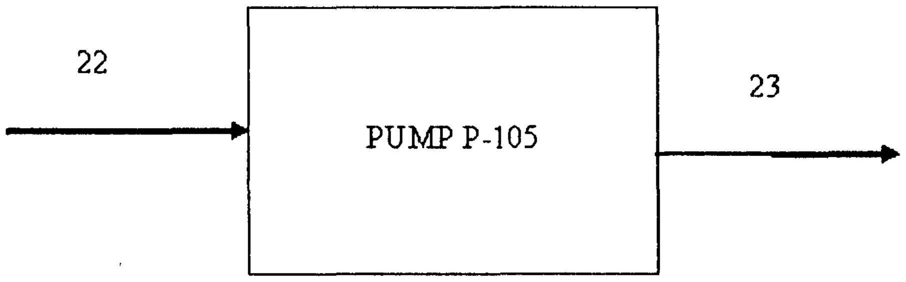
$N_{22} = 45.535 \frac{kg}{hr}$

18. PUMP P-105 ()

PUMP P-105 Assumptions

1. 100% material recovery

2.



Stream 23 (PUMP P-105 Outlet)

Phthalic anhydride in stream 23 is:

$$n_{2,23} := n_{2,21}$$

$$n_{2,23} = 0.229\frac{kg}{hr}$$

Heavy metals in stream 23 is:

$$n_{7,23} := n_{7,21}$$

$$n_{7,23} = 2.731\times 10^{-3}\cdot\frac{kg}{hr}$$

Total amount of stream 23

$$N_{23} := \sum_{s} n_{s,23}$$

$$N_{23} = 0.232\frac{kg}{hr}$$

Molecular weight of each of the components is given as:

$$Mw_s := \begin{array}{|c|}\hline 106.17\\\hline 32.00\\\hline 148.12\\\hline 18.02\\\hline 98.06\\\hline 44.01\\\hline 28.01\\\hline 76.43\\\hline \\\hline\end{array} \qquad \begin{pmatrix}\text{Oxylene}\\ \text{Oxygen}\\ \text{Phthalic\_Anhydride}\\ \text{Water}\\ \text{Maleic\_Anhydride}\\ \text{Carbon\_dioxide}\\ \text{Nitrogen}\\ \text{Heavy\_Metals}\end{pmatrix}$$

$$M_{w_s} := Mw_s \cdot \frac{kg}{kmol}$$

Molar flowrate of the components in each stream

$$z_{s,j} := \frac{n_{s,j}}{M_{w_s}}$$

Mass fraction of each component in each stream

$$x_{s,j} := \frac{n_{s,j}}{N_j}$$

Total molar flowrate of the stream

$$Z_j := \sum_s z_{s,j}$$

Molar mass fraction of each component in each stream

$$y_{s,j} := \frac{z_{s,j}}{Z_j}$$

Distillation Column 1

Reflux ratio is given by

$$R = \frac{L}{D}$$

$$4 = \frac{L}{D}$$

$$L = 4 \cdot D$$

$$Liq_{s,17} := 4 \cdot z_{s,17}$$

$$Liq_{s,17}$$

Taking total material balance across the condenser:

$$V = L + D$$

$$Vap_{s,17} := Liq_{s,17} + z_{s,17}$$

$$Liq_{mass} := \sum_{s} \left(Liq_{s,17} \cdot M_{w_s} \right)$$

$$Liq_{mass} = 0.011 \frac{kg}{s}$$

$$Vap_{mass} := \sum_{s} \left(Vap_{s,17} \cdot M_{w_s} \right)$$

$$Vap_{mass} = 0.014 \frac{kg}{s}$$

$$\sum_{s} \left(x_{s,17} \cdot M_{w_s} \right) = 98.669 \frac{kg}{kmol}$$

$$\sum_{s} \left(y_{s,17} \cdot M_{w_s} \right) = 93.812 \frac{kg}{kmol}$$

$$Z_{17} = 109.087 \frac{mol}{hr}$$

$$Z_{18} = 156.601 \frac{mol}{hr}$$

Distillation Column 2

Reflux ratio is given by

$$R = \frac{L}{D}$$

$$4 = \frac{L}{D}$$

$$L = 8 \cdot D$$

$$Liq_{s,20} := 4 \cdot z_{s,20}$$

$$Liq_{s,20}$$

Taking total material balance across the condenser:

$$V = L + D$$

$$Vap_{s,20} := Liq_{s,20} + z_{s,20}$$

$$Z_{20} = 155.019 \frac{mol}{hr}$$

$$Liq_{mass} := \sum_{s} \left(Liq_{s,20} \cdot M_{w_s} \right)$$

$$Z_{22} = 451.694 \frac{mol}{hr}$$

$$Liq_{mass} = 0.025 \frac{kg}{s}$$

$$Vap_{mass} := \sum_{s} \left(Vap_{s,20} \cdot M_{w_s} \right)$$

$$Vap_{mass} = 0.032 \frac{kg}{s}$$

CHAPTER FOUR

4.0 ENERGY BALANCES

4.1 THERMODYNAMICS PROPERTIES

4.1.1 HEAT CAPACITY COEFFICIENTS OF THE COMPONENTS

The heat capacity coefficients of the components involved in this project are as outlined below. Denoting the matrix of the heat capacity coefficients by c, we have

$$\begin{pmatrix} \text{Oxylene} \\ \text{Oxygen} \\ \text{Phthalic\_Anhydride} \\ \text{Water} \\ \text{Maleic\_Anhydride} \\ \text{Carbon\_dioxide} \\ \text{Nitrogen} \\ \text{Heavy\_Metals} \end{pmatrix}$$

$k := 0..3$ $H_{s,j} := 0\frac{J}{hr}$

FORMULATION OF ENERGY BALANCE EQUATION

The equation to be used for the energy balance is given as

$$\Delta H = n \cdot \int_{T_r}^{T_s} c_p \, dT$$

where

H = Enthalpy

C_p = Heat capacity

T = Temperature

n = Amount

T_r = Reference temperature

T_s = System temperature

If a reaction is involved, the equation becomes

$$\Delta H = n \cdot \int_{T_r}^{T_s} c_p \, dT + h_f$$

where h_f = heat of formation

It should be noted that C_p is given in terms of heat capacity coefficients as

$$C_p = a + b \cdot T + c \cdot T^2 + d \cdot T^3$$

where a, b, c and d are heat capacity coefficients (constants).

So, the enthalpy balance equation will then become

$$\Delta H = n\cdot\int_{T_r}^{T_s}\left(a + b\cdot T + c\cdot T^2 + d\cdot T^3\right) dT$$

4.2. ENERGY BALANCES CALCULATIONS

Energy Balance:

Evaluation of Species Enthalpies: the reference state is the elements at 25 ºC.

$T_r := 298 \quad K \qquad T_j \qquad T = \left(T_j\right)$

$$h\left(s,T_j\right) = z_{s,j}\cdot\left[\left[\begin{aligned}&\frac{c_{s,0}}{1}\cdot\left(\frac{T}{K}-\frac{T_r}{K}\right)+\frac{c_{s,1}}{2}\cdot\left[\left(\frac{T}{K}\right)^2-\left(\frac{T_r}{K}\right)^2\right]\ldots\\&+\frac{c_{s,2}}{3}\cdot\left[\left(\frac{T}{K}\right)^3-\left(\frac{T_r}{K}\right)^3\right]+\frac{c_{s,3}}{4}\cdot\left[\left(\frac{T}{K}\right)^4-\left(\frac{T_r}{K}\right)^4\right]\end{aligned}\right]\cdot\frac{J}{mol}+h_{f_s}\right]$$

UNIT 1 : Feed Storage Tank

Enthalpy of stream 1:

$T_r := 25°C \qquad T_1 := 30°C \qquad T := T_1$

$$H_{s,1} := z_{s,1}\cdot\left[\left[\begin{aligned}&\frac{c_{s,0}}{1}\cdot\left(\frac{T}{K}-\frac{T_r}{K}\right)+\frac{c_{s,1}}{2}\cdot\left[\left(\frac{T}{K}\right)^2-\left(\frac{T_r}{K}\right)^2\right]\ldots\\&+\frac{c_{s,2}}{3}\cdot\left[\left(\frac{T}{K}\right)^3-\left(\frac{T_r}{K}\right)^3\right]+\frac{c_{s,3}}{4}\cdot\left[\left(\frac{T}{K}\right)^4-\left(\frac{T_r}{K}\right)^4\right]\end{aligned}\right]\cdot\frac{J}{mol}\right]$$

$H_{s,1} =$

$$\begin{array}{|r|}\hline 0 \\ \hline 1.662\cdot10^{3} \\ \hline 0 \\ \hline 0 \\ \hline 0 \\ \hline 0 \\ \hline 1.136\cdot10^{4} \\ \hline 0 \\ \hline \end{array}\cdot\frac{kJ}{hr}$$

$\Delta H_1 := \sum_{s} H_{s,1}$ $\Delta H_1 = 1.303\times10^{4}\cdot\frac{kJ}{hr}$

Total energy into the Tank: $\Delta H_{in_1} := \Delta H_1$

$\Delta H_{in_1} = 1.303\times10^{4}\cdot\frac{kJ}{hr}$

Enthalpy of stream 2:

$T_r := 25°C$ $T_2 := 30°C$ $T := T_2$

$$H_{s,2} := z_{s,2}\cdot\left[\left[\frac{c_{s,0}}{1}\cdot\left(\frac{T}{K}-\frac{T_r}{K}\right)+\frac{c_{s,1}}{2}\cdot\left[\left(\frac{T}{K}\right)^2-\left(\frac{T_r}{K}\right)^2\right]\ldots\right.\right.$$
$$\left.\left.+\frac{c_{s,2}}{3}\cdot\left[\left(\frac{T}{K}\right)^3-\left(\frac{T_r}{K}\right)^3\right]+\frac{c_{s,3}}{4}\cdot\left[\left(\frac{T}{K}\right)^4-\left(\frac{T_r}{K}\right)^4\right]\right]\right]\cdot\frac{J}{mol}$$

$H_{s,2} =$

$$\begin{array}{|r|}\hline 0 \\ \hline 1.662\cdot10^{3} \\ \hline 0 \\ \hline 0 \\ \hline 0 \\ \hline 0 \\ \hline 1.136\cdot10^{4} \\ \hline 0 \\ \hline \end{array}\cdot\frac{kJ}{hr}$$

$\Delta H_2 := \sum_s H_{s,2} \qquad \Delta H_2 = 1.303\times 10^4 \cdot \frac{kJ}{hr}$

Total energyout of the Tank: $\Delta H_{out_1} := \Delta H_2$

$\Delta H_{out_1} = 1.303\times 10^4 \cdot \frac{kJ}{hr}$

Heat load:

$\Delta H_1 := \Delta H_{out_1} - \Delta H_{in_1}$

$\Delta H_1 = 0 \cdot \frac{kJ}{hr}$

UNIT 2 : MIXER

Inlet Enthalpy:

$\Delta H_{in_2} := \Delta H_{out_1}$

$\Delta H_{in_2} = 1.303\times 10^4 \cdot \frac{kJ}{hr}$

Enthalpy of stream 3:

$T_r := 25°C \qquad T_3 := 30°C \qquad T := T_3$

$$H_{s,3} := z_{s,3} \cdot \left[\left[\frac{c_{s,0}}{1}\cdot\left(\frac{T}{K}-\frac{T_r}{K}\right) + \frac{c_{s,1}}{2}\cdot\left[\left(\frac{T}{K}\right)^2 - \left(\frac{T_r}{K}\right)^2\right] \ldots \right.\right.$$
$$\left.\left. + \frac{c_{s,2}}{3}\cdot\left[\left(\frac{T}{K}\right)^3 - \left(\frac{T_r}{K}\right)^3\right] + \frac{c_{s,3}}{4}\cdot\left[\left(\frac{T}{K}\right)^4 - \left(\frac{T_r}{K}\right)^4\right]\right]\cdot\frac{J}{mol}\right]$$

$$H_{s,3} = \begin{array}{|r|}\hline 0 \\ \hline 1.662\cdot 10^3 \\ \hline 0 \\ \hline 0 \\ \hline 0 \\ \hline 0 \\ \hline 1.136\cdot 10^4 \\ \hline 0 \\ \hline \end{array} \cdot \frac{kJ}{hr}$$

$\Delta H_3 := \sum_s H_{s,3}$ $\qquad \Delta H_3 = 1.303\times 10^4 \cdot \frac{kJ}{hr}$

$\Delta H_{out_2} := \Delta H_3$

$\Delta H_{out_2} = 1.303\times 10^4 \cdot \frac{kJ}{hr}$

Heat load: $\Delta H_2 := \Delta H_{out_2} - \Delta H_{in_2}$

$\Delta H_2 = 0 \cdot \frac{kJ}{hr}$

UNIT 3 : COMPRESSOR (K-100)

Inlet Enthalpy:

$\Delta H_{in_3} := \Delta H_3$

$\Delta H_{in_3} = 1.303\times 10^4 \cdot \frac{kJ}{hr}$

Enthalpy of stream 4:

$T_r := 25°C$ $\qquad T_4 := 50°C$ $\qquad T := T_4$

$$H_{s,4} := z_{s,4} \cdot \left[\left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \ldots \right. \right. \right. \\ \left. \left. \left. + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol} \right]$$

$$H_{s,4} = \begin{pmatrix} 0 \\ 8.696\cdot 10^{3} \\ 0 \\ 0 \\ 0 \\ 0 \\ 5.878\cdot 10^{4} \\ 0 \end{pmatrix} \cdot \frac{kJ}{hr}$$

$$\Delta H_4 := \sum_{s} H_{s,4} \qquad \Delta H_4 = 6.747\times 10^{4}\cdot\frac{kJ}{hr}$$

Total energyout of the Compressor:

$$\Delta H_{out_3} := \Delta H_3$$

$$\Delta H_{out_3} = 1.303\times 10^{4}\cdot\frac{kJ}{hr}$$

Heat load: $\Delta H_3 := \Delta H_{out_3} - \Delta H_{in_3}$

$$\Delta H_3 = 0\cdot\frac{kJ}{hr}$$

UNIT 4 :FURNACE(FH-100)

Inlet Enthalpy:

$$\Delta H_{in_4} := \Delta H_{out_3}$$

$$\Delta H_{in_4} = 1.303\times 10^{4}\cdot\frac{kJ}{hr}$$

Enthalpy of stream 9:

$T_r := 25°C$ $T_9 := 300°C$ $T := T_9$

$$H_{s,9} := z_{s,9} \cdot \left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \ldots \atop + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol}$$

$$H_{s,9} = \begin{pmatrix} 0 \\ 1.58 \cdot 10^5 \\ 0 \\ 0 \\ 0 \\ 0 \\ 9.303 \cdot 10^5 \\ 0 \end{pmatrix} \cdot \frac{kJ}{hr}$$

$\Delta H_9 := \sum_s H_{s,9}$ $\Delta H_9 = 1.088 \times 10^6 \cdot \frac{kJ}{hr}$

Total energyout of the furnace: $\Delta H_{out_4} := \Delta H_9$

$\Delta H_{out_4} = 1.088 \times 10^6 \cdot \frac{kJ}{hr}$

Heat load: $\Delta H_4 := \Delta H_{out_4} - \Delta H_{in_4}$

$\Delta H_4 = 1.075 \times 10^6 \cdot \frac{kJ}{hr}$

UNIT 5 : FEED STORAGE TANK

Enthalpy of stream 5:

$T_r := 25°C$ $\qquad T_5 := 30°C$ $\qquad T := T_5$

$$H_{s,5} := z_{s,5}\cdot\left[\left[\begin{aligned}&\frac{c_{s,0}}{1}\cdot\left(\frac{T}{K}-\frac{T_r}{K}\right)+\frac{c_{s,1}}{2}\cdot\left[\left(\frac{T}{K}\right)^2-\left(\frac{T_r}{K}\right)^2\right]\cdots\\&+\frac{c_{s,2}}{3}\cdot\left[\left(\frac{T}{K}\right)^3-\left(\frac{T_r}{K}\right)^3\right]+\frac{c_{s,3}}{4}\cdot\left[\left(\frac{T}{K}\right)^4-\left(\frac{T_r}{K}\right)^4\right]\end{aligned}\right]\right]\cdot\frac{J}{mol}$$

$$H_{s,5} = \begin{pmatrix}12.86\\0\\0\\0\\0\\0\\0\\0.021\end{pmatrix}\cdot\frac{kJ}{hr}$$

$\Delta H_5 := \sum_s H_{s,5}$ $\qquad \Delta H_5 = 12.882\,\frac{kJ}{hr}$

Total energy into the Tank: $\Delta H_{in_5} := \Delta H_5$ $\qquad \Delta H_{in_5} = 12.882\,\frac{kJ}{hr}$

Enthalpy of stream 6:

$T_r := 25°C$ $\qquad T_6 := 45°C$ $\qquad T := T_6$

$$H_{s,6} := z_{s,6}\cdot\left[\left[\begin{aligned}&\frac{c_{s,0}}{1}\cdot\left(\frac{T}{K}-\frac{T_r}{K}\right)+\frac{c_{s,1}}{2}\cdot\left[\left(\frac{T}{K}\right)^2-\left(\frac{T_r}{K}\right)^2\right]\cdots\\&+\frac{c_{s,2}}{3}\cdot\left[\left(\frac{T}{K}\right)^3-\left(\frac{T_r}{K}\right)^3\right]+\frac{c_{s,3}}{4}\cdot\left[\left(\frac{T}{K}\right)^4-\left(\frac{T_r}{K}\right)^4\right]\end{aligned}\right]\right]\cdot\frac{J}{mol}$$

$$H_{s,6} = \begin{pmatrix} 51.717 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.09 \end{pmatrix} \cdot \frac{kJ}{hr}$$

$$\Delta H_6 := \sum_s H_{s,6} \qquad \Delta H_6 = 51.807 \frac{kJ}{hr}$$

Total energyout of the Tank: $\Delta H_{out_5} := \Delta H_6$

$$\Delta H_{out_5} = 51.807 \frac{kJ}{hr}$$

Heat load: $\Delta H_5 := \Delta H_{out_5} - \Delta H_{in_5}$ $\qquad \Delta H_5 = 38.926 \frac{kJ}{hr}$

UNIT 6:PUMP (P-100)

Inlet Enthalpy:

$$\Delta H_{in_6} := \Delta H_{out_5}$$

$$\Delta H_{in_6} = 51.807 \frac{kJ}{hr}$$

Enthalpy of stream 7:

$T_r := 25°C \qquad T_7 := 30°C \qquad T := T_7$

$$H_{s,7} := z_{s,7} \cdot \left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K}\right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K}\right)^2 - \left(\frac{T_r}{K}\right)^2\right] \cdots \atop + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K}\right)^3 - \left(\frac{T_r}{K}\right)^3\right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K}\right)^4 - \left(\frac{T_r}{K}\right)^4\right]\right]\right] \cdot \frac{J}{mol}$$

$$H_{s,7} = \begin{bmatrix} 12.86 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.021 \end{bmatrix} \cdot \frac{kJ}{hr}$$

$$\Delta H_7 := \sum_s H_{s,5} \qquad \Delta H_7 = 12.882 \frac{kJ}{hr}$$

Total energyout of the Pump: $\Delta H_{out_6} := \Delta H_7$

$$\Delta H_{out_6} = 12.882 \frac{kJ}{hr}$$

Heat load: $\Delta H_6 := \Delta H_{out_6} - \Delta H_{in_6}$ $\qquad \Delta H_6 = -38.926 \frac{kJ}{hr}$

UNIT 7 :HEATER(E-100)

Inlet Enthalpy:

$$\Delta H_{in_7} := \Delta H_{out_6}$$

$$\Delta H_{in_7} = 12.882 \frac{kJ}{hr}$$

Enthalpy of stream 7:

$T_r := 25°C \qquad T_7 := 120°C \qquad T := T_7$

$$H_{s,7} := z_{s,7} \cdot \left[\left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \ldots \right. \right. \right.$$
$$\left. \left. \left. + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol} \right]$$

$H_{s,7} =$

$$\begin{pmatrix} 252.288 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.541 \end{pmatrix} \cdot \frac{kJ}{hr}$$

$\Delta H_7 := \sum_s H_{s,7}$ $\qquad$ $\Delta H_7 = 252.829 \frac{kJ}{hr}$

Total energyout of the Heater: $\Delta H_{out_7} := \Delta H_7$

$\Delta H_{out_7} = 252.829 \frac{kJ}{hr}$

Heat load:

$\Delta H_7 := \Delta H_{out_7} - \Delta H_{in_7}$

$\Delta H_7 = 239.947 \frac{kJ}{hr}$

UNIT 8 :MIXER (MIX-101)

Inlet Enthalpy:

$\Delta H_{in_8} := \Delta H_{out_7} + \Delta H_{out_4}$

$\Delta H_{in_8} = 1.088 \times 10^6 \cdot \frac{kJ}{hr}$

Enthalpy of stream 10:

$T_r := 25°C$ $\qquad$ $T_{10} := 120°C$ $\qquad$ $T := T_{10}$

$$H_{s,10} := z_{s,10} \cdot \left[\left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \ldots \right. \right. \right. \\ \left. \left. \left. + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol} \right]$$

$H_{s,10} =$

$$\begin{pmatrix} 252.288 \\ 3.845\cdot 10^{4} \\ 0 \\ 0 \\ 0 \\ 0 \\ 2.497\cdot 10^{5} \\ 0.541 \end{pmatrix}\cdot\frac{kJ}{hr}$$

$\Delta H_{10} := \sum_{s} H_{s,10}$ $\qquad \Delta H_{10} = 2.884\times 10^{5}\cdot\frac{kJ}{hr}$

Total energyout of the Mixer: $\quad \Delta H_{out_8} := \Delta H_{10}$

$\Delta H_{out_8} = 2.884\times 10^{5}\cdot\frac{kJ}{hr}$

Heat load:

$\Delta H_{8} := \Delta H_{out_8} - \Delta H_{in_8}$ $\qquad \Delta H_{8} = 0\cdot\frac{kJ}{hr}$

UNIT 9 :PFR REACTOR (PFR-100)

Inlet Enthalpy:

$\Delta H_{in_9} := \Delta H_{10}$

$\Delta H_{in_9} = 2.884\times 10^{5}\cdot\frac{kJ}{hr}$

Enthalpy of stream 11:

$T_r := 25°C$ $\qquad T_{11} := 330°C$ $\qquad T := T_{11}$

$$H_{s,11} = z_{s,11}\cdot\left[\left[\left[\frac{c_{s,0}}{1}\cdot\left(\frac{T}{K}-\frac{T_r}{K}\right)+\frac{c_{s,1}}{2}\cdot\left[\left(\frac{T}{K}\right)^{2}-\left(\frac{T_r}{K}\right)^{2}\right]\ldots \atop +\frac{c_{s,2}}{3}\cdot\left[\left(\frac{T}{K}\right)^{3}-\left(\frac{T_r}{K}\right)^{3}\right]+\frac{c_{s,3}}{4}\cdot\left[\left(\frac{T}{K}\right)^{4}-\left(\frac{T_r}{K}\right)^{4}\right]\right]\right]\cdot\frac{J}{mol}+h_{f_s}\right]$$

$H_{s,11} =$

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \cdot \frac{kJ}{hr}$$

$\Delta H_{11} := \sum_{s} H_{s,11}$ $\Delta H_{11} = 0 \cdot \frac{kJ}{hr}$

Total energyout of the PFR Reator:

$\Delta H_{out_9} := \Delta H_{11}$

$\Delta H_{out_9} = 0 \cdot \frac{kJ}{hr}$

Heat load:

$\Delta H_9 := \Delta H_{out_9} - \Delta H_{in_9}$

$\Delta H_9 = -2.884 \times 10^5 \cdot \frac{kJ}{hr}$

UNIT 10 :CONDENSER 1 (E-101)

Inlet Enthalpy:

$\Delta H_{in_{10}} := \Delta H_{out_9}$

$\Delta H_{in_9} = 2.884 \times 10^5 \cdot \frac{kJ}{hr}$

Enthalpy of stream 12:

$T_r := 25°C$ $T_{12} := 45°C$ $T := T_{12}$

$$H_{s,12} := z_{s,12} \cdot \left[\left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \ldots \atop + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol} \right]$$

$$H_{s,12} = \begin{array}{|r|} \hline 4.137 \\ \hline 0 \\ \hline 144.209 \\ \hline 307.012 \\ \hline 474.624 \\ \hline 1.481 \cdot 10^3 \\ \hline 4.663 \cdot 10^4 \\ \hline 0.09 \\ \hline \end{array} \cdot \frac{kJ}{hr}$$

$$\Delta H_{12} := \sum_s H_{s,12} \qquad \Delta H_{12} = 4.904 \times 10^4 \cdot \frac{kJ}{hr}$$

Total energyout of the Condenser:

$$\Delta H_{out_{10}} := \Delta H_{12}$$

$$\Delta H_{out_{10}} = 4.904 \times 10^4 \cdot \frac{kJ}{hr}$$

Heat load: $\Delta H_{10} := \Delta H_{out_{10}} - \Delta H_{in_{10}}$ $\qquad \Delta H_{10} = 4.904 \times 10^4 \cdot \frac{kJ}{hr}$

UNIT 11: CONDENSER 2 (E-101)

Inlet Enthalpy:

$$\Delta H_{in_{11}} := \Delta H_{out_{10}}$$

$$\Delta H_{in_{11}} = 4.904 \times 10^4 \cdot \frac{kJ}{hr}$$

Enthalpy of stream 13:

$T_r := 25°C$ $T_{13} := 20°C$ $T := T_{13}$

$$H_{s,13} := z_{s,13} \cdot \left[\left[\frac{c_{s,0}}{1}\cdot\left(\frac{T}{K}-\frac{T_r}{K}\right)+\frac{c_{s,1}}{2}\cdot\left[\left(\frac{T}{K}\right)^2-\left(\frac{T_r}{K}\right)^2\right]\ldots \\ +\frac{c_{s,2}}{3}\cdot\left[\left(\frac{T}{K}\right)^3-\left(\frac{T_r}{K}\right)^3\right]+\frac{c_{s,3}}{4}\cdot\left[\left(\frac{T}{K}\right)^4-\left(\frac{T_r}{K}\right)^4\right]\right]\cdot\frac{J}{mol}\right]$$

$H_{s,13} =$

$$\begin{bmatrix} -1.025 \\ 0 \\ -35.793 \\ -77.488 \\ -109.427 \\ -344.688 \\ -1.117\cdot 10^4 \\ -0.021 \end{bmatrix} \cdot \frac{kJ}{hr}$$

$\Delta H_{13} := \sum_s H_{s,13}$ $\Delta H_{13} = -1.174\times 10^4 \cdot \frac{kJ}{hr}$

Total energyout of the Condenser:

$\Delta H_{out_{11}} := \Delta H_{13}$

$\Delta H_{out_{11}} = -1.174\times 10^4 \cdot \frac{kJ}{hr}$

Heat load: $\Delta H_{11} := \Delta H_{out_{11}} - \Delta H_{in_{11}}$

$\Delta H_{11} = -6.078\times 10^4 \cdot \frac{kJ}{hr}$

UNIT 12: SEPARATOR (V 100)

Inlet Enthalpy:

$$\Delta H_{in_{12}} := \Delta H_{out_{11}}$$

$$\Delta H_{in_{12}} = -1.174 \times 10^{4} \cdot \frac{kJ}{hr}$$

Enthalpy of stream 14:

$T_r := 25°C$ $T_{14} := 20°C$ $T := T_{14}$

$$H_{s,14} := z_{s,14} \cdot \left[\left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \ldots \atop + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol} \right]$$

$$H_{s,14} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -0.775 \\ 0 \\ -344.688 \\ -1.117 \cdot 10^{4} \\ 0 \end{bmatrix} \cdot \frac{kJ}{hr}$$

$$\Delta H_{14} := \sum_{s} H_{s,14} \qquad \Delta H_{14} = -1.151 \times 10^{4} \cdot \frac{kJ}{hr}$$

Enthalpy of stream 15:

$T_r := 25°C$ $T_{15} := 20°C$ $T := T_{15}$

$$H_{s,15} := z_{s,15} \cdot \left[\left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \dots + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol} \right]$$

$$H_{s,15} = \begin{pmatrix} -1.025 \\ 0 \\ -35.793 \\ -0.775 \\ -109.427 \\ 0 \\ 0 \\ -0.021 \end{pmatrix} \cdot \frac{kJ}{hr}$$

$$\Delta H_{15} := \sum_{s} H_{s,15} \qquad \Delta H_{15} = -147.041 \frac{kJ}{hr}$$

Total energyout of the Separator :

$$\Delta H_{out_{12}} := \Delta H_{15} + \Delta H_{14}$$

$$\Delta H_{out_{12}} = -1.166 \times 10^4 \cdot \frac{kJ}{hr}$$

Heat load: $\Delta H_{12} := \Delta H_{out_{12}} - \Delta H_{in_{12}}$ $\qquad \Delta H_{12} = 75.938 \frac{kJ}{hr}$

UNIT 13 :PUMP (P-101)

Inlet Enthalpy:

$$\Delta H_{in_{13}} := \Delta H_{15}$$

$$\Delta H_{in_{13}} = -147.041 \frac{kJ}{hr}$$

Enthalpy of stream 16:

$T_r := 25°C$ $\quad T_{16} := 20°C$ $\quad T := T_{16}$

$$H_{s,16} := z_{s,16} \cdot \left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \ldots \atop + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol}$$

$$H_{s,16} = \begin{pmatrix} -1.025 \\ 0 \\ -35.793 \\ -0.775 \\ -109.427 \\ 0 \\ 0 \\ -0.021 \end{pmatrix} \cdot \frac{kJ}{hr}$$

$\Delta H_{16} := \sum_{s} H_{s,16}$ $\qquad \Delta H_{16} = -147.041 \cdot \frac{kJ}{hr}$

Total energyout of the Pump: $\quad \Delta H_{out_{13}} := \Delta H_{16}$ $\qquad \Delta H_{out_{13}} = -147.041 \cdot \frac{kJ}{hr}$

Heat load: $\quad \Delta H_{13} := \Delta H_{out_{13}} - \Delta H_{in_{13}}$ $\qquad \Delta H_{13} = 0 \cdot \frac{kJ}{hr}$

UNIT 14: DISTILLATION COLUMN (T-101)

Inlet Enthalpy:

$\Delta H_{in_{14}} := \Delta H_{out_{13}}$

$\Delta H_{in_{14}} = -147.041 \cdot \frac{kJ}{hr}$

Enthalpy of stream 11:

$T_r := 25°C$ $\qquad T_{17} := 205°C$ $\qquad T := T_{17}$

$$H_{s,17} := z_{s,17} \cdot \left[\left[\begin{gathered} \frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] ... \\ + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \end{gathered} \right] \cdot \frac{J}{mol} \right]$$

$H_{s,17} =$

38.996	$\cdot \frac{kJ}{hr}$
0	
0	
25.119	
$6.676 \cdot 10^3$	
0	
0	
0	

$\Delta H_{17} := \sum_s H_{s,17}$ $\qquad \Delta H_{17} = 6.741 \times 10^3 \cdot \frac{kJ}{hr}$

Enthalpy of stream 18:

$T_r := 25°C$ $\qquad T_{18} := 205°C$ $\qquad T := T_{18}$

$$H_{s,18} := z_{s,18} \cdot \left[\left[\begin{gathered} \frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] ... \\ + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \end{gathered} \right] \cdot \frac{J}{mol} \right]$$

$H_{s,18} =$

$$\begin{bmatrix} 0.394 \\ 0 \\ 1.352\cdot 10^{3} \\ 0.254 \\ 136.254 \\ 0 \\ 0 \\ 1.306 \end{bmatrix} \cdot \frac{kJ}{hr}$$

$\Delta H_{18} := \sum_{s} H_{s,18}$ $\qquad$ $\Delta H_{18} = 1.49\times 10^{3}\cdot\frac{kJ}{hr}$

Total energyout of the Distillation Column

$\Delta H_{out_{14}} := \Delta H_{18} + \Delta H_{17}$

$\Delta H_{out_{14}} = 8.231\times 10^{3}\cdot\frac{kJ}{hr}$

Heat load: $\Delta H_{14} := \Delta H_{out_{14}} - \Delta H_{in_{14}}$

$\Delta H_{14} = 8.378\times 10^{3}\cdot\frac{kJ}{hr}$

UNIT15: PUMP (P-103)

Inlet Enthalpy:

$\Delta H_{in_{15}} := \left(\Delta H_{18}\right)$

$\Delta H_{in_{15}} = 1.49\times 10^{3}\cdot\frac{kJ}{hr}$

Enthalpy of stream 19:

$T_r := 25°C$ $T_{19} := 205°C$ $T := T_{19}$

$$H_{s,19} := z_{s,19} \cdot \left[\left[\frac{c_{s,0}}{1}\cdot\left(\frac{T}{K} - \frac{T_r}{K}\right) + \frac{c_{s,1}}{2}\cdot\left[\left(\frac{T}{K}\right)^2 - \left(\frac{T_r}{K}\right)^2\right] \ldots \atop + \frac{c_{s,2}}{3}\cdot\left[\left(\frac{T}{K}\right)^3 - \left(\frac{T_r}{K}\right)^3\right] + \frac{c_{s,3}}{4}\cdot\left[\left(\frac{T}{K}\right)^4 - \left(\frac{T_r}{K}\right)^4\right]\right]\right] \cdot \frac{J}{mol}$$

$H_{s,19} =$

0.394	$\cdot\frac{kJ}{hr}$
0	
$1.352\cdot10^3$	
0.254	
136.254	
0	
0	
1.306	

$\Delta H_{19} := \sum_s H_{s,19}$ $\Delta H_{18} = 1.49\times 10^3 \cdot\frac{kJ}{hr}$

Total energyout of the Pump: $\Delta H_{out_{15}} := \Delta H_{19}$

$\Delta H_{out_{15}} = 1.49\times 10^3 \cdot\frac{kJ}{hr}$

Heat load: $\Delta H_{15} := \Delta H_{out_{15}} - \Delta H_{in_{15}}$ $\Delta H_{15} = 0\cdot\frac{kJ}{hr}$

UNIT 16: DISTILLATION COLUMN (T-102)

Inlet Enthalpy:

$\Delta H_{in_{16}} := \Delta H_{out_{15}}$

$\Delta H_{in_{16}} = 1.49\times 10^3 \cdot\frac{kJ}{hr}$

Enthalpy of stream :

$T_r := 25°C$ $\qquad T_{21} := 285°C$ $\qquad T := T_{21}$

$$H_{s,21} := z_{s,21} \cdot \left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \dots \\ + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol}$$

$$H_{s,21} = \begin{bmatrix} 0 \\ 0 \\ 19.868 \\ 0 \\ 0 \\ 0 \\ 0 \\ 2.327 \end{bmatrix} \cdot \frac{kJ}{hr}$$

$\Delta H_{21} := \sum_s H_{s,21}$ $\qquad \Delta H_{21} = 22.195 \frac{kJ}{hr}$

Total energyout of the Distillat: $\Delta H_{out_{16}} := \Delta H_{21}$

$\Delta H_{out_{16}} = 22.195 \frac{kJ}{hr}$

Heat load: $\Delta H_{16} := \Delta H_{out_{16}} - \left(\Delta H_{in_{16}} \right)$

$\Delta H_{16} = -1.468 \times 10^3 \cdot \frac{kJ}{hr}$

UNIT 17: Pump (104)

Inlet Enthalpy:

$\Delta H_{in_{17}} := \Delta H_{out_{16}}$

$\Delta H_{in_{17}} = 22.195 \frac{kJ}{hr}$

Enthalpy of stream 23:

$T_r := 25°C$ $\qquad T_{23} := 285°C$ $\qquad T := T_{23}$

$$H_{s,23} := z_{s,23} \cdot \left[\left[\left[\frac{c_{s,0}}{1} \cdot \left(\frac{T}{K} - \frac{T_r}{K} \right) + \frac{c_{s,1}}{2} \cdot \left[\left(\frac{T}{K} \right)^2 - \left(\frac{T_r}{K} \right)^2 \right] \dots \atop + \frac{c_{s,2}}{3} \cdot \left[\left(\frac{T}{K} \right)^3 - \left(\frac{T_r}{K} \right)^3 \right] + \frac{c_{s,3}}{4} \cdot \left[\left(\frac{T}{K} \right)^4 - \left(\frac{T_r}{K} \right)^4 \right] \right] \right] \cdot \frac{J}{mol} \right]$$

$$H_{s,23} = \begin{pmatrix} 0 \\ 0 \\ 19.868 \\ 0 \\ 0 \\ 0 \\ 0 \\ 2.327 \end{pmatrix} \cdot \frac{kJ}{hr}$$

$\Delta H_{23} := \sum_{s} H_{s,23}$ $\qquad \Delta H_{23} = 22.195 \frac{kJ}{hr}$

Total energyout of the Pump: $\qquad \Delta H_{out_{17}} := \Delta H_{23}$

$\Delta H_{out_{17}} = 22.195 \frac{kJ}{hr}$

Heat load: $\qquad \Delta H_{17} := \Delta H_{out_{17}} - \Delta H_{in_{17}}$ $\qquad \Delta H_{17} = 0 \cdot \frac{kJ}{hr}$

CHAPTER SIX

6.0 Condenser Design

$kJ \equiv 1000 \cdot J$

$Q_{condenser} := 1.075 \times 10^{6} \cdot \frac{J}{hr}$

Heat transfer area of the condenser.

$-Q = U \cdot A_{condenser} \cdot \Delta Tm$

U = overall convection coefficient

DTm = log mean temperature difference

A = The heat transfer area

$U := 540 \frac{W}{m^2 \cdot K}$

$T_{h\_in} := 373.15K$ $T_{h\_out} := 313.15K$

$T_{c\_in} := 298.15K$ $T_{c\_out} := 323.15K$

$$\Delta Tm := \frac{(T_{h\_in} - T_{h\_out}) - (T_{c\_out} - T_{c\_in})}{\ln\left(\frac{T_{h\_in} - T_{h\_out}}{T_{c\_out} - T_{c\_in}}\right)}$$

$\Delta Tm = 39.979K$

$$A_{condenser} := \frac{Q_{condenser}}{\Delta Tm \cdot U}$$

$A_{condenser} = 0.014 \cdot m^2$

Detail chemical engineering design of the condenser

Fluids allocation

Reactor products are allocated to the tube side while water is allocated to the shell side.

Type of consenser selected

A simple square pitch and a 1 pass tube

Cooling water flowrate

$T_{h\_in} := 373.15K$ $\qquad$ $T_{h\_out} := 313.15K$

$T_{c\_in} := 298.15K$ $\qquad$ $T_{c\_out} := 323.15K$

$C_{p\_water} := 4200J\cdot kg^{-1}\cdot K^{-1}$

cooling water flow rate

$$C_{wf} := \frac{Q_{condenser}}{\int_{T_{c\_in}}^{T_{c\_out}} C_{p\_water}\,dT}$$

$$C_{wf} = 10.238\frac{kg}{hr}$$

Calculation of heat transfer area of the condenser

Heat transfer area of the condenser.

$-Q = U \cdot A_{condenser} \cdot \Delta Tm$

U = overall convection coefficient and it is given as $U := 540 \frac{W}{m^2 \cdot K}$

DTm = log mean temperature difference

A = the heat transfer area

$$\Delta Tm_i := \frac{(T_{h\_in} - T_{h\_out}) - (T_{c\_out} - T_{c\_in})}{\ln\left(\frac{T_{h\_in} - T_{h\_out}}{T_{c\_out} - T_{c\_in}}\right)}$$

$\Delta Tm_i = 39.979K$

Calculation for dimensionless temperature for one pass and two tubes passes

$R := \frac{T_{h\_in} - T_{h\_out}}{T_{c\_out} - T_{c\_in}}$ $R = 2.4$

$S := \frac{T_{c\_out} - T_{c\_in}}{T_{h\_in} - T_{c\_in}}$ $S = 0.333$

Temperature correlation factor from graph $F_t := 0.8$

Therefore Actual ΔTm

$\Delta Tm := F_t \cdot \Delta Tm_i$

$\Delta Tm = 33.982K$

$$A_{trial} := \frac{Q_{condenser}}{\Delta Tm \cdot U}$$

$A_{trial} = 0.016 \cdot m^2$

The above area calculated is the trial area At

'From standard then following parameters were chosen

Internal diameter	$D_i := 16mm$	$D_i = 0.016m$
Outer diameter	$D_o := 20mm$	$D_o = 0.02m$
Tube length	$L_{tb} := 550mm$	$L_{tb} = 0.55m$
Allowance for welding	$A_{fw} := 10mm$	$A_{fw} = 0.01m$
Actual tube length	$L_{atb} := L_{tb} - A_{fw}$	$L_{atb} = 0.54m$
Area of one tube	$A_s := D_o \cdot \pi \cdot L_{atb}$	$A_s = 0.034m^2$
Number of tubes	$N_t := \frac{A_{tria}}{A_s}$	$N_t = 0.48$
Using square pitch and a 1 pass tube.	$P_t := 1.25 \cdot D_o$	$P_t = 0.025m$
	$K_1 := 0.21$	$n_1 := 2.20$
Tube bundle diameter	$D_b := D_o \cdot \left(\frac{N_t}{K_1}\right)^{\frac{1}{n_1}}$	$D_b = 0.029m$

Allow bundle clearance of of 10mm. therefore

Bundle clearance	$B_c := 10mm$	$B_c = 0.01m$

Number of tube in the center row (Nr)	$N_r := \frac{D_b}{P_t}$	$N_r = 1.151$
Shell side diameter	$D_s := B_c + D_b$	$D_s = 0.039\text{m}$

Tube side calculations;

water mean temperature	$T_t := \frac{T_{c\_in} + T_{c\_out}}{2}$	$T_t = 310.65\text{K}$
Tube cross sectional area	$T_{csa} := \frac{\pi}{4} \cdot D_i^2$	$T_{csa} = 2.011 \times 10^{-4}\,\text{m}^2$
Tube per pass	$T_{pp} := \frac{N_t}{2}$	$T_{pp} = 0.24$
Total flow area	$A_{tf} := T_{pp} \cdot T_{csa}$	$A_{tf} = 4.822 \times 10^{-5}\,\text{m}^2$
Water flow rate	$C_{wf} = 2.844 \times 10^{-3}\,\frac{\text{kg}}{\text{s}}$	
Water mass velocity	$W_{mv} := \frac{C_{wf}}{A_{tf}}$	$W_{mv} = 58.983\frac{\text{kg}}{\text{m}^2 \cdot \text{s}}$
Density of water	$\rho_{water} := 1000 \cdot \frac{\text{kg}}{\text{m}^3}$	
Water viscousity	$\mu_w := 8 \times 10^{-4} \cdot \frac{\text{N} \cdot \text{s}}{\text{m}^2}$	
Water linear velocity	$V_L := \frac{W_{mv}}{\rho_{water}}$	$V_L = 0.059\frac{\text{m}}{\text{s}}$
Heat transfer coefficient	$H_i = C_{p\_water} \cdot \left(\frac{1.35 + D_o T_t}{D_i^2} \right) \cdot V_L^{0.8}$	

$$T_t = 310.65\text{K} - 273.15 = 37.5°\text{C}$$

$$H_i := 4200\cdot\left(\frac{1.35 + 0.02\cdot310.65}{0.016^2}\right)\cdot0.058983^{0.8}\cdot\frac{\text{W}}{\text{m}^2\text{K}}$$

$$H_i = 1.289\times10^7\cdot\frac{\text{W}}{\text{m}^2\text{K}}$$

Reynolds $\quad R_{ey} := \frac{W_{mv}\cdot D_i}{\mu_w} \qquad R_{ey} = 1.18\times10^3$

Shell side calculations

Mean temperature of shell side $\quad T_s := \frac{T_{h\_in} + T_{h\_out}}{2} \qquad T_s = 343.15\text{K}$

Choice of baffle spacing $\quad B_{sc} := \frac{D_s}{5} \qquad B_{sc} = 7.754\times10^{-3}\text{m}$

Using square pitch and a 1 pass tube. $\quad P_t := 1.25\cdot D_o \qquad P_t = 0.025\text{m}$

Cross flow area $\quad A_{cf} := \left[\frac{(P_t - D_o)\cdot B_{sc}\cdot D_s}{P_t}\right] \qquad A_{cf} = 6.012\times10^{-5}\text{m}^2$

Mass flow rate of reactor product $\quad F_{2a} := 0.016\text{kg}\cdot\text{s}^{-1}$

Mass velocity $\quad O_{mv} := \frac{F_{2a}}{A_{cf}} \qquad O_{mv} = 266.136\frac{\text{kg}}{\text{m}^2\cdot\text{s}}$

Equivalent Diameter $\quad D_{eq} := \frac{1.27}{D_o}\cdot\left(P_t^2 - D_o^2\right) \qquad D_{eq} = 0.014\text{m}$

Viscousity	$\mu_{oil} := 6.92 \cdot 10^{-4} N \cdot m^{-2} s$	
Density	$\rho_{ow} := 876.43 kg \cdot m^{-3}$	
Linear velocity	$V_{L\_oil} := \dfrac{O_{mv}}{\rho_{ow}}$	$V_{L\_oil} = 0.304 \dfrac{m}{s}$
Heat capacity	$C_{ap} := 7200 J \cdot kg^{-1} \cdot K^{-1}$	
Thermal conductivity	$K_f := 1.242 W \cdot m^{-1} K^{-1}$	
Reynolds	$Re := \dfrac{O_{mv} \cdot D_{eq}}{\mu_{oil}}$	$Re = 5.495 \times 10^3$
Prandtle Number	$Pr := \dfrac{C_{ap} \cdot \mu_{oil}}{K_f}$	$Pr = 4.012$

From chart at15% baffle cut $j_h := 2.5 \cdot 10^{-2}$

Take into account viscousity correction the heat transfer coefficient h_s can be calculated from Nusselt equation

$$Nu = h_s \cdot \frac{D_{eq}}{K_f} = j_h \cdot Re \cdot Pr^{0.33} \left(\frac{\mu_{oil}}{\mu_w} \right)^{0.14}$$

This implies that

$$h_s := j_h \cdot Re \cdot Pr^{0.33} \cdot \left(\frac{\mu_{oil}}{\mu_w} \right)^{0.14} \cdot \frac{K_f}{D_{eq}}$$

$h_s = 1.851\times 10^4\cdot\frac{W}{m^2K}$

Estimate tube wall temperature

Mean temperature difference

$T_{md} := T_s - T_t$

$T_{md} = 32.5K$

Heat transfer coefficient $U := 540\frac{W}{m^2\cdot K}$

Mean temperature difference across the oil film

$T_{mc} := \left(\frac{U}{h_s}\right)\cdot T_{md}$

$T_{mc} = 0.948K$

Mean wall temperature

$T_{mw} := T_s - T_{mc}$

$T_{mw} = 342.202K$

Thermal conductivity K_w of tube wall material (aluminium alloy) $K_w := \alpha$

Inside fluid coefficient $h_{id} := 10800W\cdot m^{-2}K^{-1}$

outside fluid coefficient $h_{od} := 10800W\cdot m^{-2}K^{-1}$

6.1 Distillation Column 1 Design

Overal heat transfer coefficient U_{ov} is given by the relationship below

Sieve-Tray Design for Distillation Column 1 Design

This equipment design calculation program calculates the diameter of a sieve-tray tower to satisfy an approach to flooding criterium, and estimates of the tray efficiency.

Entering Data Related to the Gas and Liquid Streams

Entering liquid flow rate, mL, in kg/s

$mL := 0.01 \cdot kg \cdot sec^{-1}$

Entering gas flow rate, mG, in kg/s

$mG := 0.014 kg \cdot sec^{-1}$

$\rho L := 791 \cdot kg \cdot m^{-3}$

$U_{ov} = 1.629 \cdot \frac{W}{m^2 K}$

$$U_{ov} = \frac{1}{\frac{1}{h_s} + \frac{1}{h_{od}} + \frac{D_o \cdot \ln\left(\frac{D_o}{D_i}\right)}{2K_w} + \frac{\frac{D_o}{D_i}}{h_{id}} + \frac{\frac{D_o}{D_i}}{H_i}}$$

$$U_{ov} := \frac{1}{\frac{1}{1.7002} + \frac{1}{10800} + \frac{0.02 \cdot \ln\left(\frac{D_o}{D_i}\right)}{2 \times 275.9} + \frac{\frac{D_o}{D_i}}{10800} + \frac{\frac{D_o}{D_i}}{48.90640}} \cdot \frac{W}{m^2 K}$$

New heat transfer area for the condenser is given by

New Area $A_{new} := \frac{Q_{condenser}}{U_{ov} \cdot \Delta Tm}$

$A_{new} = 5.395 m^2$

This show a great reduction in the heat transfer area required for the condenser

Entering liquid density, in kg/m3

Entering gas density, kg/m3

$\rho G := 1.18 \cdot kg \cdot m^{-3}$

Entering gas viscosity, Pa-s

$\mu G := 1.05 \cdot 10^{-5} \cdot Pa \cdot sec$

Entering temperature, T, in K

$T := 353 \cdot K$

Entering total pressure, P, in Pa

$P := 101300 Pa$

Entering liquid surface tension, in dyne/cm

$\sigma := 21 \cdot \frac{dyne}{cm}$

Molar gas constant

$R := 8.314510 \cdot \frac{joule}{mole \cdot K}$

Gas Flowrate

$QG := \frac{mG}{\rho G}$

Liquid Flowrate

$$qL := \frac{mL}{\rho L}$$

Entering foaming factor, dimensionless

$FF := 0.9$

Enter water density at T, kg/m3

$\rho W := 970 \cdot kg \cdot m^{-3}$

$g = 9.807 \frac{m}{s^2}$

Entering local slope of equilibrium curve

$me := 0.42$

Entering molecular weights of gas and liquid

$ML := 32$ $\qquad$ $MG := 34.2$

Entering diffusivities of gas and liquid

$DG := 0.158 \frac{cm^2}{sec}$ $\qquad$ $DL := 2.07 \cdot 10^{-5} \cdot \frac{cm^2}{sec}$

Entering data related to the tray design

Enter hole diameter and pitch

$do := 4.5 \cdot mm$ $\qquad$ $p := 12 \cdot mm$

Entering plate thickness

$l := 2 \cdot mm$

Entering weir height

$hw := 5 \cdot cm$

Entering fractional approach to flooding

$f := 0.8$

Calculating flow parameter, X

$$X := \frac{mL}{mG}\cdot\sqrt{\frac{\rho G}{\rho L}}$$

$X = 0.028$

Specifying the ratio of downcomer area to total area, AdAt

$AdAt := 0.1$

$AdAt = 0.1$

If X is smaller than 0.1, use X = 0.1 in equation (4-31)

$X := 0.1$

$X = 0.1$

Calculating the ratio of hole to active area, Ah/Aa

$$AhAa := 0.907\cdot\left(\frac{do}{p}\right)^2$$

$AhAa = 0.128$

Calculating FHA

$$FHA := \begin{cases} 5\cdot AhAa + 0.5 & \text{if } AhAa < 0.1 \\ 1 & \text{otherwise} \end{cases}$$

$FHA = 1$

Calculating FST

$$FST := \left(\frac{\sigma}{20\cdot\frac{dyne}{cm}}\right)^{0.2}$$

$FST = 1.01$

$C1 := FST\cdot FHA\cdot FF$

$C1 = 0.909$

Entering parameters

$\alpha1 := 0.0744\mathrm{m}^{-1}$ $\qquad\qquad$ $\alpha2 := 0.0117$

$\beta1 := 0.0304\mathrm{m}^{-1}$ $\qquad\qquad$ $\beta2 := 0.01$

Iterating to find diameter and tray spacing

$\alpha(t) := \alpha1 \cdot t + \alpha2$

$\beta(t) := \beta1 \cdot t + \beta2$

$CF(t) := \alpha(t)\cdot\log\left(X^{-1}\right) + \beta(t)$ $\qquad\qquad$ $C(t) := C1\cdot CF(t)\cdot\dfrac{m}{sec}$

$$vGF(t) := C(t)\cdot\sqrt{\frac{\rho L - \rho G}{\rho G}}$$

Initial Estimates of Tray Spacing and Diameter

$D := 2\cdot m$ $\qquad\qquad$ $t := 0.5\cdot m$

Given

$$D = \sqrt{\frac{4\cdot QG}{f\cdot vGF(t)\cdot(1 - AdAt)\cdot\pi}}$$

Use is made here of the step function F(x) to define the recommended values of tray spacing.

$$\begin{aligned} t = {} & 0.5\cdot m\cdot\Phi(1\cdot m - D) + 0.6\cdot m\cdot(\Phi(3\cdot m - D) - \Phi(1\cdot m - D)) \ldots \\ & + 0.75\cdot m\cdot(\Phi(4\cdot m - D) - \Phi(3\cdot m - D)) \ldots \\ & + 0.9\cdot m\cdot(\Phi(20\cdot m - D) - \Phi(4\cdot m - D)) \end{aligned}$$

$$\begin{pmatrix} D \\ t \end{pmatrix} := \mathrm{Find}(D, t)$$

Diameter of the Column

$D = 0.106\mathrm{m}$ $\qquad\qquad$ $t = 0.5\mathrm{m}$

Calculating some further details of the tray design

$$At := \frac{\pi\cdot D^2}{4}$$

Total area

$At = 8.857\times 10^{-3}\,m^2$

Downcomer area

$Ad := AdAt \cdot At$

$Ad = 8.857\times 10^{-4}\,m^2$

Active area

$Aa := At - 2 \cdot Ad$

$Aa = 7.085\times 10^{-3}\,m^2$

Hole Area

$Ah := AhAa \cdot Aa$

$Ah = 9.037\times 10^{-4}\,m^2$

first estimate

$\theta 1 := 1.2 \cdot rad$

Given

$$AdAt = \frac{\theta 1 - \sin(\theta 1)}{2 \cdot \pi}$$

$\theta 1 := Find(\theta 1)$ $\qquad$ $\theta 1 = 1.627$

Weir Length

$$Lw := D \cdot \sin\left(\frac{\theta 1}{2}\right)$$

$Lw = 0.077m$

distance from tower center to weir

$$rw := \frac{D}{2} \cdot \left(\cos\left(\frac{\theta 1}{2}\right)\right)$$

$rw = 0.036m$

Estimating the gas-pressure drop through the tray

Dry Tray Head Loss, hd

Calculating orifice gas velocity, vo

$$vo := \frac{QG}{Ah}$$

$$vo = 13.129\frac{m}{s}$$

Calculating orifice coefficient, Co,

$$Co := 0.85032 - 0.04231\frac{do}{l} + 0.0017954\left(\frac{do}{l}\right)^{2}$$

$$Co = 0.764$$

$$hd := 0.0051\left(cm\cdot m\cdot\frac{sec^{2}}{kg}\right)\cdot\left(\frac{vo}{Co}\right)^{2}\cdot\rho G\frac{\rho W}{\rho L}\cdot\left(1 - Ah/Aa^{2}\right)$$

$$hd = 0.021\cdot m$$

Equivalent head of clear liquid, hl

Calculating gas velocity based on active area, va

$$va := \frac{QG}{Aa}$$

$$va = 1.675\frac{m}{s}$$

Calculating capacity parameter, Ks

$$qL = 1.264\times 10^{-5}\frac{m^{3}}{s}$$

$$Ks := va\cdot\sqrt{\frac{\rho G}{\rho L - \rho G}}$$

$$Ks = 0.065\frac{m}{s}$$

Calculating froth density ϕe

$$\phi e := \exp\left[-12.55\left(\frac{Ks}{1\cdot m\cdot sec^{-1}}\right)^{0.91}\right]$$

$$\phi e = 0.354$$

$$CL1 := 50.12\,cm\cdot sec^{\frac{2}{3}}\cdot m^{\frac{-4}{3}}$$

$$CL2 := 43.89\,cm\cdot sec^{\frac{2}{3}}\cdot m^{\frac{-4}{3}}$$

$$CL := CL1 + CL2\cdot\exp\left(-1.378\,cm^{-1}\cdot hw\right)$$

$$hl := \phi e\cdot\left[hw + CL\cdot\left(\frac{qL}{Lw\cdot\phi e}\right)^{\frac{2}{3}}\right]$$

$$hl = 0.019m$$

Head loss due to surface tension, h

$$h\sigma := \frac{6\cdot\sigma}{g\cdot\rho L\cdot do}$$

$$h\sigma = 3.61\times 10^{-3}m$$

Total head loss, ht

$$ht := hd + hl + h\sigma$$

$$ht = 0.044m$$

Converting head loss to pressure drop, DP

$$\Delta P := ht\cdot\rho L\cdot g$$

$$\Delta P = 339.633Pa$$

Tray Design for Excessive Weeping

Checking tray design for excessive weeping: calculating orifice Froude number, Fro

If Fro > 0.5 there is no weeping problem.

$$\mathrm{Fro} := \sqrt{\frac{\rho G \mathrm{vo}^2}{\rho L \cdot g \cdot \mathrm{hl}}}$$

$$\mathrm{Fro} = 1.183$$

Fractional entrainment, E

$$\kappa := 0.5 \cdot \left(1 - \tanh\left(1.3 \cdot \ln\left(\frac{\mathrm{hl}}{\mathrm{do}}\right) - 0.15\right)\right)$$

$$\kappa = 0.032$$

$$\mathrm{h2}\phi := \frac{\mathrm{hl}}{\phi e} + 7.79 \left[1 + 6.9 \cdot \left(\frac{\mathrm{do}}{\mathrm{hl}}\right)^{1.85}\right] \cdot \frac{\mathrm{Ks}^2}{\phi e \cdot g \cdot \mathrm{AhAa}}$$

$$\mathrm{h2}\phi = 0.163\mathrm{m}$$

$$E := 0.00335 \left(\frac{\mathrm{h2}\phi}{t}\right)^{1.1} \cdot \left(\frac{\rho L}{\rho G}\right)^{0.5} \cdot \left(\frac{\mathrm{hl}}{\mathrm{h2}\phi}\right)^{\kappa}$$

$$E = 0.024$$

Point efficiency, EOG

$$\mathrm{ReFe} := \frac{\rho G \mathrm{vo} \cdot \mathrm{hl}}{\mu G \cdot \phi e}$$

$$\mathrm{ReFe} = 7.82 \times 10^4$$

$$cG := \frac{\rho G}{MG}$$

$$cG = 0.035 \cdot \frac{kg}{m^3}$$

$$cL := \frac{\rho L}{ML}$$

$$cL = 24.719 \frac{kg}{m^3}$$

$a1 := 0.413$ $\quad a2 := 0.607$ $\quad a3 := -0.319$

$$EOG := 1 - \exp\left[\frac{-0.0029}{1 + me\cdot\frac{cG}{cL}\cdot\sqrt{DG\cdot\frac{1-\phi e}{DL\cdot AhAa}}}\cdot ReFe^{a1}\cdot\left(\frac{hl}{do}\right)^{a2}\cdot AhAa^{a3}\right]$$

$EOG = 0.717$

Calculating Murphree tray efficiency, EMG

Checking the degree of vapor mixing; calculate PeG.

If PeG > 50, or if t Ð h2f < 0, vapor is unmixed.

$t - h2\phi = 0.337m$ $\qquad DEG := 0.01\cdot\frac{m^2}{sec}$

$PeG := \frac{4\cdot QG\cdot rw^2}{DEG\cdot Aa\cdot(t - h2\phi)}$ $\qquad PeG = 2.646$

Calculate PeL

$DEL := 0.1\cdot\sqrt{g\cdot h2\phi^3}$ $\qquad DEL = 0.021\frac{m^2}{s}$

$PeL := \frac{4\cdot qL\cdot rw^2}{Aa\cdot hl\cdot DEL}$ $\qquad PeL = 0.025$

$N := \frac{PeL + 2}{2}$ $\qquad N = 1.012$

$\lambda := me\cdot\frac{mG}{mL}\cdot\frac{ML}{MG}$ $\qquad \lambda = 0.55$

For mixed vapor

$EMGmixed := \frac{\left(1 + \frac{\lambda\cdot EOG}{N}\right)^N - 1}{\lambda}$ $\qquad EMGmixed = 0.718$

For unmixed vapor

$EMGunmixed := EMGmixed\left(1 - 0.0335\lambda^{1.07272}\cdot EOG^{2.51841}\cdot PeL^{0.17524}\right)$

$EMGunmixed = 0.716$

$$EMG := \begin{cases} EMGmixed & \text{if } 0 < PeG < 50 \\ EMGunmixed & \text{otherwise} \end{cases}$$

$EMG = 0.718$

Correcting efficiency for entrainment

$$EMGE := EMG\left(1 - 0.8 \cdot EOG\lambda^{1.543} \cdot \frac{E}{me}\right)$$

$EMGE = 0.709$

Atmospheric Distillation Column Number of Stages and Position of the Feed Stage Determination

In the distillation process at low temperatures differences between the top and the bottom of the column, we may suppose that the vaporization pressure of species may be constant in the whole apparatus. Because of that, we say:

...vapor pressure of the lighter component.

$$Pvl := \exp\left(18.5242 - \frac{3578.91}{303 + -50.50}\right) \cdot kPa \qquad Pvl = 0.901 \cdot mmHg$$

...vapor pressure of the heavier component (Pvl must be greater than Pvh).

$$Pvh := \exp\left(18.3036 - \frac{3816.44}{303 + -46.13}\right) \cdot kPa \qquad Pvh = 0.365 \, mmHg$$

And in the same way, lets define the pressure inside the column:

$P := 5.526687 bar$

5.5

With the statements above, we call the quotient as the relative volatility coefficient, which is evaluated as

$$\alpha := \left(\frac{Pvl}{Pvh}\right) \qquad \alpha = 2.47$$

With all the previous conditions, we may trace an equilibrium curve in a diagram y vs. x, where y is the composition of the lighter component in the gas phase and x is the lighter component composition in the liquid phase. This curve will have the next equation:

$ye(xe) := \dfrac{\alpha \cdot xe}{1 + (\alpha - 1) \cdot xe}$ ...both ye and xe design "y in equilibrium with x"

If the enthalpy of vaporization for both the heavier and lighter components is similar, the conditions of the McCabe-Thiele distillation are valid, and we may use a "graphical" solution to the problem:

$F := 160.691 \dfrac{mol}{hr}$ ...feed rate.

$zf := 0.08$ ...feed composition of lighter component

Design Parameters:

$xd := 99.95\%$ ...lighter component composition at the top.

$xb := 1 \cdot \%$ ...bottom composition of lighter component.

$r := 0.99\%$ ...lighter component recuperation in the process.

$q := 1.032732$ ...thermodynamic constant of feed;

$$q := \frac{Hv - Hf}{Hv - Hl}$$

where Hv ...saturated vapor enthalpy at feed temperature.

Hl ...saturated liquid enthalpy at feed temperature.

Hf ...feed enthalpy.

$$\infty \equiv 10^{100}$$

$q := q \cdot \left(1 + \dfrac{1}{\infty}\right)$ this correction for q is made to avoid division by zero later in the electronic sheet.

Heat and Mass Balances:

$D := 109.087 \dfrac{mol}{hr}$ ...Distillate Flowrate

$B := 156.601\frac{mol}{hr}$, ...Bottom Flowrate

$kmol \equiv 1000\, mole$

in the condition of minimal reflux ratio,

$xi := 0.5$ Given $ye(xi) = \frac{q}{q-1}\cdot xi - \frac{zf}{q-1}$ $xi := Find(xi)$ and $yi := ye(xi)$

where the point given by (xi,yi) is the intersection of q, DOL, ROL and equilibrium lines.

The minimal reflux ratio will be

$$Rmin := \frac{xd}{xd - xd\cdot\frac{xd-yi}{xd-xi}} - 1 \qquad Rmin = 8.165$$

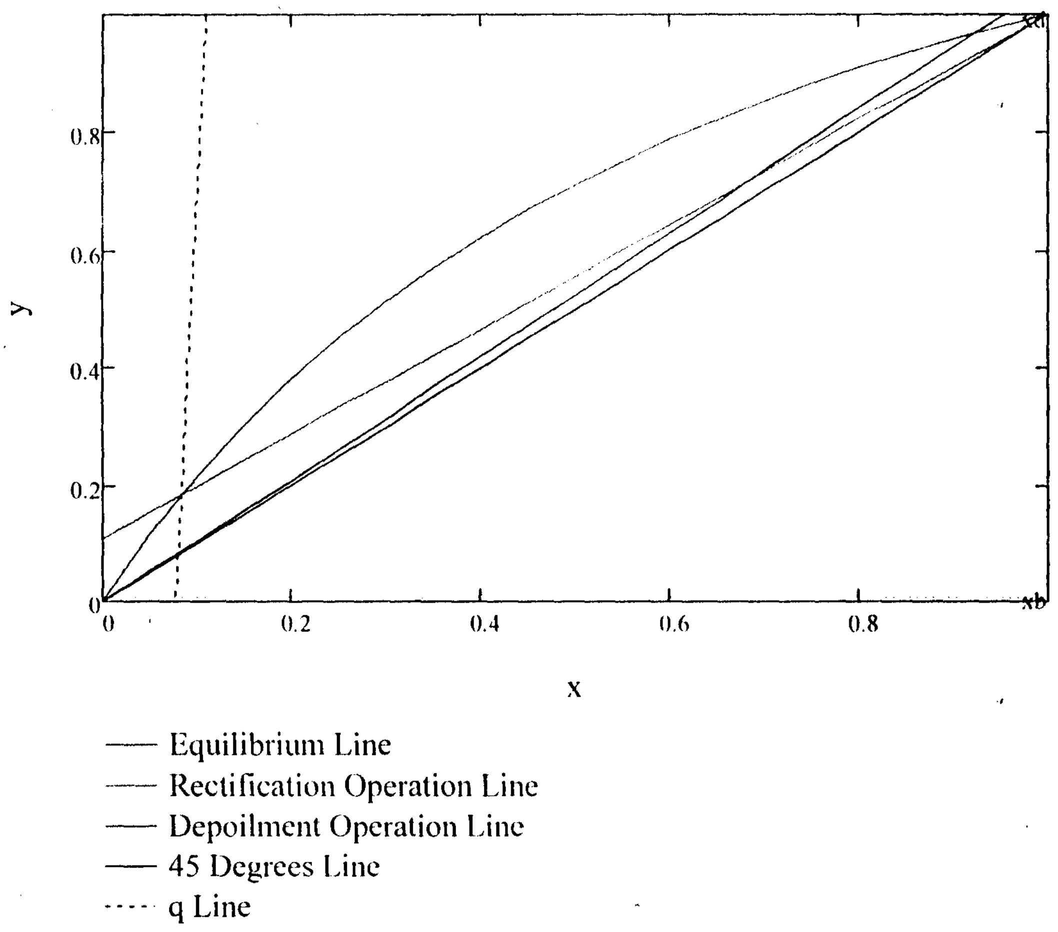
$Lr := Rmin\cdot D$ ...the liquid flow in the rectification section of the column $Lr = 14.845\frac{mol}{min}$

$Vr := Lr + D$ ...the vapor flow in the rectification section of the column. $Vr = 16.663\frac{mol}{min}$

$Ld := F\cdot q + Lr$ ...the liquid flow in the depoilment section of the column. $Ld = 17.61\frac{mol}{min}$

$Vd := F\cdot(q-1) + Vr$

$x := 0, 0.05..1$ ...the vapor flow in the depoilment section of the column. $Vd = 16.75\frac{mol}{min}$



Real Reflux Ratio Calculation.

$Rr := 6$ ...which must be greater than $Rmin = 8.165$

With the new reflux ratio, we may redefine Vr, Lr, Ld and Vd as

$Vr := D\cdot(Rr + 1)$ $\quad Lr := Vr\cdot\left(\frac{Rr}{Rr + 1}\right)$ $\quad Ld := F\cdot q + Lr$ $\quad Vd := F\cdot(q - 1) + Vr$

...and other quantities of interest as

$i := 0..200$ $\quad xp_0 := xd$ $\quad yp_0 := xd$

$$xq := \frac{\frac{D\cdot xd}{Vr} + \frac{B\cdot xb}{Vd}}{\frac{Ld}{Vd} - \frac{Lr}{Vr}} \qquad yq := \frac{Lr\cdot xq + D\cdot xd}{Vr}$$

$$Vf_i := \Phi(xp_i - xq) \qquad Nf := \frac{\sum Vf + 1}{2} \qquad \begin{pmatrix} yp_{i+1} \\ xp_{i+1} \end{pmatrix} := \begin{bmatrix} \text{if}\left(xp_i > xq, \frac{Lr\cdot xp_i + D\cdot xd}{Vr}, \frac{Ld\cdot xp_i - B\cdot xb}{Vd}\right) \\ \frac{yp_i}{\alpha - (\alpha - 1)\cdot yp_i} \end{bmatrix}$$

$$Vn_i := \Phi(xp_i - xb) \qquad Nt := \frac{\sum Vn + 1}{2}$$

Units

$MW \equiv 1$ $\quad MPa \equiv 10^6\cdot Pa$ $\quad kPa \equiv 10^3\cdot Pa$ $\quad J \equiv joule$ $\quad bar \equiv 10^5\cdot Pa$ $\quad kJ \equiv 1000 joule$

$Rg \equiv 8.314510\frac{J}{MW\cdot gm\cdot K}$ $\quad mol \equiv MW\cdot gm$ $\quad kgmol \equiv mol\cdot 1000$ $\quad cP \equiv 10^{-2}\cdot poise$ $\quad \mu P \equiv 10^{-6}\cdot poise$

$s \equiv sec$ $\quad lt \equiv liter$ $\quad N \equiv newton$ $\quad mmHg \equiv in\_Hg\cdot 25.4$

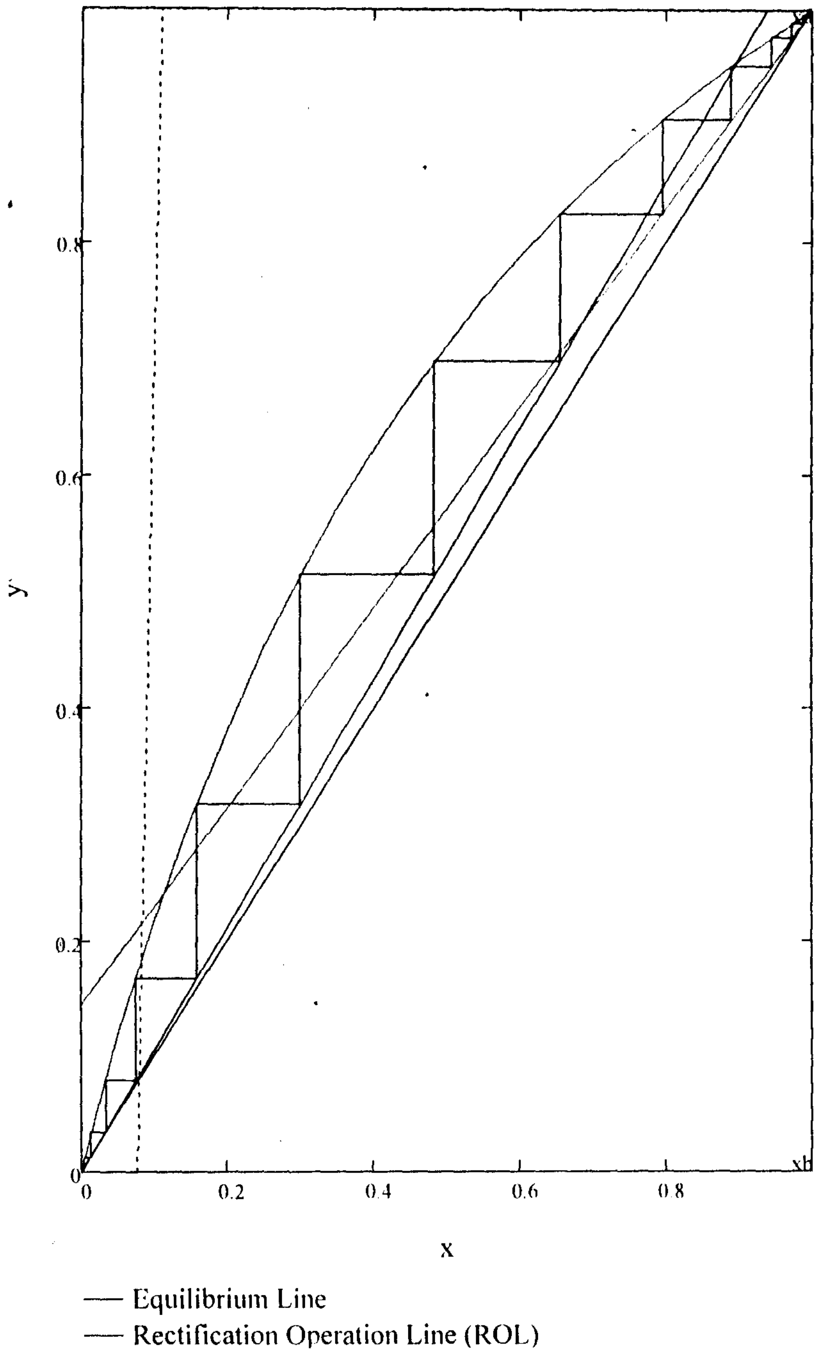
$Vr = 12.727\frac{mol}{min}$ $\quad Lr = 10.909\frac{mol}{min}$ $\quad Vd = 12.814\frac{mol}{min}$ $\quad Ld = 13.675\frac{mol}{min}$

Position of the Feed Stage

$Nf = 9$ ...Feed Stage.

Actual Number of Stages

$Nt = 16$ ...Total number of theoretical trays.



Column efficiency:

Col_Eff := 80%

$$Actual\_Number\_of\_Trays := \frac{Nt}{Col\_Eff}$$

Col_Eff = 0.8

6.1 Distillation Column 2 Design

$\text{Actual\_Number\_of\_Trays} = 20$

Sieve-Tray Design for Distillation Column 1 Design

Column Height

This equipment design calculation program calculates the diameter of a sieve-tray tower to

Column height = [Number of actual trays] x [Tray spacing] + Additional elevation of
satisfy an approach to flooding criterium, and estimates of the tray efficiency.

the liquid holdup in the base of the column.

Entering Data Related to the Gas and Liquid Streams

$\text{Tray\_Spacing} := 0.5\ \text{m}$

Entering liquid flow rate, mL, in kg/s

Additional elevation of the liquid holdup in the base of the column (Z_A)

$mL = 0.025\,\text{kg}\cdot\text{sec}^{-1}$

$Z_A := 0.5\ \text{m}$

Entering gas flow rate, mG, in kg/s

Column height (H) is finally calculated as

$mG = 0.032\,\text{kg}\cdot\text{sec}^{-1}$

$\text{Column\_Height} := \left[\left[(\text{Actual\_Number\_of\_Trays})\cdot\text{Tray\_Spacing}\right] + Z_A\right]$ Column_H

Entering liquid density, in kg/m3

$\rho L = 891\cdot\text{kg}\cdot\text{m}^{-3}$

$\text{Column\_Height} = 10.5\text{m}$

Entering gas density, kg/m3

$\rho G = 1.28\,\text{kg}\cdot\text{m}^{-3}$

Entering gas viscosity, Pa-s

$\mu G = 1.07\cdot 10^{-5}\cdot\text{Pa}\cdot\text{sec}$

Entering temperature, T, in K

$T = 353\,\text{K}$

Entering total pressure, P, in Pa

$P = 101300\text{Pa}$

Entering liquid surface tension, in dyne/cm

$\sigma = 21\cdot\frac{\text{dyne}}{\text{cm}}$

Molar gas constant

$R = 8.314510\frac{\text{joule}}{\text{mole}\cdot\text{K}}$

Gas Flowrate

$QG = \frac{mG}{\rho G}$

Liquid Flowrate

$$qL = \frac{mL}{\rho L}$$

Entering foaming factor, dimensionless

$FF = 0.9$

Enter water density at T, kg/m3

$\rho W = 970 \cdot kg \cdot m^{-3}$

$$g = 9.807 \frac{m}{s^2}$$

Entering local slope of equilibrium curve

$me = 0.42$

Entering molecular weights of gas and liquid

$ML = 32$ $\quad\quad$ $MG = 34.2$

Entering diffusivities of gas and liquid

$$DG = 0.158 \frac{cm^2}{sec} \qquad DL = 2.07 \cdot 10^{-5} \cdot \frac{cm^2}{sec}$$

Entering data related to the tray design

Enter hole diameter and pitch

$do = 4.5 \cdot mm$ $\quad\quad$ $p = 12 \cdot mm$

Entering plate thickness

$l = 2 \cdot mm$

Entering weir height

$hw = 5 \cdot cm$

Entering fractional approach to flooding

$f = 0.8$

Calculating flow parameter, X

$$X = \frac{mL}{mG} \cdot \sqrt{\frac{\rho G}{\rho L}}$$

$X = 0.03$

Specifying the ratio of downcomer area to total area, AdAt

$AdAt = 0.1$

$AdAt = 0.1$

If X is smaller than 0.1, use X = 0.1 in equation (4-31)

$X = 0.1$

$X = 0.1$

Calculating the ratio of hole to active area, Ah/Aa

$$AhAa = 0.907 \cdot \left(\frac{do}{p}\right)^2$$

$AhAa = 0.128$

Calculating FHA

$$FHA = \begin{cases} 5 \cdot AhAa + 0.5 & \text{if } AhAa < 0.1 \\ 1 & \text{otherwise} \end{cases}$$

$FHA = 1$

Calculating FST

$$FST = \left(\frac{\sigma}{20 \cdot \frac{dyne}{cm}}\right)^{0.2}$$

$FST = 1.01$

$C1 = FST \cdot FHA \cdot FF$

$C1 = 0.909$

Entering parameters ,

$\alpha 1 = 0.0744\,\mathrm{m}^{-1}$ $\qquad\qquad \alpha 2 = 0.0117$

$\beta 1 = 0.0304\,\mathrm{m}^{-1}$ $\qquad\qquad \beta 2 = 0.01$

Iterating to find diameter and tray spacing

$\alpha(t) = \alpha 1 \cdot t + \alpha 2$

$\beta(t) = \beta 1 \cdot t + \beta 2$

$CF(t) = \alpha(t)\,\log\left(X^{-1}\right) + \beta(t)$ $\qquad\qquad C(t) = C1 \cdot CF(t) \cdot \frac{m}{sec}$

$$vGF(t) = C(t) \cdot \sqrt{\frac{\rho L - \rho G}{\rho G}}$$

Initial Estimates of Tray Spacing and Diameter

$D = 2 \cdot m$ $\qquad\qquad t = 0.5 \cdot m$

Given

$$D = \sqrt{\frac{4 \cdot QG}{f \cdot vGF(t) \cdot (1 - AdAt) \cdot \pi}}$$

Use is made here of the step function F(x) to define the recommended

values of tray spacing.

$$t = 0.5 \cdot m \cdot \Phi(1 \cdot m - D) + 0.6 \cdot m \cdot (\Phi(3 \cdot m - D) - \Phi(1 \cdot m - D)) \ldots$$
$$+ 0.75 \cdot m \cdot (\Phi(4 \cdot m - D) - \Phi(3 \cdot m - D)) \ldots$$
$$+ 0.9 \cdot m \cdot (\Phi(20 \cdot m - D) - \Phi(4 \cdot m - D))$$

$$\begin{pmatrix} D \\ t \end{pmatrix} = \mathrm{Find}(D,t)$$

Diameter of the Column

D = 2.

$D = 2.5\,\mathrm{m}$ $\qquad\qquad t = 0.5\,\mathrm{m}$

Calculating some further details of the tray design

$$At = \frac{\pi \cdot D^2}{4}$$

Total area

$At = 4.909m^2$

Downcomer area

$Ad = AdAt \cdot At$

$Ad = 0.491m^2$

Active area

$Aa = At - 2 \cdot Ad$

$Aa = 3.927m^2$

Hole Area

$Ah = AhAa \cdot Aa$

$Ah = 0.501m^2$

first estimate

$\theta 1 = 1.2 \cdot rad$

Given

$$AdAt = \frac{\theta 1 - \sin(\theta 1)}{2 \cdot \pi}$$

$\theta 1 = Find(\theta 1)$ $\theta 1 = 1.627$

Weir Length

$$Lw = D \cdot \sin\left(\frac{\theta 1}{2}\right)$$

$Lw = 1.817m$

distance from tower center to weir

$$rw = \frac{D}{2} \cdot \left(\cos\left(\frac{\theta 1}{2}\right)\right)$$

$rw = 0.859m$

Estimating the gas-pressure drop through the tray

Dry Tray Head Loss, hd

Calculating orifice gas velocity, vo

$$vo = \frac{QG}{Ah}$$

$$vo = 0.05\frac{m}{s}$$

Calculating orifice coefficient, Co,

$$Co = 0.85032 - 0.04231\frac{do}{l} + 0.0017954\left(\frac{do}{l}\right)^2$$

$$Co = 0.764$$

$$hd = 0.0051\cdot\left(cm\cdot m\cdot\frac{sec^2}{kg}\right)\cdot\left(\frac{vo}{Co}\right)^2\cdot\rho G\frac{\rho W}{\rho L}\cdot\left(1 - AhAa^2\right)$$

$$hd = 2.982\times 10^{-7}\cdot m$$

Equivalent head of clear liquid, hl

Calculating gas velocity based on active area, va

$$va = \frac{QG}{Aa}$$

$$va = 6.366\times 10^{-3}\frac{m}{s}$$

Calculating capacity parameter, Ks

$$qL = 2.806\times 10^{-5}\frac{m^3}{s}$$

$$Ks = va\cdot\sqrt{\frac{\rho G}{\rho L - \rho G}}$$

$$Ks = 2.415\times 10^{-4}\frac{m}{s}$$

Calculating froth density ϕe

$$\phi e = \exp\left[-12.55\left(\frac{Ks}{1\cdot m\cdot sec^{-1}}\right)^{0.91}\right]$$

$$\phi e = 0.994$$

$$CL1 = 50.12\,cm\cdot sec^{\frac{2}{3}}\cdot m^{\frac{-4}{3}}$$

$$CL2 = 43.89\,cm\cdot sec^{\frac{2}{3}}\cdot m^{\frac{-4}{3}}$$

$$CL = CL1 + CL2\cdot\exp\left(-1.378\,cm^{-1}\cdot hw\right)$$

$$hl = \phi e\cdot\left[hw + CL\cdot\left(\frac{qL}{Lw\cdot\phi e}\right)^{\frac{2}{3}}\right]$$

$$hl = 0.05m$$

Head loss due to surface tension, h

$$h\sigma = \frac{6\cdot\sigma}{g\cdot\rho L\cdot do}$$

$$h\sigma = 3.204\times 10^{-3}m$$

Total head loss, ht

$$ht = hd + hl + h\sigma$$

$$ht = 0.053m$$

Converting head loss to pressure drop, DP

$$\Delta P = ht\cdot\rho L\cdot g$$

$$\Delta P = 464.809Pa$$

Tray Design for Excessive Weeping

Checking tray design for excessive weeping; calculating orifice Froude number, Fro

If Fro > 0.5 there is no weeping problem.

$$Fro = \sqrt{\frac{\rho Gvo^2}{\rho Lg \cdot hl}}$$

$$Fro = 2.702 \times 10^{-3}$$

Fractional entrainment, E

$$\kappa = 0.5 \cdot \left(1 - \tanh\left(1.3 \cdot \ln\left(\frac{hl}{do}\right) - 0.15\right)\right)$$

$$\kappa = 2.573 \times 10^{-3}$$

$$h2\phi = \frac{hl}{\phi e} + 7.79\left[1 + 6.9 \cdot \left(\frac{do}{hl}\right)^{1.85}\right] \cdot \frac{Ks^2}{\phi e \cdot g \cdot AhAa}$$

$$h2\phi = 0.05m$$

$$E = 0.00335\left(\frac{h2\phi}{t}\right)^{1.1} \cdot \left(\frac{\rho L}{\rho G}\right)^{0.5} \cdot \left(\frac{hl}{h2\phi}\right)^{\kappa}$$

$$E = 7.069 \times 10^{-3}$$

Point efficiency, EOG

$$ReFe = \frac{\rho Gvo \cdot hl}{\mu G \cdot \phi e}$$

$$ReFe = 300.408$$

$$cG = \frac{\rho G}{MG}$$

$$cG = 0.037 \frac{kg}{m^3}$$

$$cL = \frac{\rho L}{ML}$$

$$cL = 27.844 \frac{kg}{m^3}$$

$a1 = 0.413$ $a2 = 0.607$ $a3 = -0.319$

$$EOG = 1 - \exp\left[\frac{-0.0029}{1 + me\cdot\frac{cG}{cL}\cdot\sqrt{DG\cdot\frac{1-\phi e}{DL\cdot AhAa}}}\cdot ReFe^{a1}\cdot\left(\frac{hl}{do}\right)^{a2}\cdot AhAa^{a3}\right]$$

$EOG = 0.224$

Calculating Murphree tray efficiency, EMG

Checking the degree of vapor mixing; calculate PeG.

If PeG > 50, or if t D h2f < 0, vapor is unmixed.

$t - h2\phi = 0.45m$ $DEG = 0.01\cdot\frac{m^2}{sec}$

$$PeG = \frac{4\cdot QG\cdot rw^2}{DEG\cdot Aa\cdot(t - h2\phi)}$$ $PeG = 4.177$

Calculate PeL

$DEL = 0.1\cdot\sqrt{g\cdot h2\phi^3}$ $DEL = 3.534\times 10^{-3}\frac{m^2}{s}$

$$PeL = \frac{4\cdot qL\cdot rw^2}{Aa\cdot hl\cdot DEL}$$ $PeL = 0.119$

$$N = \frac{PeL + 2}{2}$$ $N = 1.06$

$$\lambda = me\cdot\frac{mG}{mL}\cdot\frac{ML}{MG}$$ $\lambda = 0.503$

For mixed vapor

$$EMGmixed = \frac{\left(1 + \frac{\lambda\cdot EOG}{N}\right)^{N} - 1}{\lambda}$$ $EMGmixed = 0.224$

For unmixed vapor

$$EMGunmixed = EMGmixed\left(1 - 0.0335\lambda^{1.07272}\cdot EOG^{2.51844}\cdot PeL^{0.17524}\right)$$

$EMGunmixed = 0.224$

$$\mathrm{EMG} = \begin{cases} \mathrm{EMGmixed} \text{ if } 0 < \mathrm{PeG} < 50 \\ \mathrm{EMGunmixed} \text{ otherwise} \end{cases}$$

$$\mathrm{EMG} = 0.224$$

Correcting efficiency for entrainment

$$\mathrm{EMGE} = \mathrm{EMG}\left(1 - 0.8\cdot \mathrm{EOG}\lambda^{1.543}\cdot\frac{E}{me}\right)$$

$$\mathrm{EMGE} = 0.224$$

Atmospheric Distillation Column Number of Stages and Position of the Feed Stage Determination

In the distillation process at low temperatures differences between the top and the bottom of the column, we may suppose that the vaporization pressure of species may be constant in the whole apparatus. Because of that, we say:

...vapor pressure of the lighter component.

$$\mathrm{Pvl} = \exp\left(19.1543 - \frac{3786.91}{343 + -65.50}\right)\cdot \mathrm{kPa} \qquad \mathrm{Pvl} = 2.867\cdot \mathrm{mmHg}$$

...vapor pressure of the heavier component (Pvl must be greater than Pvh).

$$\mathrm{Pvh} = \exp\left(19.0675 - \frac{3916.44}{323 + -49.13}\right)\cdot \mathrm{kPa} \qquad \mathrm{Pvh} = 1.367\cdot \mathrm{mmHg}$$

And in the same way, lets define the pressure inside the column:

$$P = 5.526687\mathrm{bar}$$

5.5

With the statements above, we call the quotient as the relative volatility coefficient, which is evaluated as

$$\alpha = \left(\frac{\mathrm{Pvl}}{\mathrm{Pvh}}\right) \qquad \alpha = 2.097$$

With all the previous conditions, we may trace an equilibrium curve in a diagram y vs. x, where y is the composition of the lighter component in the gas phase and x is the lighter component composition in the liquid phase. This curve will have the next equation:

$$ye(xe) = \frac{\alpha \cdot xe}{1 + (\alpha - 1) \cdot xe}$$ ...both ye and xe design "y in equilibrium with x"

If the enthalpy of vaporization for both the heavier and lighter components is similar, the conditions of the McCabe-Thiele distillation are valid, and we may use a "graphical" solution to the problem:

$F = 160.691 \frac{mol}{hr}$ ...feed rate.

$zf = 0.08$ ...feed composition of lighter component

Design Parameters:

$xd = 99.95\%$ ...lighter component composition at the top.

$xb = 1 \cdot \%$ ...bottom composition of lighter component.

$r = 0.99\%$ ...lighter component recuperation in the process.

$q = 1.032732$ ...thermodynamic constant of feed:

$$q = \frac{Hv - Hf}{Hv - Hl}$$

where Hv ...saturated vapor enthalpy at feed temperature.

Hl ...saturated liquid enthalpy at feed temperature.

Hf ...feed enthalpy.

$$\infty \equiv 10^{100}$$

$q = q \cdot \left(1 + \frac{1}{\infty}\right)$ this correction for q is made to avoid division by zero later in the electronic sheet.

Heat and Mass Balances:

$D = 155.019 \frac{mol}{hr}$ ...Distillate Flowrate

$B = 451.694\frac{mol}{hr}$ ...Bottom Flowrate

$kmol \equiv 1000 mol$

in the condition of minimal reflux ratio,

$xi = 0.5$ Given $ye(xi) = \frac{q}{q-1} \cdot xi - \frac{zf}{q-1}$ $xi = Find(xi)$ and $yi = ye(xi)$

where the point given by (xi,yi) is the intersection of q, DOL, ROL and equilibrium lines.

The minimal reflux ratio will be

$$Rmin = \frac{xd}{xd - xd \cdot \frac{xd - yi}{xd - xi}} - 1 \qquad Rmin = 11.041$$

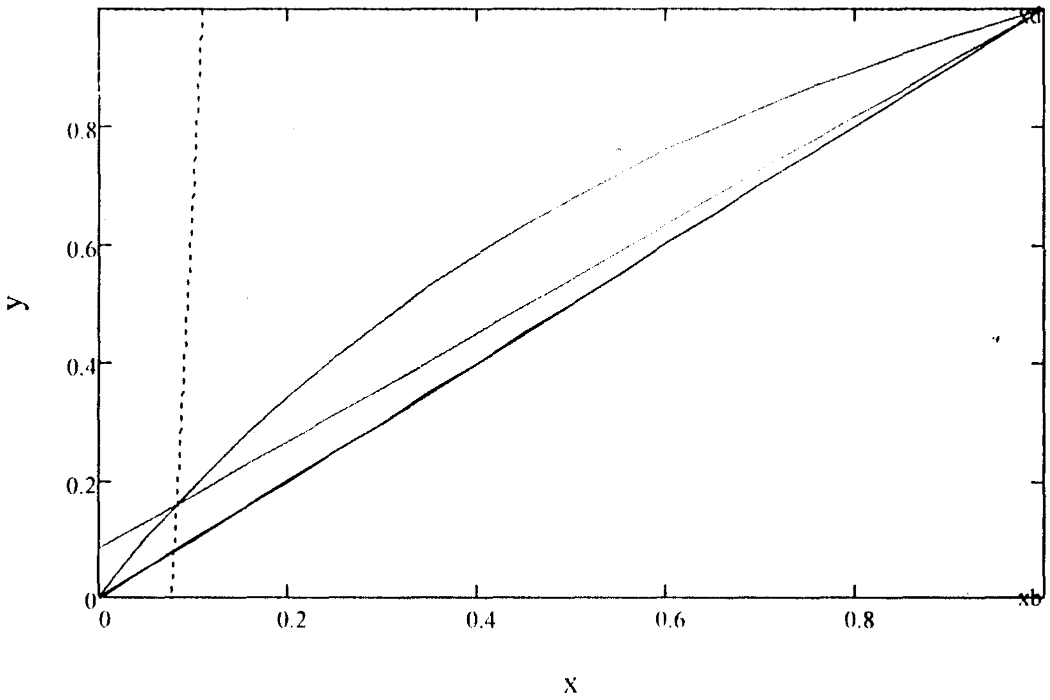
$Lr = Rmin \cdot D$ ...the liquid flow in the rectification section of the column $Lr = 28.526\frac{mol}{min}$

$Vr = Lr + D$ ...the vapor flow in the rectification section of the column $Vr = 31.11\frac{mol}{min}$

$Ld = F \cdot q + Lr$ ...the liquid flow in the depoilment section of the column. $Ld = 31.292\frac{mol}{min}$

$Vd = F \cdot (q - 1) + Vr$

$x = 0, 0.05 .. 1$ ...the vapor flow in the depoilment section of the column. $Vd = 31.198\frac{mol}{min}$



—— Equilibrium Line
—— Rectification Operation Line
—— Depoilment Operation Line
—— 45 Degrees Line
----- q Line

Real Reflux Ratio Calculation.

$Rr = 6$ ...which must be greater than $Rmin = 11.041$

With the new reflux ratio, we may redefine Vr, Lr, Ld and Vd as

$Vr = D\cdot(Rr + 1)$ $\quad Lr = Vr\cdot\left(\frac{Rr}{Rr + 1}\right)$ $\quad Ld = F\cdot q + L$ $\quad Vd = F\cdot(q - 1) + V$

...and other quantities of interest as

$i = 0..20$ $\quad xp_0 = xc$ $\quad yp_0 = xd$

$$xq = \frac{\frac{D\cdot xd}{Vr} + \frac{B\cdot xb}{Vd}}{\frac{Ld}{Vd} - \frac{Lr}{Vr}} \qquad yq = \frac{Lr\cdot xq + D\cdot xd}{Vr}$$

$$\begin{pmatrix} yp_{i+1} \\ xp_{i+1} \end{pmatrix} = \begin{bmatrix} \text{if}\left(xp_i > xq, \frac{Lr\cdot xp_i + D\cdot xd}{Vr}, \frac{Ld\cdot xp_i - B\cdot xb}{Vd}\right) \\ \frac{yp_i}{\alpha - (\alpha - 1)\cdot yp_i} \end{bmatrix}$$

$$Vf_i = \Phi(xp_i - xq) \qquad Nf = \frac{\sum Vf + 1}{2}$$

$$Vn_i = \Phi(xp_i - xb) \qquad Nt = \frac{\sum Vn + 1}{2}$$

Units

$MW \equiv 1$ $\quad MPa \equiv 10^6\cdot Pa$ $\quad kPa \equiv 10^3\cdot Pa$ $\quad J \equiv joule$ $\quad bar \equiv 10^5\cdot Pa$ $\quad kJ \equiv 1000 joule$

$Rg \equiv 8.314510\frac{J}{MW\cdot gm\cdot K}$ $\quad mol \equiv MW\cdot gm$ $\quad kgmol \equiv mol\cdot 100$ $\quad cP \equiv 10^{-2}\cdot poise$ $\quad \mu P \equiv 10^{-6}\cdot poise$

$s \equiv sec$ $\quad lt \equiv lite$ $\quad N \equiv newton$ $\quad mmHg \equiv in\_Hg\cdot 25.$

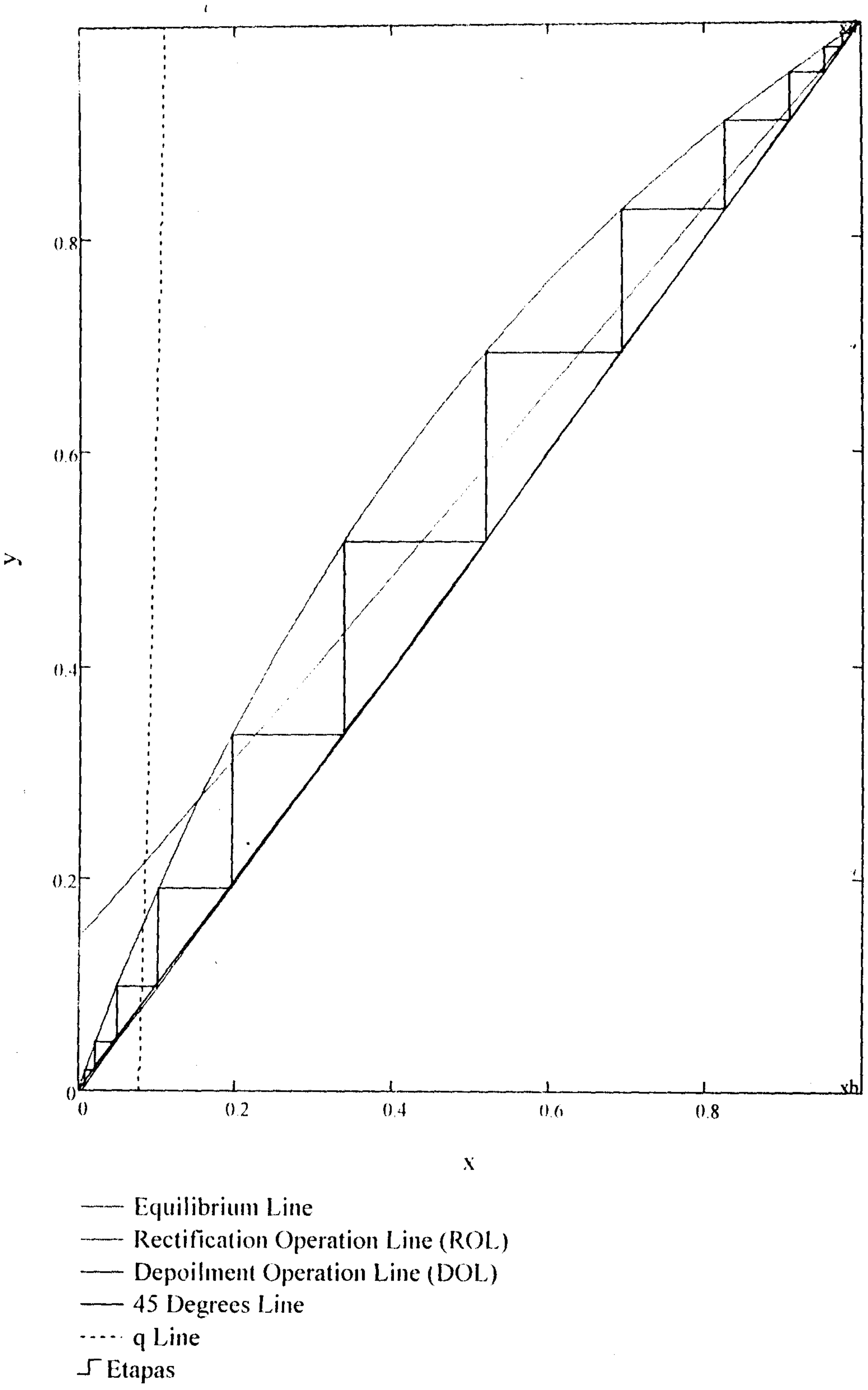
$Vr = 18.086\frac{mol}{min}$ $\quad Lr = 15.502\frac{mol}{min}$ $\quad Vd = 18.173\frac{mol}{min}$ $\quad Ld = 18.268\frac{mol}{min}$

6.2.7 Position of the Feed Stage

$Nf = 5$ ...Feed Stage.

6.2.8 Actual Number of Stages

$Nt = 17$ ...Total number of theoretical trays.



Column efficiency:

Col_Eff = 80%

$$\text{Actual\_Number\_of\_Trays} = \frac{\text{Nt}}{\text{Col\_Eff}} \qquad \text{Col\_Eff} = 0.8$$

$\text{Actual\_Number\_of\_Trays}_i = 21.25$

6.2 Fluidized Bed Reactor Design:

Reactor Conditions

$P = 840 \cdot torr$

$\text{Tray\_Spacing} = 0.5 \ m$

Additional elevation of the liquid holdup in the base of the column (Z_A)

$T = (320 + 273) \cdot K$

$Z_A = 0.5 \ m \qquad D_t = 11.4 cm$

Column height (H) is finally calculated as

Reactor distributor plate is porous stainless steel.

$\text{Column\_Height} = \left[[(\text{Actual\_Number\_of\_Trays}) \cdot \text{Tray\_Spacing}] + Z_A \right]$

Column_I

Flowrate of Reactant

$\text{Column\_Height} = 11.125 m$

Mass flow rate of O-xylene,

$$M_{Oxylene} = 3.791 \times 10^4 \cdot \frac{kg}{hr}$$

Density of O-xylene

$P = 2 \quad bar \quad T_K = (330 + 273) K \quad M = 795.98 \quad \frac{kg}{kmol}$

$$\rho_{Oxylene} = \left(\frac{P \cdot M}{0.08205 \cdot T_K} \right) \cdot \frac{kg}{m^3}$$

$$\rho_{Oxylene} = 32.176 \frac{kg}{m^3}$$

Volumetric flow rate of O-xylene in m^3/hr

$$V_{Oxylene} = \frac{M_{Oxylene}}{\rho_{Oxylene}}$$

$$V_{Oxylene} = 1.178 \times 10^3 \cdot \frac{m^3}{hr}$$

Mass flow rate of Air,

$$M_{Air} = 3.791 \times 10^4 \cdot \frac{kg}{hr}$$

Density of Air,

$$P = 2 \quad bar \qquad T_K = (330 + 273)K \quad M = 777.0 \frac{kg}{kmol}$$

$$\rho_{Air} = \left(\frac{P \cdot M}{0.08205 \cdot T_K} \right) \cdot \frac{kg}{m^3}$$

$$\rho_{Air} = 31.409 \frac{kg}{m^3}$$

Volumetric flow rate of Air in m^3/hr

$$V_{Air} = \frac{M_{Air}}{\rho_{Air}}$$

$$V_{Air} = 1.207 \times 10^3 \cdot \frac{m^3}{hr}$$

Volumetric flow rate of reactant in liter/min

$$v_0 = V_{Oxylene} + V_{Air}$$

$$v_0 = 6.625 \times 10^5 \cdot \frac{cm^3}{s}$$

$$V_o = v_0$$

$$V_o = 6.625 \times 10^5 \cdot \frac{cm^3}{s}$$

Catalyst particle diameter

$d_p = 105\mu m \qquad (0.015cm)$

$\psi = 0.6$ (assumed)

$\rho_p = 2.06 \frac{g}{cm^3}$

$h_s = 38.9cm$

$-r_A = kC_{Oxylene}$

$k_{cat} = 0.0858s^{-1}$ at reaction conditions

$\rho_g = 7.85 \times 10^{-4} \frac{g}{cm^3}$

$\mu_g = 2.98 \times 10^{-4} \frac{g}{cm \cdot s}$

$D_{AB} = 0.618 \frac{cm^2}{s}$

$G = 980 \frac{cm}{s^2}$

Fluidized Bed Reactor Design Calculation

Mechanical Characteristics of Bed

Gravitation term,η

$$\eta = G \cdot (\rho_p - \rho_g)$$

$$\eta = 2.018 \times 10^3 \cdot \frac{g}{(s^2) \cdot (cm^2)}$$

Porosity of Bed at minimum fluidization.ε_{mf}

$$\varepsilon = 0.586\psi^{-0.72}\cdot\left(\frac{\mu_g^{\;2}}{\rho_g\cdot\eta\cdot d_p^{\;3}}\right)^{0.029}\cdot\left(\frac{\rho_g}{\rho_p}\right)^{0.021}$$

$$\varepsilon = 0.657$$

Gas velocity at minimum fluidization.u_{mf}

$$u_{mf} = \frac{\left(\psi\cdot d_p\right)^2}{150\cdot\mu_g}\cdot\eta\cdot\frac{\varepsilon^3}{1-\varepsilon}$$

$$u_{mf} = 1.484\cdot\frac{cm}{s}$$

Entering gas velocity u_o

$$A_c = \frac{\pi\ D_t^{\;2}}{4}$$

$$u_o = \frac{V_o}{A_c}$$

$$u_o = 6.491\times10^3\cdot\frac{cm}{s}$$

Maximum fluidization gas velocity

$$u_t = \left(\frac{1.78\cdot10^{-2}\cdot\eta^2}{\rho_g\cdot\mu_g}\right)^{\frac{1}{3}}\cdot\left(d_p\right)$$

$$u_t = 71.054\cdot\frac{cm}{s}$$

$$N_{Re} = \frac{d_p \cdot \rho_g \cdot u_{mf}}{\mu_g}$$

At u_{mf} $\quad N_{Re} = 0.041$

$$N_{Re} = \frac{d_p \cdot \rho_g \cdot u_t}{\mu_g}$$

At u_t $\quad N_{Re} = 1.965$ $\quad$ (Ok.Since $0.4 < N_{Re} < 500$)

Thus u_o is 5.4 times u_{mf} ,and well below u_t.

Bubble sizes, d_{bo},d_{bm},and d_b.

$$\kappa = 0.00376 \frac{s^2}{cm}$$

$$d_{bo} = \kappa \left(u_o - u_{mf}\right)^2$$

$$d_{bo} = 1.584 \times 10^{5} \cdot cr$$

$$\tau = 0.652 \frac{s^{0.4}}{cm^{0.2}}$$

$$d_{bm} = \tau \left[A_c \cdot \left(u_o - u_{mf}\right)\right]^{0.4}$$

$$d_{bm} = 138.898 \cdot cr$$

Since this is smaller than Column diameter, Slugging will not occur.

Bubble sizes, d_{bo},d_{bm},and d_b.

The expanded bed height will probably be 40-50% greater,say ~60cm.We therefore will assume the average bubble size will be taken as the one calculated for (h/2) =30cm.

Average bubble diameter

$$h = 30\text{cm}$$

$$d_b = d_{bm} - \left(d_{bm} - d_{bo}\right)e^{\frac{-0.3 \cdot h}{D_t}}$$

$$d_b = 7.198 \times 10^4 \cdot \text{cm}$$

Rise velocity of single bubble.

$$u_{br} = (0.71)\left(g \cdot d_b\right)^{\frac{1}{2}}$$

$$u_{br} = 5.965 \times 10^3 \cdot \frac{\text{cm}}{\text{s}}$$

Rise velocity of a bubble when many bubbles are present.

$$u_b = u_o - u_{mf} + (0.71)\left(g \cdot d_b\right)^{\frac{1}{2}}$$

$$u_b = 1.245 \times 10^4 \cdot \frac{\text{cm}}{\text{s}}$$

From (Fromet, 2003),glass spheres with d_b=0.105 mm, then $\alpha = 0.4$

Fraction of bed in bubble phase:

$$\alpha = 0.4$$

$$\delta = \frac{\left(u_o - u_{mf}\right)}{\left[u_b - u_{mf}(1 + \alpha)\right]}$$

$$\delta = 0.521$$

Bed height:

$W = 30000g$ W = Mass of catalyst in bed.

$$\left(h \cdot A_c\right) \cdot (1 - \delta) \cdot (1 - \varepsilon) \cdot \rho_p = W$$

$$h = \frac{W}{(1 - \delta) \cdot (1 - \varepsilon) \cdot A_c \cdot \rho_p}$$

$$h = 8.692 \cdot m$$

Mass Transfer and Reaction Parameters:

Bubble-Cloud mass transfer coefficient.

$$K_{bc} = 4.5\left(\frac{u_{mf}}{d_b}\right) + 5.85\left(\frac{D_{AB}^{\frac{1}{2}} \cdot g^{\frac{1}{4}}}{d_b^{\frac{5}{4}}}\right)$$

$$K_{bc} = 1.146 \times 10^{-4} \cdot s^{-1}$$

Cloud-emulsion mass transfer coefficient.

$$K_{ce} = 6.78\left(\frac{\varepsilon \cdot D_{AB} \cdot u_b}{d_b^{3}}\right)^{\frac{1}{2}}$$

$$K_{ce} = 2.497 \times 10^{-5} \cdot s^{-1}$$

Volume of Catalysts in the bubble per volume of bubble.

$$\gamma_b = 0.01 \qquad \text{(Assumed)}$$

Volume of Catalysts in Cloud and wakes/ cm^3 of bubbles.

$$\gamma_c = (1-\varepsilon)\left[\left[\left[3\frac{\left(\frac{u_{mf}}{\varepsilon}\right)}{u_b} - \left(\frac{u_{mf}}{\varepsilon}\right)\cdot\frac{s}{m}\right]\right] + \alpha\right]$$

$$\gamma_c = 0.13$$

Volume of Catalysts in emulsion/cm^3 of bubbles.

$$\gamma_e = (1-\varepsilon)\left[\frac{(1-\delta)}{\delta}\right] - \gamma_c - \gamma_b$$

$$\gamma_c = 0.175$$

Calculate K_R and X

$$K_R = \gamma_b + \cfrac{1}{\cfrac{k_{cat}}{K_{bc}} + \cfrac{1}{\cfrac{1}{\cfrac{1}{\gamma_e} + \cfrac{k_{cat}}{K_{ce}}} + \gamma_c}}$$

$$K_R = 17462 \cdot K_R$$

$K_R = 197.703$

6.3Design of Furnace

$kJ \equiv 10^3 \cdot J$

$$X = 1 - \exp\left(\frac{-K_R \cdot k_{cat} \cdot h}{u_b}\right)$$

Given below is the mass in, mass out and mass of the gas out of the furnace.

$X = 0.693874$

mass in

mass out

mass of gas out

$$\begin{pmatrix} O_2 \\ N_2 \end{pmatrix} \qquad m_{in} := \begin{pmatrix} 34.66533 \\ 114.10673 \end{pmatrix} \cdot \frac{kg}{hr} \qquad m_{out} := \begin{pmatrix} 34.66533 \\ 114.10673 \end{pmatrix} \cdot \frac{kg}{hr} \qquad m_{gout} := \begin{pmatrix} 34.66533 \\ 114.10673 \end{pmatrix} \cdot \frac{kg}{hr}$$

where

$$A = \mu_{in} \cdot e^{\left(\frac{-B}{T_{in}}\right)}$$

$$B = \frac{\ln\left(\frac{\mu_{in}}{\mu_{out}}\right)}{\left(\frac{1}{T_{in}} - \frac{1}{T_{out}}\right)}$$

μ_{new} is the corrected viscosity

μ_{in} is the inlet viscosity

μ_{out} outlet viscosity

T_{new} is the temperatre at new condition

T_{in} is the temperature at the inlet

T_{in} is the temperature at inlet

T_{out} is the temperature at outlet

In this case,

$$\mu_{in} := 0.1057 \cdot \text{poise}$$

$$\mu_{out} := 0.107 \cdot \text{poise}$$

$$T_{in} := 1500 \cdot K$$

$$T_{out} := 1100 \cdot K$$

$$B := \frac{\ln\left(\frac{\mu_{in}}{\mu_{out}}\right)}{\left(\frac{1}{T_{in}} - \frac{1}{T_{out}}\right)} \qquad B = 50.42K$$

$$A := \mu_{in} \cdot e^{\left(\frac{-B}{T_{in}}\right)} \qquad A = 0.01 \cdot \frac{kg}{m \cdot s}$$

$$T_{new} := 1200 \cdot K$$

$$\mu_{new} := A \cdot e^{\left(\frac{B}{T_{new}}\right)} \qquad \mu_{new} = 0.01 \cdot \frac{kg}{m \cdot s}$$

INTUBE PRESSURE DROP

The intube pressure drop may be calculated by any number of methods available today, but the following procedures should give sufficient results for furnace design. The pressure loss in furnace tubes and fittings is normally calculated by first converting the fittings to an equivalent length of pipe. Then the average properties for a segment of piping and fittings can be used to calculate a pressure drop per foot to apply to the overall equivalent length. This pressure drop per foot value can be improved by correcting it for inlet and outlet specific volumes.

The friction loss is given by:

$$\Delta_p = \frac{0.00517}{d_i} \cdot G_2 \cdot V_{lm} \cdot F \cdot L_{equiv}$$

where

Δ_p is the pressure drop

d_i is inside diameter of the tube

G is the mass velocity of fluid

V_{lm} is the log mean specific volume correction

F is the Fanning friction factor

L_{equiv} is the equivalent length of pipe run

The log mean specific volume correction is given by

$$V_{lm} = \frac{(V_2 - V_1)}{\ln\left(\frac{V_2}{V_1}\right)}$$

where

V_1 is the specific volume at start of run

V_2 is the specific volume at end of run

Density of Oxygen:

$$\rho_1 := 1.2875 \cdot \frac{kg}{m^3}$$

Density of Nitrogen:

$$\rho_2 := 1.1266 \cdot \frac{kg}{m^3}$$

Given that, ρ

$$V_1 := \sum \overrightarrow{\frac{m_{in}}{\rho}} \qquad V_1 = 128.21 \cdot \frac{m^3}{hr}$$

$$V_2 := \sum \overrightarrow{\frac{m_{out}}{\rho}} \qquad V_2 = 128.21 \cdot \frac{m^3}{hr}$$

$$V_{lm} := \frac{(V_2 - V_1)}{\ln\left(\frac{V_2}{V_1}\right)} \qquad V_{lm} = 0.00 m^{3.00} \cdot s^{-1.00}$$

Fanning Friction Factor:

The Moody friction factor, for a non-laminar flow, may be calculated by using the Colebrook equation relating the friction factor to the Reynolds number and relative roughness. And the Fanning friction factor is 1/4 the Moody factor. For a clean pipe or tube, the relative roughness value for an inside diameter given in inches is normally 0.0018 inch. With this, the friction factor was found to be 0.00457 (that is, $F := \frac{0.00457}{m^2 \cdot s}$).

Equivalent Length Of Return Bends:

The equivalent length of a return bend may be obtained from the following curves based on Maxwell

table and can be corrected using the Reynolds number correction factor.

$$L_{equiv} = Fact_{Nre} \cdot L_{rb}$$

where

$Fact_{Nre}$ Reynolds number correction

L_{rb} Equivalent length of return bend

If

$Fact_{Nre} := 0.11$

$L_{rb} := 2.3 \cdot m$

$L_{equiv} := Fact_{Nre} \cdot L_{rb}$

$L_{equiv} = 0.26m$

Given

$d_i := 0.153 \cdot m$

Assuming that, $G_2 := 1.034 \times 10^3 \cdot \frac{kg}{m^2 \cdot s}$, the friction is, therefore, calculated as

$$\Delta_p := \frac{0.00517}{d_i} \cdot G_2 \cdot V_{lm} \cdot F \cdot L_{equiv}$$

$$\Delta_p = 0.00s^{-1.00} \cdot \frac{N}{m^2}$$

HEAT TRANSFER COEFFICIENTS

The inside film coefficient needed for the thermal calculations may be estimated by several different methods. The API RP530, Appendix C provides the following methods,

For vapour flow with Re >= 10,000,

$$h_v = 0.021 \cdot \left(\frac{k}{d_i}\right) \cdot Re^{0.8} \cdot Pr^{0.4} \cdot \left(\frac{T_b}{T_w}\right)^{0.5}$$

where

h_v is the vapour phase heat transfer coefficient

k is the thermal conductivity

T_b is the bulk temperature of vapour

T_w is the wall temperature of the vapour

Re is the Reynolds number which is calculated as

$$Re = \frac{d_i \cdot G}{\mu_b}$$

and Pr is the Prandtl number calculated as $Pr = \frac{C_p \cdot \mu_b}{k}$

$$d_i = 0.15m$$

$$k := 3.808\times 10^{-5} \cdot \frac{kJ}{s \cdot m \cdot K}$$

$$G_2 = 1034.00 \cdot \frac{kg}{m^2 \cdot s} \qquad G := G_2$$

$$\mu_b := 5.002\times 10^{-6} \cdot \frac{kg}{m \cdot s}$$

$$C_p := 1.279 \cdot \frac{kJ}{kg \cdot K}$$

So,

$$Re := \frac{d_i \cdot G}{\mu_b} \qquad Re = 31627748.90$$

$$Pr := \frac{C_p \cdot \mu_b}{k} \qquad Pr = 0.17$$

$$T_b := 367 \cdot K$$

$$T_w := 378 \cdot K$$

$$h_v := 0.021 \cdot \left(\frac{k}{d_i}\right) \cdot Re^{0.8} \cdot Pr^{0.4} \cdot \left(\frac{T_b}{T_w}\right)^{0.5} \qquad h_v = 2.52 \cdot \frac{kJ}{s \cdot m^2 \cdot K}$$

Bare Tube Pressure Loss:

For bare tubes, the method presented by Winpress (Hydrocarbon Processing, 1963) can be used. In the method,

$$\Delta P = \frac{P_v}{2} \cdot N_r$$

where,

ΔP is the pressure drop

P_v is the velocity head of gas

N_r is the number of tube rows

The velocity head can be described as,

$$P_v = 0.0002317 \cdot \left(\frac{G_n}{1000}\right)^2 \cdot \rho_g$$

where

G_n is the mass velocity of gas

ρ_g is the density of gas

$$G_n = \frac{W_g}{A_n}$$

where

W_g is the mass gas flow

A_n is the net free area

$$A_n = A_d - \frac{d_o}{12} \cdot L_c \cdot N_t$$

$$A_d = \left(N_t \cdot \frac{P_t}{12} \right) \cdot L_c$$

A_d is the convection box area

d_o is the outside tube diameter

L_c is the tube length

P_t is the transverse pitch of tubes

N_t is the number of tubes per row

Now,

$N_t := 4$

$P_t := 0.203 \cdot m$

$L_c := 7.925 \cdot m$

$$A_d := \left(N_t \cdot \frac{P_t}{12} \right) \cdot L_c \qquad A_d = 0.54 m^{2.00}$$

Also,

$d_o := 0.114 \cdot m$

$$A_n := A_d - \frac{d_o}{12} \cdot L_c \cdot N_t \qquad A_n = 0.24 m^{2.00}$$

$$W_g := \sum m_{gout}$$

$$G_n := \frac{W_g}{A_n} \qquad G_n = 0.18 \cdot \frac{kg}{m^2 \cdot s}$$

$$\rho_g := 0.308 \cdot \frac{kg}{m^3}$$

$$P_v := \frac{0.0002317 \cdot \left(\frac{G_n}{1000}\right)^2}{\rho_g} \qquad P_v = 0.00 \cdot \frac{N}{m^2}$$

$$N_r := 4$$

$$\Delta P := \frac{P_v}{2} \cdot N_r \qquad \Delta P = 0.00 \cdot \frac{N}{m^2}$$

Fin Tube Pressure Loss:

For the fin tube pressure drop, the Escoa method will be used

$$\Delta P = \frac{\left[(f + a) \cdot G_n^2 \cdot N_r\right]}{r_b \cdot 1.083 \cdot 10^9}$$

For inline layouts,

where

ΔP is the pressure drop

ρ_b is the density of bulk gas

ρ_{out} is the density of outlet gas

ρ_{in} is the density of inlet gas

G_n is the mass gas flow

Nr is the number of tube rows

d_o is the outside tube diameter

d_f is the outside fin diameter

$$f = C_2 \cdot C_4 \cdot C_6 \cdot \left(\frac{d_f}{d_o} \right)$$

$$a = \left[\frac{(1 + B_2)}{(4 \cdot N_r)} \right] \cdot \rho_b \cdot \left[\left(\frac{1}{\rho_{out}} \right) - \left(\frac{1}{\rho_{in}} \right) \right]$$

$$B = \frac{A_n}{A_d}$$

For staggered tubes with corbels or inlune tubes.

$$A_d = \left(\frac{N_t \cdot P_t}{12} \right) \cdot L_e$$

Net Free Area, A_n:

$$A_n = A_d - A_c \cdot L_e \cdot N_t$$

A_d is the cross sectional area of box

A_c is the fin tube cross sectional area per m,

L_e is the effective tube length

N_t is the number tubes wide

and

$$A_c = \frac{(d_o + 2 \cdot l_f \cdot t_f \cdot n_f)}{12}$$

t_f is the fin thickness

n_f is the number of fins

Reynolds correction factor, C_2:

$$C_2 = 0.07 + 8 \cdot Re - 0.4$$

$$R_e = \frac{G_n \cdot d_o}{12 \cdot \mu_b}$$

μ_b is the gas dynamic viscosity

Geometry correction

C_4: For segmented fin tubes arranged in, for an inline pattern,

$$C_4 = 0.80 \cdot \left(0.15 \cdot \frac{P_t}{d_o}\right) \cdot \left[-1.1 \cdot \left(\frac{l_f}{s_f}\right)^{0.20}\right]$$

where

l_f is the fin height

s_f is the fin spacing

Non-equilateral & row correction

C6: For fin tubes arranged in, an inline pattern,

$$C_6 = 1.6 + \left[0.75 - 1.5 \cdot e^{\left(-0.70 \cdot N_r\right)}\right] \cdot e^{\left[-2.0 \left(\frac{P_l}{P_t}\right)^2\right]}$$

N_r is the number of tube rows

P_l is the longitudinal tube pitch

P_t is the transverse tube pitch

$P_l := 0.176 \cdot m$

$P_t = 0.20m$

$N_r = 4.00$

$$C_6 := 1.6 + \left[0.75 - 1.5 \cdot e^{\left(-0.70 \cdot N_r\right)}\right] \cdot e^{\left[-2.0\left(\frac{P_l}{P_t}\right)^2\right]} \qquad C_6 = 1.75$$

$l_f := 0.019 \cdot m$

$s_f := 0.0013 \cdot m$

$$C_4 := 0.80 \cdot \left(0.15 \cdot \frac{P_t}{d_o}\right) \cdot \left[1.1 \cdot \left(\frac{l_f}{s_f}\right)^{0.20}\right] \qquad C_4 = 0.40$$

$$R_e := \frac{G_n \cdot d_o}{12 \cdot \mu_b} \qquad R_e = 333.83$$

$C_2 := 0.07 + 8 \cdot Re - 0.4 \qquad C_2 = 253021990.82$

$t_f := 0.012$

$n_f := 4$

$$A_c := \frac{\left(d_o + 2 \cdot l_f \cdot t_f \cdot n_f\right)}{12} \qquad A_c = 0.01m$$

$$A_n := A_d - A_c \cdot L_e \cdot N_t \qquad A_n = 0.23m^{2.00}$$

$$A_d := \left(\frac{N_t \cdot P_t}{12}\right) \cdot L_e \qquad A_d = 0.54m^{2.00}$$

$$B := \frac{A_n}{A_d} \qquad B = 0.43$$

$$\rho_b := 0.394 \cdot \frac{kg}{m^3}$$

$$\rho_{in} := 0.327 \cdot \frac{kg}{m^3}$$

$$\rho_{out} := 0.497 \cdot \frac{kg}{m^3}$$

$$a := -\left[\frac{\left(1 + B^2\right)}{\left(4 \cdot N_r\right)}\right] \cdot \rho_b \cdot \left[\left(\frac{1}{\rho_{out}}\right) - \left(\frac{1}{\rho_{in}}\right)\right]$$

$$a = 0.03$$

$$d_f := 0.0127 \cdot m$$

$$f := C_2 \cdot C_4 \cdot C_6 \cdot \left(\frac{d_f}{d_o}\right)$$

$$f = 19785785.06$$

$$\Delta P := \frac{\left[(f + a) \cdot G_n^{\,2} \cdot N_r\right]}{\rho_b \cdot 1.083 \cdot 10^9}$$

$$\Delta P = 0.01 \cdot \frac{N}{m^2}$$

Stud Tube Pressure Loss:

For the stud tube pressure loss, the Muhlenforth method will be used. The general equation for staggered

or inline tubes is given as,

$$\Delta P = N_r \cdot 0.0514 \cdot n_s \cdot \left[\frac{\left(C_{min} - d_o - 0.8 \cdot l_s\right)}{\left[n_s \cdot \left(C_{min} - d_o - 1.2 \cdot l_s\right)^2\right]^{0.555}}\right]^{1.8} \cdot G_s \cdot \left(\frac{T_g}{1460}\right)$$

where,

ΔP is the pressure drop across tubes

N_r is the number of tube rows

C_{min} is the minimum tube space, diagonal or transverse

$d_0$outside tube diameter

l_s is the length of stud

G is the mass gass velocity

T_g is the average gas Temperature

Correction for inline tubes

$$\Delta P = \Delta P \cdot \left[\left(\frac{d_o}{C_{min}}\right)^{0.333}\right]^2$$

$$G = \frac{Wg}{(A_n \cdot 3600)}$$

$$A_n = L_e \cdot N_t \cdot \frac{\left[P_t - d_o - \frac{(l_s \cdot r_s \cdot r_s)}{12}\right]}{12}$$

where,

W_g is the mass flow of gas

A_n is the net free area of tubes

L_e is the length of tubes

N_t is the number of tubes wide

P_t is the transverse tube pitch

l_s is the length of stud

t_s is the diameter of stud

r_s is the rows of studs

$l_s := 0.0127 \cdot m$

$r_s := 4$

$t_s := 0.0127 \cdot m$

$P_t = 0.20m$

$d_o = 0.11m$

$$A_n := L_e \cdot N_t \cdot \frac{\left[P_t - d_o - \frac{(l_s \cdot t_s \cdot r_s)}{12 \cdot m}\right]}{12}$$

$$A_n = 0.23m^{2.00}$$

$$G := \frac{W_g}{(A_n \cdot 3600)}$$

$$G = 0.00 \cdot \frac{kg}{m^2 \cdot s}$$

Assuming that the tube space is $C_{min} := 50 \cdot mm$

$$\Delta P := \Delta P \cdot \left[\left(\frac{d_o}{C_{min}}\right)^{0.333}\right]^2$$

$$\Delta P = 0.01 \cdot \frac{N}{m^2}$$

PRESSURE LOSS ACROSS STACK ENTRY

This pressure loss can normally be considered as a sudden entry since the area of the outlet gas plenum in the heater is usually much greater than the area of the inlet to the transition. A sudden entry pressure loss can be approximated by the following equation.

$$\Delta P = 0.34 \cdot V_h$$

ΔP is the pressure drop

V_h is the velocity head at inlet area

PRESSURE LOSS ACROSS DAMPER

This pressure loss is normally accounted for by rule of thumb. This may be 0.5 or 0.25 velocity head. Assuming 0.25.

$$\Delta P = 0.25 \cdot V_h$$

where

ΔP is the pressure drop

V_h is the average velocity head of stack

Stack friction loss:

For the stack friction loss, we can use the following equation.

$$\Delta P = \frac{\left(0.002989 \cdot 0.018 \cdot r_g \cdot V_g^{2}\right)}{D_S \cdot L_S}$$

where

ΔP is the pressure drop

V_g is the average velocity of stack

r_g is the density of flue gas

D_S is the stack diameter

L_S is the stack length

Stack draft gain:

The draft gain will be taken based on the height, "A" on above sketch.

$$G_d = \frac{(\rho_a - \rho_g)'}{5.2} \cdot H_g$$

where

G_d is the draft gain

ρ_g is the density of flue gas

ρ_a is the density of ambient air

H_g = Height of gas path

Pressure loss across stack exit:

This pressure loss, since it normally exits to atmosphere, can be considered as a sudden exit. A sudden exit pressure loss can be approximated by the following equation.

$$\Delta P = 10 \cdot V_h$$

where

ΔP is the pressure drop

V_h is the velocity head at inlet area

Velocity head of gas:

$$V_h = V_g^2 \cdot \frac{\rho_g}{2 \cdot 32.2 \cdot 144} \cdot 27.6778$$

Now, calculating,

$$V_g := 2.365 \cdot \frac{kg}{s}$$

$$V_h := V_g^2 \cdot \frac{\rho_g}{2 \cdot 32.2 \cdot 144 \cdot \frac{kg^2}{m^2}} \cdot 27.6778 \qquad V_h = 0.01 \cdot \frac{N}{m^2}$$

$$\Delta P := 10 \cdot V_h$$

$$\Delta P = 0.05 \cdot \frac{N}{m^2}$$

$$\rho_a := 1.216 \cdot \frac{kg}{m^3}$$

$$H_g := 0.914 \cdot m$$

$$G_d := \frac{(\rho_a - \rho_g)}{5.2} \cdot H_g$$

$$G_d = 0.16 m^{-2.00} \cdot kg$$

$$D_s := 0.863 \cdot m$$

$$L_s := 6.325 \cdot m$$

$$\Delta P := \frac{\left(0.002989 \cdot 0.018 \cdot \rho_g \cdot V_g^2\right)}{D_s \cdot L_s}$$

$$\Delta P = 0.00 m^{-4.00} \cdot kg^{2.00} \cdot \frac{N}{m^2}$$

Ducting Pressure Losses

Furnace designers utilize ducting for many purposes in a fired heater design. They are used for connecting flue gas plenums to stacks, distributing combustion air to burners, transfering flue gas to and from air preheat systems, etc. The pressure losses through ducting pieces may be individually analyzed or the may be analyzed as a system.

Straight duct run friction loss:

$$\Delta P = \left(0.002989 \cdot F_r \cdot r_g \cdot V_g^2\right) \cdot \frac{L_e}{D_e}$$

where,

ΔP is the pressure drop

F_f is the Moody friction factor

r_g is the average gas density

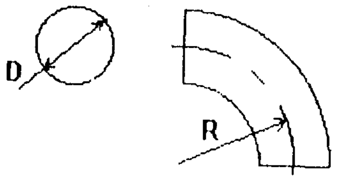
V_g is the velocity of gas

L_e is the equivalent length of piece

D_e is the equivalent diameter of piece

For round duct, D_e = diameter

90° Round section elbow loss:



$$\Delta P = V_h \cdot C_l$$

where

V_h is the velocity head of gas

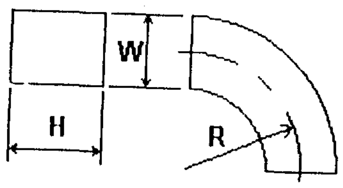
C_l is the loss coefficient

For $C_l := 0.33$

$$\Delta P := V_h \cdot C_l$$

$$\Delta P = 0.00 \cdot \frac{N}{m^2}$$

90° Rectangular section elbow loss:



$$\Delta P = V_h \cdot C_l$$

where

V_h is the velocity head of gas

C_l is the loss coefficient

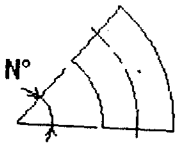
For $C_l := 0.37$

$$\Delta P := V_h \cdot C_l$$

$$\Delta P = 0.00 \cdot \frac{N}{m^2}$$

Elbow of any degree turn loss:

This may be used for a rectangular or round duct elbow of N ° turn.



$$\Delta P = V_h \cdot C_{90} \cdot \frac{N}{90}$$

where

V_h is the velocity head of gas

C_{90} is the loss coefficient from above for 90° turn

N is the number of degrees of turn

Given that,

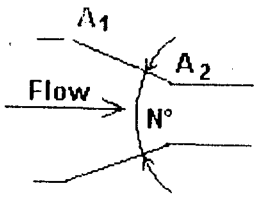
$C_{90} := 0.25$

$N' := 90$

$\Delta P := V_h \cdot C_{90} \cdot \frac{N'}{90}$

$\Delta P = 0.00 \cdot \frac{N}{m^2}$

Gradual contraction loss:



$\Delta P = V_h \cdot C_l$

where

V_h is the velocity head of gas

C_l is the loss coefficient

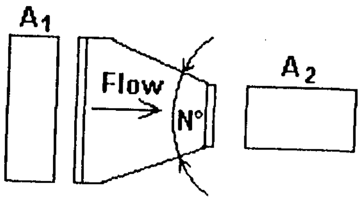
Given that,

$C_l := 0.04$

$\Delta P := V_h \cdot C_l$

$\Delta P = 0.00 \cdot \frac{N}{m^2}$

No contraction change of axis loss:



$\Delta P = V_h \cdot C_l$

where

V_h is the velocity head of gas

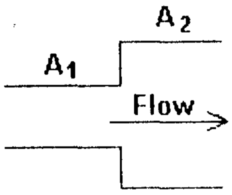
C_l is the loss coefficient

Given that,

$C_l := 0.1$

$\Delta P := V_h \cdot C_l$ $\Delta P = 0.00 \cdot \frac{N}{m^2}$

Sudden enlargement loss:



$\Delta P = V_h \cdot C_l$

where

V_h is the velocity head of gas

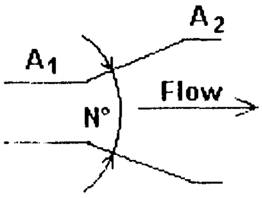
C_l is the loss coefficient

Given that,

$C_l := 0.4$

$\Delta P := V_h \cdot C_l$ $\Delta P = 0.00 \cdot \frac{N}{m^2}$

Gradual enlargement loss:



$\Delta P = V_h \cdot C_l$

where

V_h is the velocity head of gas

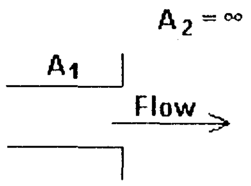
C_l is the loss coefficient

Given that,

$$C_l := 0.50$$

$$\Delta P := V_h \cdot C_l \qquad \Delta P = 0.00 \cdot \frac{N}{m^2}$$

Sudden exit loss:



$\Delta P = V_h \cdot C_l$

where

V_h is the velocity head of gas

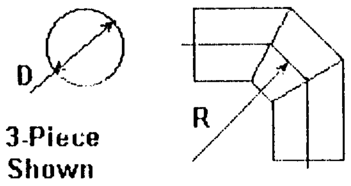
C_l is the loss coefficient

Given that,

$$C_l := 1.0$$

$$\Delta P := V_h \cdot C_l \qquad \Delta P = 0.01 \cdot \frac{N}{m^2}$$

90° Round miter elbow loss:



$\Delta P = V_h \cdot C_l$

where

V_h is the velocity head of gas

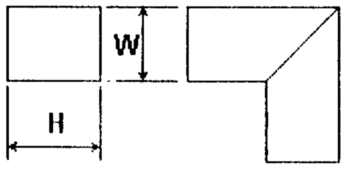
C_l is the loss coefficient

Given that,

$$C_l := 0.47$$

$\Delta P := V_h \cdot C_l$ $\qquad \Delta P = 0.00 \cdot \frac{N}{m^2}$

90° Rectangular miter elbow loss:



$\Delta P = V_h \cdot C_l$

where

V_h is the velocity head of gas

C_l is the loss coefficient

Given that,

$C_l := 1.5$

$\Delta P := V_h \cdot C_l$

$\Delta P = 0.01 \cdot \frac{N}{m^2}$

TUBE WALL TEMPERATURE CALCULATION

The temperature of the tube wall may be calculated using the following equations. This method does not take coking into account.

$$T_w = \text{Flux} \cdot \frac{d_o}{d_i} \cdot R_{fi} + \text{Flux} \cdot \frac{d_o}{d_i} \cdot \frac{1}{h_i} + \text{flux} \cdot \frac{d_o}{(d_o - t_w) \cdot \frac{t_w}{(k_w \cdot 12)}} + T_f$$

where

T_w is the tube wall temperature

Flux is the flux rateof bare tube

d_o is the outside tube diameter

d_i is the inside tube diameter

t_w is the tube wall thickness

R_{fi} is the inside fouling factor

h_i is the fluid film coefficient

k_w is the thermal conductivity of tube wall

T_f is the bulk process fluid temperature

$\text{Flux} := 1.136 \times 10^5 \cdot \frac{kJ}{hr \cdot m^2}$

$$R_{fi} := 4.892\times 10^{-5}\cdot\frac{hr\cdot m^2\cdot K}{kJ}$$

$$h_i := 1.635\times 10^4\cdot\frac{kJ}{hr\cdot m^2\cdot K}$$

$$T_{di} := 0.102\cdot m$$

$$T_{do} := 0.114\cdot m$$

$$t_w := T_{do} - T_{di}$$

$$k_w := 155.766\cdot\frac{kJ}{hr\cdot m\cdot K}$$

$$T_f := 533\cdot K$$

$$T_w := Flux\cdot\frac{d_o}{d_i}\cdot R_{fi} + Flux\cdot\frac{d_o}{d_i}\cdot\frac{1}{h_i} + Flux\cdot\frac{d_o}{\left(d_o - t_w\right)}\cdot\frac{t_w}{\left(k_w\cdot 12\right)} + T_f$$

$$T_w = 543.13K$$

The minimum volume of the furnace can be calculated with the knowledge of the mass and densityof the materials inside it. Therefore, if the densities of the components, having given the mass before as

$$m_{in} = \begin{pmatrix} 34.67 \\ 114.11 \end{pmatrix}\cdot\frac{kg}{hr}$$

The volume occupied by each material can thus be calculated as

$$Vol := \sum\overrightarrow{\frac{m_{in}}{\rho}}$$

$$Vol = 128.21\cdot\frac{m^3}{hr}$$

The minimum volume of the furnace is thus equal to

$$V_{furnace} := Vol$$

$$V_{furnace} = 128.21 \cdot \frac{m^3}{hr}$$

In order to estimate the diameter, height and area of the furnace tube, an assumption that the tube is cylindrical will be made.

If the tube of the furnace is assumed to be cylindrical, its volume is given as

$$V = \pi \cdot R^2 \cdot H$$

and, since

$$R = \frac{D}{2}$$

$$V = \pi \cdot \left(\frac{D}{2}\right)^2 \cdot h$$

$$V = \pi \cdot \frac{D^2}{4} \cdot h$$

Assming that H= kD, where k is a constant

substituting for H yields,

$$V = \pi \cdot \frac{D^2}{4} \cdot (k \cdot D)$$

$$4 \cdot V = k \cdot \pi \cdot D^3$$

Making d the subject of the formular

$$D = \left(\frac{4 \cdot V}{k \cdot \pi}\right)^{\frac{1}{3}}$$

For a standard tube, $k := 2$

$$V_{furnace} := V_{furnace} \cdot hr$$

6.4Pump Sizing

Sizing of Pump P101

$$D_{furnace} := \left(\frac{4 \cdot V_{furnace}}{k \cdot \pi}\right)^{\frac{1}{3}} \qquad D_{furnace} = 4.34m$$

From

$$H_{furnace} := k \cdot D_{furnace}$$

$$H_{furnace} = 8.68m$$

The area of the furnace is therefore,

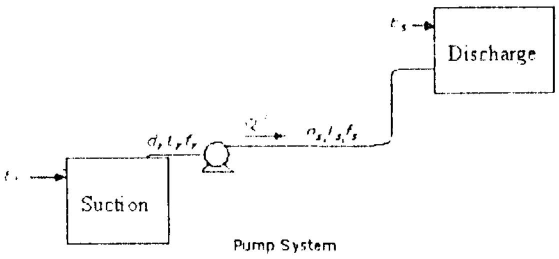
$$A_{furnace} := 2\pi \cdot \frac{D_{furnace}}{2} \cdot H_{furnace} + 2\pi \cdot \left(\frac{D_{furnace}}{2}\right)^2 \qquad A_{furnace} = 147.78m^2$$

Parameters

Mass flow rate of o-xylene to the pump:

$$F_w := 27.343\frac{kg}{hr}$$

$$F_w = 2.397\times 10^5 \cdot \frac{kg}{yr}$$



Pump System

Density of o-xylene (hyprotech, 1999):

$$\rho_{Feed} := 897\cdot\frac{kg}{m^3}$$

Volumetric flow rate of o-xylene

$$Q := \frac{F_w}{\rho_{Feed}}$$

$$Q = 0.03\frac{m^3}{hr}$$

Flowrate: $Q := 2500\frac{gal}{min}$

Fluid specific weight:: $\gamma := 84.13\frac{lbf}{ft^3}$

	Suction:	Discharge
Elevation:	$E_r := 1.5 \cdot m$	$E_s := 5 \cdot m$
Pipe diameter:	$d_r := 0.203 m$	$d_s := 0.254 m$
Pipe length:	$l_r := 5 \cdot m$	$l_s := 10 \cdot m$
Pipe friction factor:	$f_r := 0.02$	$f_s := 0.01$

Results

The solution is found by first writing the energy equation

$$\frac{V_r^2}{2 \cdot g} + \frac{P_r}{\gamma} + E_r + E_p = \frac{V_s^2}{2 \cdot g} + \frac{P_s}{\gamma} + E_s + h_L$$

Where:
V_r, V_s = velocity
P_r, P_s = pressure
E_r, E_s = elevation
= fluid density
E_p = pump energy
h_L = head loss

Now, solve this equation for pump energy

$$E_p = \left(\frac{V_s^2}{2 \cdot g} - \frac{V_r^2}{2 \cdot g}\right) + \left(\frac{p_s}{\gamma} - \frac{p_r}{\gamma}\right) + \left(E_s - E_r\right) + h_L$$

assuming that the velocity and pressure head are negligible.

$$E_p = \left(E_s - E_r\right) + h_L$$

The head loss in this equation can be found using the Darcy-Weisbach equation.

$$h_L = f\cdot\frac{L}{d}\cdot\left(\frac{Q}{\pi\cdot\frac{d^2}{4}}\right)^2\cdot\frac{1}{2\cdot g}$$

rewriting as a *function*

$$h_L(f,L,d,Q) := f\cdot\frac{L}{d}\cdot\left(\frac{Q}{\pi\cdot\frac{d^2}{4}}\right)^2\cdot\frac{1}{2\cdot g}$$

Now, by substitution of the Darcy-Weisbach equation into the energy equation the pump head is calculated as:

$$E_p := \left(E_s - E_r\right) + h_L\left(f_r, L_r, d_r, Q\right) + h_L\left(f_s, L_s, d_s, Q\right)$$

$$E_p = 4.291\cdot m$$

The horsepower required is the product of the fluid specific weight, flowrate, and pump energy.

$$HP := \gamma\cdot Q\cdot E_p$$

$$HP = 11.995\,hp$$

The hydraulic grade line is calculated by first defining a number N of points to evaluate at

Number of points: $N := 200$

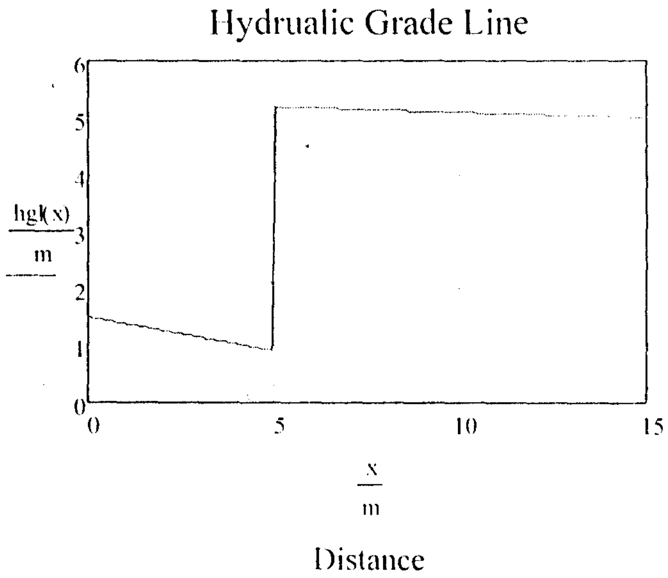
defining a *range* of distances x along the pipeline from zero to total combined length of pipe from the river to the storage reservoir

$$x := 0 \cdot L_r, \left(\frac{L_r + L_s}{N}\right) .. \left(L_r + L_s\right)$$

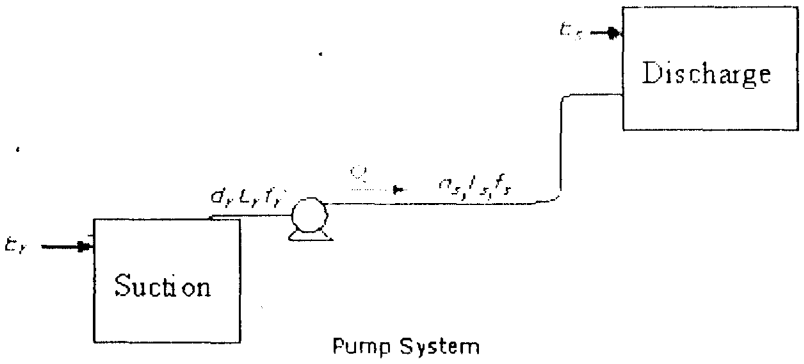
and then using an *if statement* to control calculation of the hydraulic grade line as the calculations proceed through the range of distances.

$$\mathrm{hgl}(x) := \mathrm{if}\left(x < L_r, E_r - h_L\left(f_r, x, d_r, Q\right), E_r - h_L\left(f_r, L_r, d_r, Q\right) \ldots \right.$$
$$\left. + E_p - h_L\left(f_s, x - L_r, d_s, Q\right)\right)$$

Now, the hydraulic grade line can be *graphed*.



Sizing of Pump P102



Pump System

Parameters

Mass flow rate of feed to the pump:

$$F_W := 33.325 \frac{kg}{hr}$$

Density of feed to the pump (hyprotech, 1999):

$$\rho_{Feed} := 894 \frac{kg}{m^3}$$

Volumetric flow rate of the feed to the pump

$$Q := \frac{F_W}{\rho_{Feed}}$$

$$Q = 0.037 \frac{m^3}{hr}$$

Flowrate: $$Q = 0.164 \frac{gal}{min}$$

Fluid specific weight:: $$\gamma := 62.4 \frac{lbf}{ft^3}$$

	Suction:	Discharge
Elevation:	$E_r := 0.5 \cdot m$	$E_s := 2.5 \cdot m$
Pipe diameter:	$d_r := 0.203 m$	$d_s := 0.254 m$
Pipe length:	$L_r := 6 \cdot m$	$L_s := 6 \cdot m$
Pipe friction factor:	$f_r := 0.02$	$f_s := 0.01$

Results

The solution is found by first writing the energy equation.

$$\frac{V_r^2}{2 \cdot g} + \frac{P_r}{\gamma} + E_r + E_p = \frac{V_s^2}{2 \cdot g} + \frac{P_s}{\gamma} + E_s + h_l$$

Where: V_r, V_s = velocity

P_r, P_s = pressure

E_r, E_s = elevation

= fluid density

E_p = pump energy

h_L = head loss

Now, solve this equation for pump energy

$$E_p = \left(\frac{V_s^2}{2 \cdot g} - \frac{V_r^2}{2 \cdot g} \right) + \left(\frac{P_s}{\gamma} - \frac{P_r}{\gamma} \right) + \left(E_s - E_r \right) + h_l$$

assuming that the velocity and pressure head are negligible.

$$E_p = \left(E_s - E_r \right) + h_L$$

The head loss in this equation can be found using the Darcy-Weisbach equation.

$$h_L = f \cdot \frac{L}{d} \cdot \left(\frac{Q}{\pi \cdot \frac{d^2}{4}} \right)^2 \cdot \frac{1}{2 \cdot g}$$

rewriting as a *function*

$$h_L(f, L, d, Q) := f \cdot \frac{L}{d} \cdot \left(\frac{Q}{\pi \cdot \frac{d^2}{4}} \right)^2 \cdot \frac{1}{2 \cdot g}$$

Now, by substitution of the Darcy-Weisbach equation into the energy equation the pump head is calculated as:

$$E_p := \left(E_s - E_r\right) + h_L\left(f_r, L_r, d_r, Q\right) + h_L\left(f_s, L_s, d_s, Q\right)$$

$$E_p = 2 \cdot m$$

The horsepower required is the product of the fluid specific weight, flowrate, and pump energy.

$$HP := \gamma \cdot Q \cdot E_p$$

$$HP = 2.722 \times 10^{-4} \cdot hp$$

The hydraulic grade line is calculated by first defining a number N of points to evaluate at

Number of points: $N := 20($

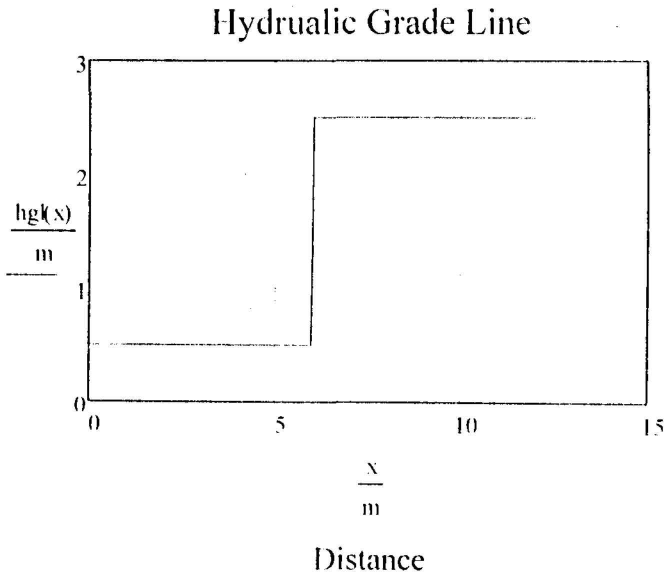
defining a *range* of distances x along the pipeline from zero to total combined length of pipe from the river to the storage reservoir

$$x := 0 \cdot L_r, \left(\frac{L_r + L_s}{N}\right) .. \left(L_r + L_s\right)$$

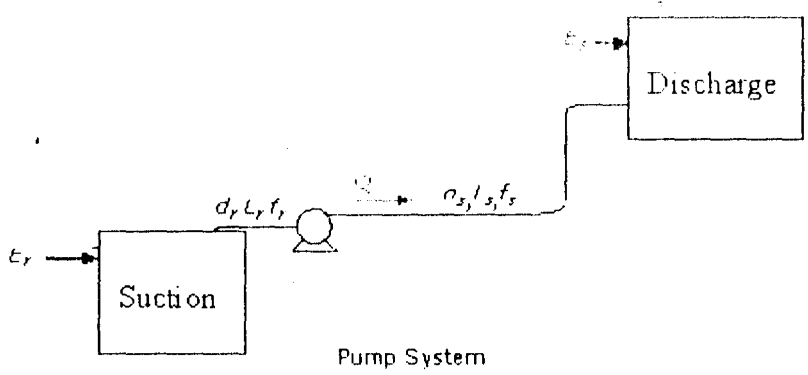
and then using an *if statement* to control calculation of the hydraulic grade line as the calculations proceed through the range of distances.

$$hgl(x) := \mathrm{if}\left(x < L_r, E_r - h_L\left(f_r, x, d_r, Q\right), E_r - h_L\left(f_r, L_r, d_r, Q\right) \ldots + E_p - h_L\left(f_s, x - L_r, d_s, Q\right)\right)$$

Now, the hydraulic grade line can be *graphed.*



Sizing of Pump P103



Parameters

Mass flow rate of feed to the pump:

$$F_w := 23.092 \frac{kg}{hr}$$

Density of Feed (hyprotech, 1999):

$$\rho_{Feed} := 923.14 \frac{kg}{m^3}$$

Volumetric flow rate of the Feed

$$Q := \frac{F_w}{\rho_{Feed}}$$

$$Q = 0.025 \frac{m^3}{hr}$$

Flowrate:

Fluid specific weight:: $\gamma := 62.4 \frac{lbf}{ft^3}$

	Suction:	Discharge
Elevation:	$E_r := 0.5 \cdot m$	$E_s := 2 \cdot m$
Pipe diameter:	$d_r := 0.203 m$	$d_s := 0.254 m$
Pipe length:	$l_r := 5 \cdot m$	$l_s := 5 \cdot m$
Pipe friction factor:	$f_r := 0.02$	$f_s := 0.01$

Results

The solution is found by first writing the energy equation from the river to the storage reservoir.

$$\frac{V_r^2}{2 \cdot g} + \frac{P_r}{\gamma} + E_r + E_p = \frac{V_s^2}{2 \cdot g} + \frac{P_s}{\gamma} + E_s + h_l$$

Where: V_r, V_S = velocity
P_r, P_S = pressure
E_r, E_S = elevation
= fluid density
E_p = pump energy
h_L = head loss

Now, solve this equation for pump energy

$$E_p = \left(\frac{V_s^2}{2 \cdot g} - \frac{V_r^2}{2 \cdot g} \right) + \left(\frac{P_s}{\gamma} - \frac{P_r}{\gamma} \right) + \left(E_s - E_r \right) + h_L$$

assuming that the velocity and pressure head are negligible.

$$E_p = \left(E_s - E_r \right) + h_L$$

The head loss in this equation can be found using the Darcy-Weisbach equation.

$$h_L = f \cdot \frac{L}{d} \cdot \left(\frac{Q}{\pi \cdot \frac{d^2}{4}} \right)^2 \cdot \frac{1}{2 \cdot g}$$

rewriting as a *function*

$$h_L(f, L, d, Q) := f \cdot \frac{L}{d} \cdot \left(\frac{Q}{\pi \cdot \frac{d^2}{4}} \right)^2 \cdot \frac{1}{2 \cdot g}$$

Now, by substitution of the Darcy-Weisbach equation into the energy equation the pump head is calculated as:

$$E_p := \left(E_s - E_r\right) + h_L\left(f_r, L_T, d_r, Q\right) + h_L\left(f_s, L_s, d_s, Q\right)$$

$$E_p = 1.5 \cdot m$$

The horsepower required is the product of the fluid specific weight, flowrate, and pump energy.

$$HP := \gamma \cdot Q \cdot E_p$$

$$HP = 1.37 \times 10^{-4} \cdot hp$$

The hydraulic grade line is calculated by first defining a number N of points to evaluate at

Number of points: $N := 20$

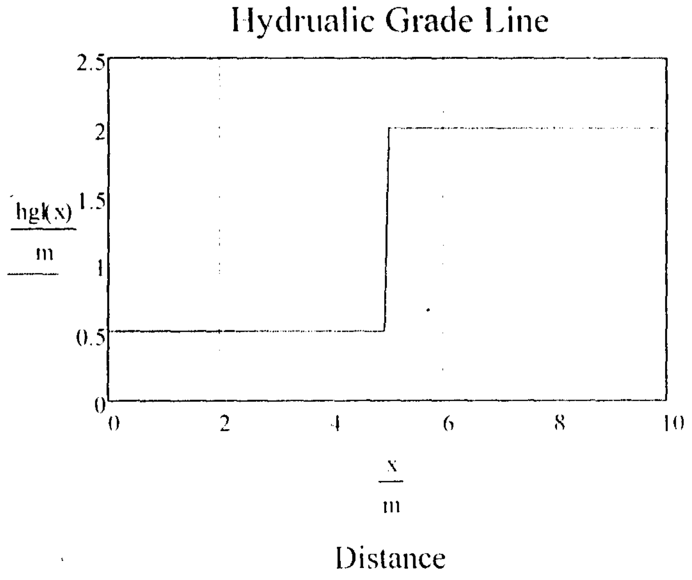
defining a *range* of distances x along the pipeline from zero to total combined length of pipe from the river to the storage reservoir

$$x := 0 \cdot L_r, \left(\frac{L_r + L_s}{N} \right) .. \left(L_r + L_s \right)$$

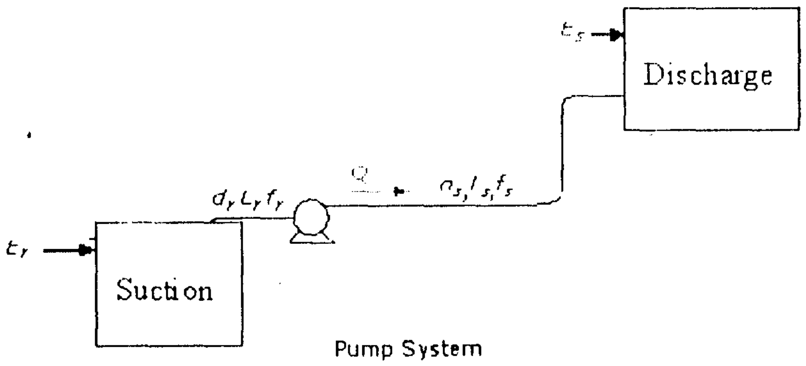
and then using an *if statement* to control calculation of the hydraulic grade line as the calculations proceed through the range of distances.

$$\mathrm{hgl}(x) := \mathrm{if}\left(x < L_r, E_r - h_L\left(f_r, x, d_r, Q\right), E_r - h_L\left(f_r, L_r, d_r, Q\right) \dots \atop + E_p - h_L\left(f_s, x - L_r, d_s, Q\right) \right)$$

Now, the hydraulic grade line can be *graphed*.



Sizing of Pump P104



Pump System

Parameters

Mass flow rate of the feed to the pump:

$$F_W := 45.535 \frac{kg}{hr}$$

Density of feed (hyprotech, 1999):

$$\rho_{Feed} := 902.567 \frac{kg}{m^3}$$

Volumetric flow rate of the feed

$$Q := \frac{F_W}{\rho_{Feed}}$$

$$Q = 0.05 \frac{m^3}{hr}$$

Flowrate: $Q = 0.222 \frac{gal}{min}$

Fluid specific weight:: $\gamma := 62.4 \frac{lbf}{ft^3}$

	Suction:	Discharge
Elevation:	$E_r := 0.8 \cdot m$	$E_s := 2.4 \cdot m$
Pipe diameter:	$d_r := 0.203 m$	$d_s := 0.254 m$
Pipe length:	$L_r := 8 \cdot m$	$L_s := 8 \cdot m$
Pipe friction factor:	$f_r := 0.02$	$f_s := 0.01$

Results

The solution is found by first writing the energy equation.

$$\frac{V_r^2}{2 \cdot g} + \frac{P_r}{\gamma} + E_r + E_p = \frac{V_s^2}{2 \cdot g} + \frac{P_s}{\gamma} + E_s + h_L$$

Where: V_r, V_s = velocity
P_r, P_s = pressure
E_r, E_s = elevation
= fluid density
E_p = pump energy
h_L = head loss

Now, solve this equation for pump energy

$$E_p = \left(\frac{V_s^2}{2 \cdot g} - \frac{V_r^2}{2 \cdot g} \right) + \left(\frac{p_s}{\gamma} - \frac{p_r}{\gamma} \right) + \left(E_s - E_r \right) + h_L$$

assuming that the velocity and pressure head are negligible.

$$E_p = \left(E_s - E_r \right) + h_L$$

The head loss in this equation can be found using the Darcy-Weisbach equation.

$$h_L = f\cdot\frac{L}{d}\cdot\left(\frac{Q}{\pi\cdot\frac{d^2}{4}}\right)^2\cdot\frac{1}{2\cdot g}$$

rewriting as a *function*

$$h_L(f,L,d,Q) := f\cdot\frac{L}{d}\cdot\left(\frac{Q}{\pi\cdot\frac{d^2}{4}}\right)^2\cdot\frac{1}{2\cdot g}$$

Now, by substitution of the Darcy-Weisbach equation into the energy equation the pump head is calculated as:

$$E_p := \left(E_s - E_r\right) + h_L\left(f_r, L_r, d_r, Q\right) + h_L\left(f_s, L_s, d_s, Q\right)$$

$$E_p = 1.6\,\mathrm{m}$$

The horsepower required is the product of the fluid specific weight, flowrate, and pump energy.

$$HP := \gamma\cdot Q\cdot E_p$$

$$HP = 2.947\times 10^{-4}\cdot \mathrm{hp}$$

The hydraulic grade line is calculated by first defining a number N of points to evaluate at

Number of points: $N := 20($

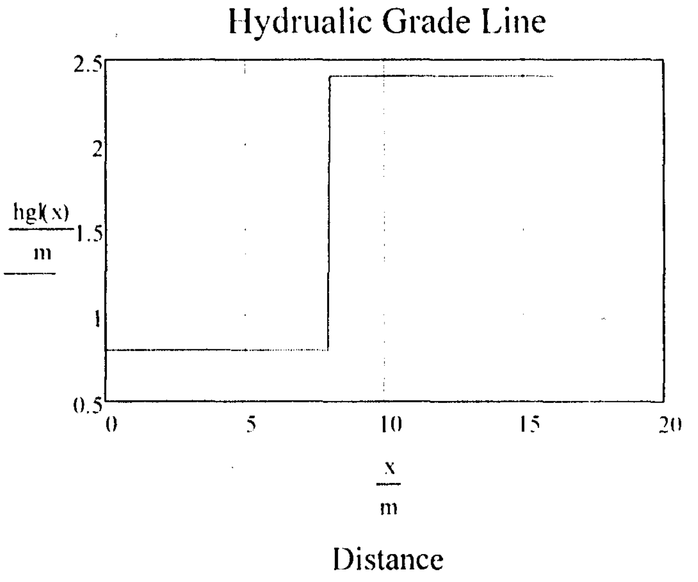
defining a *range* of distances x along the pipeline from zero to total combined length of pipe from the river to the storage reservoir

$$x := 0 \cdot L_r, \left(\frac{L_r + L_s}{N}\right) .. \left(L_r + L_s\right)$$

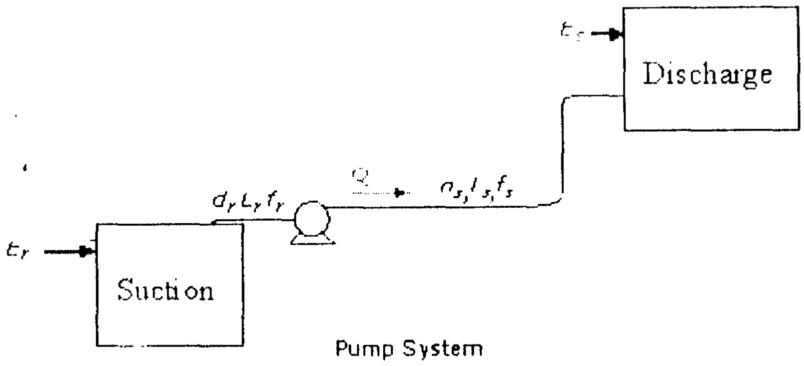
and then using an *if statement* to control calculation of the hydraulic grade line as the calculations proceed through the range of distances.

$$\text{hgl}(x) := \text{if}\left(x < L_r, E_r - h_L\left(f_r, x, d_r, Q\right), E_r - h_L\left(f_r, L_r, d_r, Q\right) \ldots \atop + E_p - h_L\left(f_s, x - L_r, d_s, Q\right)\right)$$

Now, the hydraulic grade line can be *graphed*.



Sizing of Pump P105



Pump System

Parameters

Mass flow rate of feed to the pump:

$$F_W := 0.232 \frac{kg}{hr}$$

Density of feed to the pump (hyprotech, 1999):

$$\rho_{Feed} := 882.19 \frac{kg}{m^3}$$

Volumetric flow rate of the feed to the pump

$$Q := \frac{F_W}{\rho_{Feed}}$$

$$Q = 2.63 \times 10^{-4} \cdot \frac{m^3}{hr}$$

Flowrate: $Q = 1.158 \times 10^{-3} \cdot \frac{gal}{min}$

Fluid specific weight:: $\gamma := 62.4 \frac{lbf}{ft^3}$

	Suction:	Discharge
Elevation:	$E_r := 0.5 \cdot m$	$E_s := 2 \cdot m$
Pipe diameter:	$d_r := 0.203 m$	$d_s := 0.254 m$
Pipe length:	$l_r := 5 \cdot m$	$l_s := 5 \cdot m$
Pipe friction factor:	$f_r := 0.02$	$f_s := 0.01$

Results

The solution is found by first writing the energy equation.

$$\frac{V_r^2}{2 \cdot g} + \frac{P_r}{\gamma} + E_r + E_p = \frac{V_s^2}{2 \cdot g} + \frac{P_s}{\gamma} + E_s + h_l$$

Where: V_r, V_s = velocity
P_r, P_s = pressure
E_r, E_s = elevation
= fluid density
E_p = pump energy
h_L = head loss

Now, solve this equation for pump energy

$$E_p = \left(\frac{V_s^2}{2 \cdot g} - \frac{V_r^2}{2 \cdot g} \right) + \left(\frac{p_s}{\gamma} - \frac{p_r}{\gamma} \right) + \left(E_s - E_r \right) + h_l$$

assuming that the velocity and pressure head are negligible.

$$E_p = \left(E_s - E_r \right) + h_L$$

The head loss in this equation can be found using the Darcy-Weisbach equation.

$$h_L = f \cdot \frac{L}{d} \cdot \left(\frac{Q}{\pi \cdot \frac{d^2}{4}} \right)^2 \cdot \frac{1}{2 \cdot g}$$

rewriting as a *function*

$$h_L(f, L, d, Q) := f \cdot \frac{L}{d} \cdot \left(\frac{Q}{\pi \cdot \frac{d^2}{4}} \right)^2 \cdot \frac{1}{2 \cdot g}$$

Now, by substitution of the Darcy-Weisbach equation into the energy equation the pump head is calculated as:

$$E_p := \left(E_s - E_r\right) + h_L\left(f_r, L_r, d_r, Q\right) + h_L\left(f_s, L_s, d_s, Q\right)$$

$$E_p = 1.5 \cdot m$$

The horsepower required is the product of the fluid specific weight, flowrate, and pump energy.

$$HP := \gamma \cdot Q \cdot E_p$$

$$HP = 1.44 \times 10^{-6} \cdot hp$$

The hydraulic grade line is calculated by first defining a number N of points to evaluate at

Number of points: $N := 200$

defining a *range* of distances x along the pipeline from zero to total combined length of pipe from the river to the storage reservoir

6.5 Sizing of storage tanks

$$x := 0 \cdot L_r, \left(\frac{L_r + L_s}{N}\right) .. \left(L_r + L_s\right)$$

Storage tank A: Air storage tank

Flow rate of water to the air storage tank

$$F_a := \left(148.772 \frac{kg}{hr}\right)$$

and then using an *if statement* to control calculation of the hydraulic grade line as the

Density of air in the storage tank

calculations proceed through the range of distances.

$$\rho_a := 1.234 \frac{kg}{m^3}$$

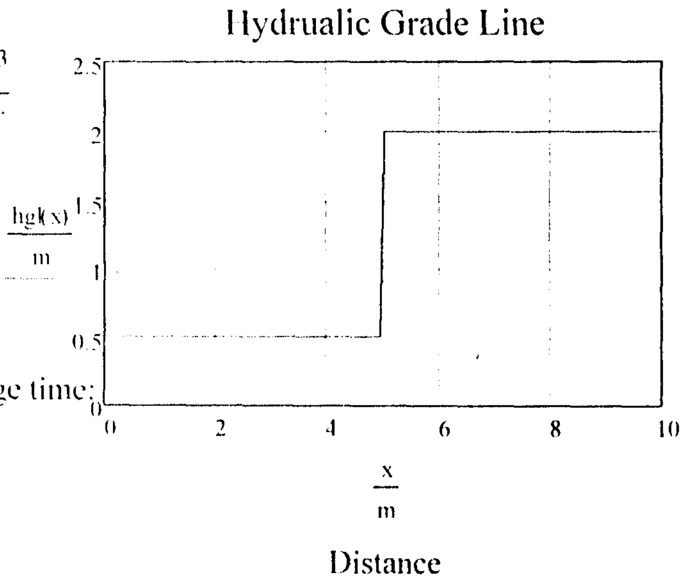
$$hgl(x) := if\left(x < L_r, E_r - h_L(f_r, x, d_r, Q), E_r - h_L(f_r, L_r, d_r, Q) \dots + E_p - h_L(f_s, x - L_r, d_s, Q)\right)$$

Volumetric flow rate of tank A

Now, the hydraulic grade line can be *graphed*.

$$V_3 := \frac{F_a}{\rho_a}$$

$$V_3 = 120.561 \frac{m^3}{hr}$$



Storage time, τ:

$$\tau := 30 \cdot day$$

$$\tau = 720 hr$$

Volume of the tank required for the storage time:

$$V := V_3 \cdot \tau$$

$$V = 8.68 \times 10^7 L$$

The optimum proportions for a cylindrical container. A classical example of the optimization of a simple function.

The surface are, A, of a closed cylinder is:

$$A = \pi \times D \times L + 2\frac{\pi}{4}D^2$$

Where D = vessel diameter

L = vessel length (or height)

This will be the objective function which is to be minimized; simplified:

$$f(D \times L) = D \times L + \frac{D^2}{2}$$

For a given volume, V, the diameter and length are related by:

$$V = \frac{\pi}{4}D^2 \times L$$

and

$$L = 4\frac{V}{\pi D^2}$$

and the objective function becomes

$$f(D) = 4\frac{V}{\pi D} + \frac{D^2}{2}$$

Setting the differential of this function zero will give the optimum value for D

$$-4\frac{V}{\pi D^2} + D = 0$$

$$D := \sqrt[3]{4\frac{V}{\ }}$$

Allowing for 30% safety allowance:

$$D = \sqrt[3]{4\frac{\frac{V}{0.7}\ 119.632}{3.142}}$$

$$V = 1.24 \times 10^8\ L$$

$$D = 54.048\mathrm{m}$$

From literature, Cerebro, 2003 ratio of tank diameter to tank height (D/H) is:

$$\mathrm{Ratio} = \frac{D}{H} = 0.8$$

$$\mathrm{Ratio} := 0.8$$

$$H := \frac{D}{\mathrm{Ratio}}$$

$$H = 65.119\mathrm{m}$$

Storage tank B: O-Xylene storage tank

Flow rate of o-xylene to the O-xylene storage tank

$$F_o := 27.34\frac{\mathrm{kg}}{\mathrm{hr}}$$

Density of O-xylene in the storage tank

$$\rho_o := 882.19\frac{\mathrm{kg}}{\mathrm{m}^3}$$

Volumetric flow rate of tank A

$$V_3 := \frac{F_o}{\rho_o}$$

$$V_3 = 0.031\frac{\mathrm{m}^3}{\mathrm{hr}}$$

Storage time, τ:

$$\tau := 30\cdot\mathrm{day}$$

$$\tau = 720\cdot\mathrm{hr}$$

Volume of the tank required for the storage time:

$$V := V_3\cdot\tau$$

$$V = 2.231 \times 10^4 L$$

Allowing for 30% safety allowance:

$$V := \frac{V}{0.7}$$

$$V = 3.188 \times 10^4 L$$

The optimum proportions for a cylindrical container. A classical example of the optimization of a simple function.

The surface are, A, of a closed cylinder is:

$$A = \pi \times D \times L + 2\frac{\pi}{4} D^2$$

Where D = vessel diameter

L = vessel length (or height)

This will be the objective function which is to be minimized; simplified:

$$f(D \times L) = D \times L + \frac{D^2}{2}$$

For a given volume, V, the diameter and length are related by:

$$V = \frac{\pi}{4} D^2 \times L$$

and

$$L = 4\frac{V}{\pi D^2}$$

and the objective function becomes

$$f(D) = 4\frac{v}{\pi D} + \frac{D^2}{2}$$

Setting the differential of this function zero will give the optimum value for D

$$-4\frac{V}{\pi D^2} + D = 0$$

$$D := \sqrt[3]{4\frac{V}{\pi}}$$

$$D = \sqrt[3]{4\frac{119.632}{3.142}}$$

$$D = 3.437\text{m}$$

From literature, Cerebro, 2003 ratio of tank diameter to tank height (D/H) is:

$$\text{Ratio} = \frac{D}{H} = 0.83$$

$$\text{Ratio} := 0.83$$

$$H := \frac{D}{\text{Ratio}}$$

$$H = 5.341\cdot 0.83$$

$$H = 4.14\text{m}$$

Storage tank C: Phthalic Anhydride Storage Tank

Flow rate of Phthalic Anhydride to the Phthalic Anhydride storage tank

$$F_p := 22.904\frac{kg}{hr}$$

Density of Phthalic Anhydride in the storage tank

$$\rho_p := 882.19\frac{kg}{m^3}$$

Volumetric flow rate of tank A

$$V_3 := \frac{F_p}{\rho_p}$$

$$V_3 = 0.026\frac{m^3}{hr}$$

Storage time, τ:

$$\tau := 5\cdot day$$

$$\tau = 120\,hr$$

Volume of the tank required for the storage time:

$$V := V_3\cdot\tau$$

$$V = 3.116\times 10^3\,L$$

Allowing for 30% safety allowance:

$$V := \frac{V}{0.7}$$

$$V = 4.451\times 10^3\,L$$

The optimum proportions for a cylindrical container. A classical example of the optimization of a simple function.

The surface are, A, of a closed cylinder is:

$$A = \pi \times D \times L + 2\frac{\pi}{4}D^2$$

Where D = vessel diameter

L = vessel length (or height)

This will be the objective function which is to be minimized: simplified:

$$f(D \times L) = D \times L + \frac{D^2}{2}$$

For a given volume, V, the diameter and length are related by:

$$V = \frac{\pi}{4}D^2 \times L$$

and

$$L = 4\frac{V}{\pi D^2}$$

and the objective function becomes

$$f(D) = 4\frac{V}{\pi D} + \frac{D^2}{2}$$

Setting the differential of this function zero will give the optimum value for D

$$-4\frac{V}{\pi D^2} + D = 0$$

$$D := \sqrt[3]{4\frac{V}{\pi}}$$

$$D = \sqrt[3]{4\frac{119.63}{3.142}}$$

$$D = 1.783\text{m}$$

From literature, Cerebro, 2003 ratio of tank diameter to tank height (D/H) is:

$$\mathrm{Ratio} = \frac{D}{H} = 0.83$$

$$\mathrm{Ratio} := 0.83$$

$$H := \frac{D}{\mathrm{Ratio}}$$

$$H = 5.341 \cdot 0.83$$

$$H = 2.148\mathrm{m}$$

CHAPTER SEVEN

7.0 REACTOR/EQUIPMENT OPTIMIZATION

In optimizing any equipment, the first step is clearly to define the objective. That is, the criterion to be used to judge the performance of the system. In engineering design, the objective of optimizing any reactor or equipment must be an economical one. This is because for any chemical plant set up, the primary objective is to maximize profits.

7.1 REACTOR OPTIMIZATION

The optimization of the reactor, which is used in the conversion of o-xylene to phthalic anhydride will be carried out in two ways.

7.1.1 OPTIMIZING THE REACTOR BY DETERMINING CONVERSIONS AT VARIOUS THERMODYNAMIC CONDITIONS

The relationship for the detemination of vapour pressures of o-xylene at various conversions is given as

$$P'''_A = P\cdot\frac{(1 - X)}{(1 + X)} \qquad \mathrm{kPa} \equiv 10^3\cdot\mathrm{Pa}$$

where P'''_A = "vapour pressure"

X = "conversions"

P = "operating pressure"

In this case, $P := 37\cdot\mathrm{kPa}$

Now, evaluating, given the conversions

$$X := \begin{pmatrix} 0 \\ 0.05 \\ 0.1 \\ 0.15 \\ 0.2 \\ 0.25 \\ 0.3 \\ 0.35 \\ 0.4 \\ 0.45 \\ 0.5 \\ 0.55 \\ 0.6 \\ 0.65 \\ 0.7 \\ 0.75 \\ 0.8 \\ 0.85 \\ 0.9 \\ 0.95 \\ 1 \end{pmatrix}$$

$$P'''_A := \overrightarrow{\left[P\cdot\frac{(1-X)}{(1+X)}\right]}$$

$P'''_A =$

	0
0	37
1	33.476
2	30.273
3	27.348
4	24.667
5	22.2
6	19.923
7	17.815
8	15.857
9	14.034
10	12.333
11	10.742
12	9.25
13	7.848
14	6.529
15	...

$\cdot kPa$

So, the relationship between the conversion and vapour pressure can be summarized as shown below

$$X\_P := \text{augment}\left(X, \frac{P'''_A}{kPa}\right)$$

$X\_P =$

	0	1
0	0	37
1	0.05	33.476
2	0.1	30.273
3	0.15	27.348
4	0.2	24.667
5	0.25	22.2
6	0.3	19.923
7	0.35	...

Furthermore, to know the relationship between the height of the reactor and the conversion as well as the vapour pressures, the procedure is shown thus.

Knowing that,

$$Z = HRU \cdot \ln\left(\frac{P_{A1} - P'''_A}{P_{A2} - P'''_A}\right)$$

and

$$P'''_A = P \cdot \frac{(1 - X)}{(1 + X)}$$

substituting the expression of P'''_A into the equation of Z, we have

$$Z = HRU \cdot \ln\left[\frac{P_{A1} - P \cdot \frac{(1 - X)}{(1 + X)}}{P_{A2} - P \cdot \frac{(1 - X)}{(1 + X)}}\right]$$

which on simplifying yields

$$Z = HRU \cdot \ln\left[\frac{(P_{A1} + P_{A1} \cdot X - P + P \cdot X)}{(P_{A2} + P_{A2} \cdot X - P + P \cdot X)}\right]$$

Having that

$P_{A1} := 37 \cdot kPa$ $\quad P_{A2} := 10 \cdot kPa$ $\quad HRU := 0.0171 \cdot m$

$X := 0.1, 0.15 .. 1$ $\quad P = 37 \cdot kPa$

$$Z(X) := HRU \cdot \ln\left[\frac{(P_{A1} + P_{A1} \cdot X - P + P \cdot X)}{(P_{A2} + P_{A2} \cdot X - P + P \cdot X)}\right]^{3.5}$$

Iterations were carried out to find the optimum height of the reactor. The outputs of the iterations are as shown below, in tabular and graphical form. It should be noted that absolute values of the height of the reactor were taken to avoid having height in the complex or negative form.

X =

0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0.55
0.6
0.65
0.7
0.75
0.8
...

$$|Z(X)| = \begin{pmatrix} 1.152 \\ 0.998 \\ 0.945 \\ 0.946 \\ 0.989 \\ 1.078 \\ 1.231 \\ 1.5 \\ 2.054 \\ 4.002 \\ 1.53 \\ 0.489 \\ 0.258 \\ 0.164 \\ 0.114 \\ 0.085 \\ 0.066 \\ 0.053 \\ 0.044 \end{pmatrix} \text{m}$$

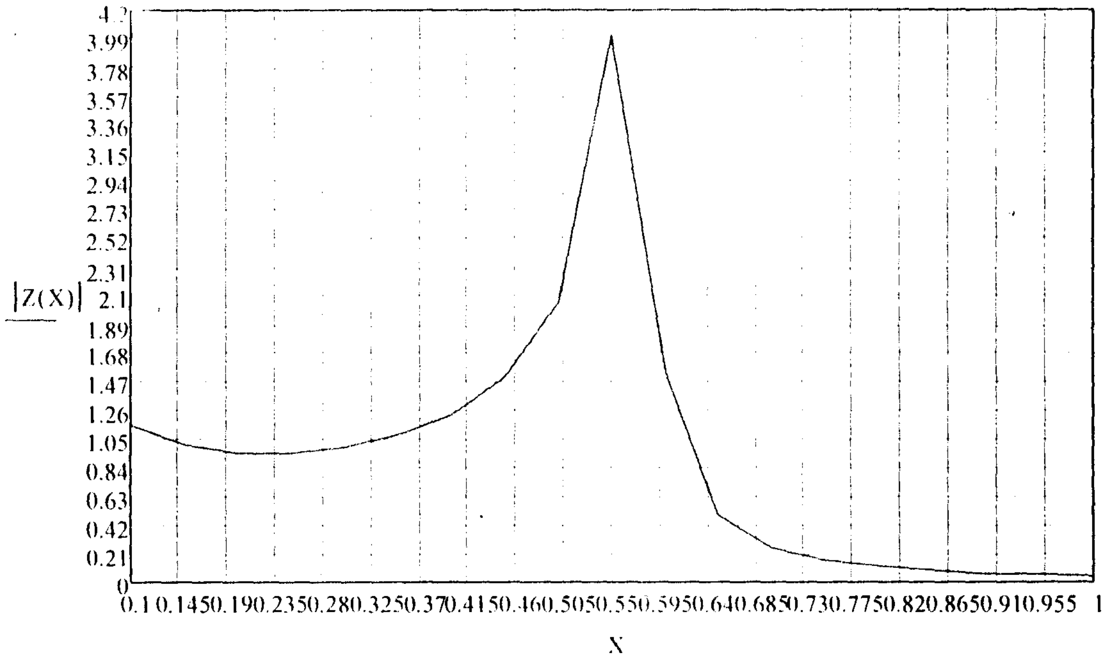


Fig. 7.1: Graph of height of reactor against conversion

7.1.2 OPTIMIZATION OF THE CONVERTER USING THE PRINCIPLE OF MINIMIZING THE LENGTH AND DIAMETER

The reactor can also be optimized using the fact that, in order to minimize cost of construction of the converter, the length and diameter of the reactor must be kept at minimum.

Since the reactor is a tubular type, it is said to have a cylindrical shape.

That is, the total surface area of the reactor is given as

$$A_r = 2\cdot\pi\cdot r^2 + 2\cdot\pi\cdot r\cdot H$$

and $r = \frac{D}{2}$

where r = "radius of the reactor tube"
D = "diameter of the reactor"
H = "height of the reactor"
π = "pie, a constant"

So, the formula becomes

$$A_r = 2\cdot\pi\cdot r^2 + 2\cdot\pi\cdot r\cdot H$$

$$A_r = 2\cdot\pi\cdot\left(\frac{D}{2}\right)^2 + 2\pi\cdot\frac{D}{2}\cdot H$$

$$A_r = 2\cdot\pi\cdot\frac{D^2}{4} + 2\cdot\pi\cdot\frac{D}{2}\cdot H$$

$$A_r = \pi\cdot\frac{D^2}{2} + \pi\cdot D\cdot H$$

One can now say that the area of the reactor is a function of the diameter and length of the reactor. That is, mathematically,

$$A_r = f(D,H)$$

where $A_r = \pi \cdot \frac{D^2}{2} + \pi \cdot D \cdot H$ is the objective function and D = minimum and H = minimum are the constraints that are to be minimized.

so that the equation of A_t becomes

$$f(D,H) = \pi \cdot \frac{D^2}{2} + \pi \cdot D \cdot H$$

Noting that the volume of the reactor is given as

$$V_r = \pi \cdot r^2 \cdot H$$

with $r = \frac{D}{2}$

$$V_r = \pi \cdot \left(\frac{D}{2}\right)^2 \cdot H$$

$$V_r = \pi \cdot \frac{D^2}{4} \cdot H$$

Making H the subject of the formula in the above equation,

$$H = \frac{4 \cdot V_r}{\pi \cdot D^2}$$

substituting the expression of H into the equation of total area of the reactor which is a function

of distance, D, and height ,H, it is obtained that

$$f(D,H) = \pi \cdot \frac{D^2}{2} + \pi \cdot D \cdot \frac{4 \cdot V_r}{\pi \cdot D^2}$$

Simplifying,

$$f(D,H) = \pi \cdot \frac{D^2}{2} + \pi \cdot \frac{4 \cdot V_r}{\pi \cdot D}$$

Now, it can be observed that the term of H has disappeared. That is to say that the total surface area is now a function of only the diameter, D. As such, the expression can be rewritten as

$$f(D) = \pi \cdot \frac{D^2}{2} + \pi \cdot \frac{4 \cdot V_r}{\pi \cdot D}$$

Since the aim here is to optimize, it may either be maximizing or minimizing. In this case, the aim is to maximize buy to minimize the dimension of the reactor so that the construct can be less, consequently, the profit can be much.

Differentiating the above equation,

$$\frac{d}{dD}f(D) = \pi \cdot D - \frac{4}{D^2} \cdot V_r$$

To optimize, the differential will be equated to zero, that is,

$$\frac{d}{dD}f(D) = \pi \cdot D - \frac{4}{D^2} \cdot V_r = 0$$

Taking the last two expressions,

$$\pi \cdot D - \frac{4}{D^2} \cdot V_r = 0$$

simplifying and making D the subject of the formula

$$\pi \cdot D = \frac{4}{D^2} \cdot V_r$$

$$D^2 \cdot D = \frac{4 \cdot V_r}{\pi}$$

$$D^3 = \frac{4 \cdot V_r}{\pi}$$

$$D = \sqrt[3]{\frac{4 \cdot V_r}{\pi}}$$

The above expression is now the optimized diameter of the reactor.

Using the relatioship between the height of the reactor and the diameter given as

$$H = \frac{4 \cdot V_r}{\pi \cdot D^2}$$

Substituting for D in this expression yields

$$H = \frac{4 \cdot V_r}{\pi \cdot \left(\sqrt[3]{\frac{4 \cdot V_r}{\pi}} \right)^2}$$

Simplifying,

$$H = \frac{V_r^{\left(\frac{1}{3}\right)}}{\pi^{\left(\frac{1}{3}\right)}} \cdot \sqrt[3]{2^2}$$

Numerically, with

$$V_r := 45m^3$$

$$D := \sqrt[3]{\frac{4 \cdot V_r}{\pi}} \qquad D = 3.855m$$

$$H := \frac{V_r^{\left(\frac{1}{3}\right)}}{\pi^{\left(\frac{1}{3}\right)}} \cdot \sqrt[3]{2^2} \qquad H = 3.855m$$

Thus, it, therefore, means that the optimum diameter and height of the reactor are the

same and have the same value of $D = 3.855m$ and $H = 3.855m$.

Taking cost as the objective function, which is always the primary objective of any set-up, the optimum dimension is almost given as $H = 2 \cdot D$

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 phthalic 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 PHTHALIC 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 phthalic 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.

MATERIAL INVENTORY

Regarding the material inventory, the followings are present:

i. Oxygen, which support combustion.

ii. Ortho-xylene

iii. phthalic

8.1.1.2 EQUIPMENT INVENTORY

In this case, the followings are present:

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

ii. Heat exchangers, which accommodate hot steam.

iii. Compressors, in which leakages of product gas which are flammable and thus become unfriendly to the environment.

iv. Phthalic column in which the separation of the maleic-phthalic mixture is separated.

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 phthalic plant designed.

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. Since o-xylene, and oxygen are in gaseous form, there is the possibility of explosion occurring.

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 combustible components like o-xylene and oxygen present in the phthalic plant to prevent fire from occurrence. In order words, the temperature of the reactor should be controlled not to exceed the flash point of the materials.

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.

Chemical splash has to do with the corrosive caustic soda, which is used in the pre-treatment of air. Its attach can be felt on the equipment, the pipelines and, even, on the skin of the personnel.

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 pthalic 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 serviçe 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.

CHAPTER NINE

9.0 PROCESS CONTROL AND INSTRUMENTATION

Instrumentation is provided to monitor the key process variables during plant operations. They may be incorporated in automatic control loops or used for manual monitoring. Critical process variables are usually fitted with automatic alarms (sinnott, 2000).

It is desirable that the process variables to be monitored be measured directly. This is often impractical and some dependent variable that is easier to measure is monitored in lieu of the desiored variable. In the control of distillation columns for instance, the continous on line analysis of the overhead product is desirable but difficult and expensive to achieve reliably. As a result of this, temperature is often monitored as an indication of composition (sinnott, 2000)

9.2 OBJECTIVES OF CONTROL

The primary objective of the designer when specifying instrumentation and control are:

Safe plant operation:

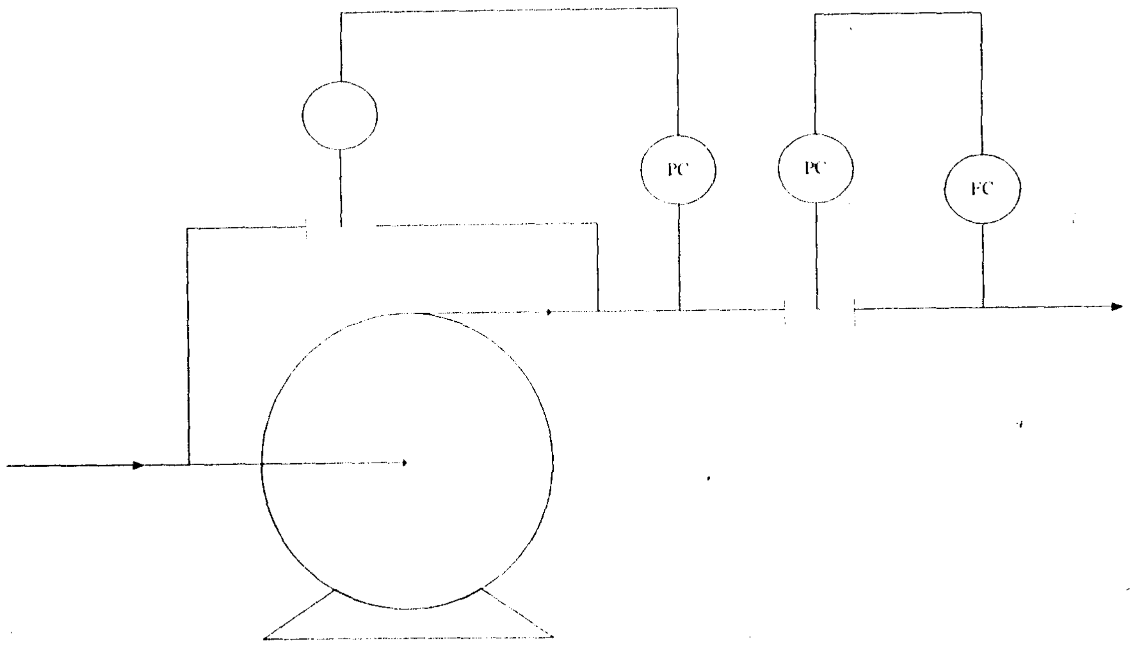
- To achieve the design product output
- To maintain the product composition within the specified quality standards.
- To operate at the lowest production cost commensurate with the other objectives.
- To optimize plant operation
- The following sections proffer a comprehensive discussion of process control with respect to the proposed p[hthalic anhydride plant.

9.3 CONTROL SYSTEMS AND LOOPS

The units are considered individually and only the crucial plant units are treated. All the loops are feed back control loops.

- **Pump / compressor control**

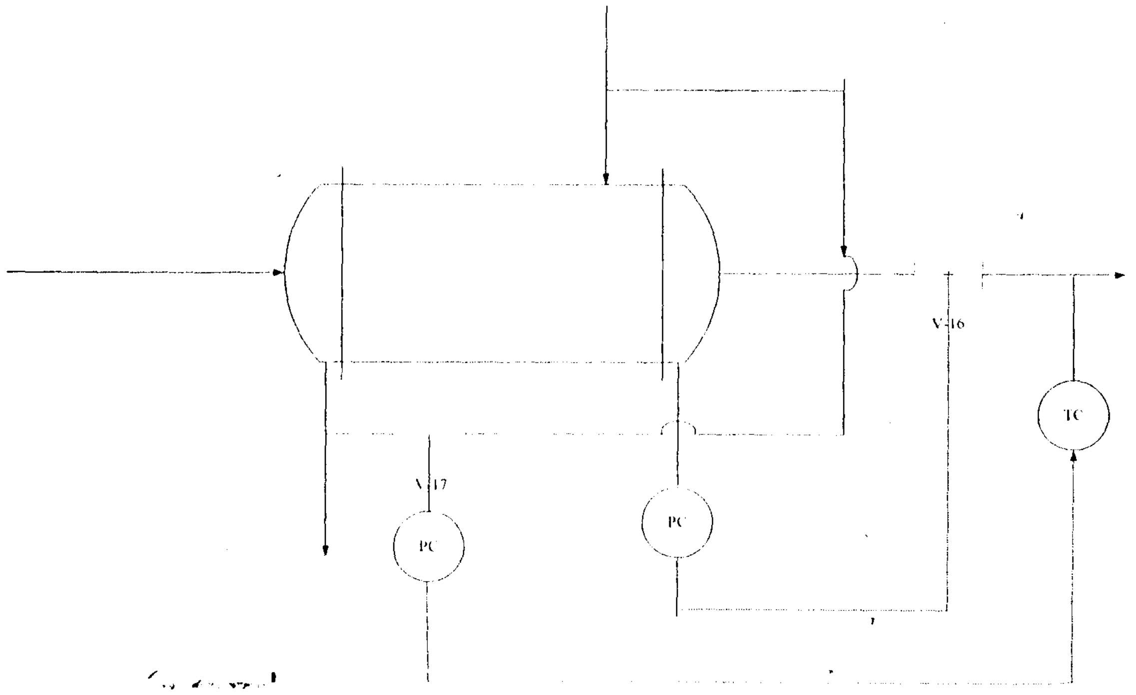
Normally a by pass control is used to provide flow control on a compressor or pump running at a fixed speed and supplying near constant volume output. The control loop is as shown below for a centrifugal compressor or pump.



The pressure controller (PC) measures the pump outlet pressure. A rise above the set point prompts the control loop to divert a portion of the flow such that at the mixing point (mixing tee), the desired pressure is achieved. The flow controller (FC) controls flow to the unit being fed by the pump.

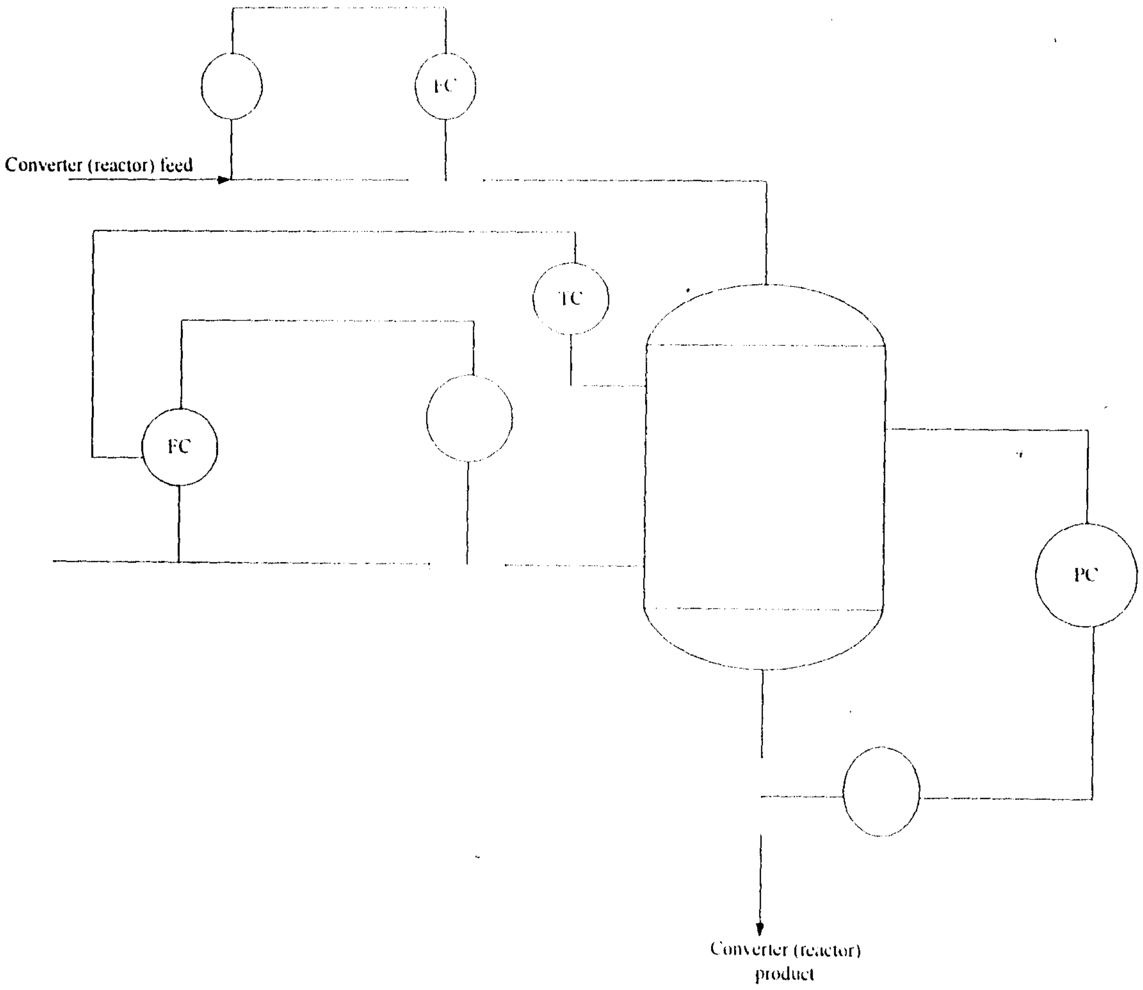
- **Heat Exchanger Controller.**

Varying the flow of the cooling of heating medium controls the temperature of the heat exchanger. The exchanger in the heat exchangers in the proposed plant is between two process streams whose flows are fixed. Hence, by pass control as shown in the fig below



- **Reactor**

The reactor feed enters the fluidized bed reactor at a reactor temperature of 380c^0 and a pressure of 4bar. In other to keep to keep the desired feed rate constant, FIC as shown directly measures the flow) of the feed mixture. Should the flow rise above the set point (desired rate), the flow feed back controller loop makes adjustment to the valve by closing it to reduce the flow rate to some magnitude in the neighbourhood of the set point valve.

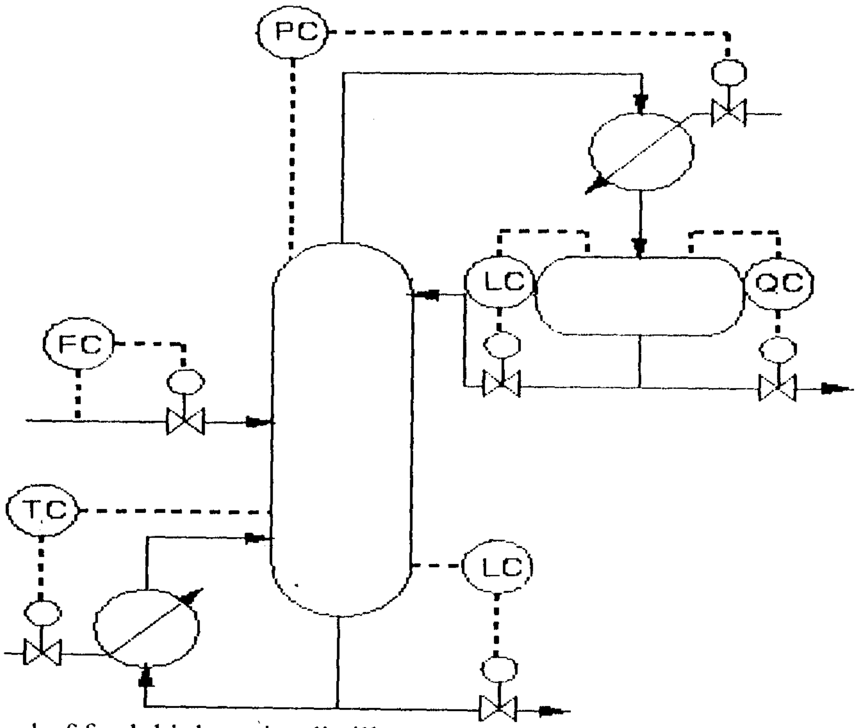


The reaction occurring in the reactor is highly exothermic. The molten salt flows counter to the flow of the flue gases.

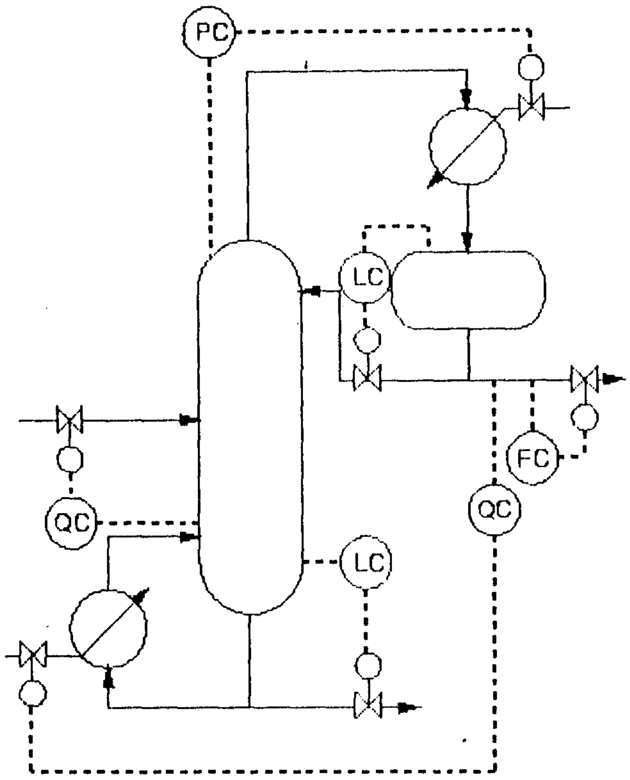
The temperature of the reactor is to be kept fixed at 380. Regulating the flow of the cooling medium however, normally control reactor temperature. Temperature controller (TC) measures the temperature of the reactor and interacts with FIC. If the reactor temperature rises above the design valve, FIC interacts with the control valve such that the flow of the flow of molten salt is increased to bring down the reactor temperature.

- **Distillation columns control**

The flow at the top of the distillation column is normally controlled by the control loop of the auxillary equipment at the top. The column in the proposed operates at vacuum pressure. The pressure controller PIC controls the column pressure by manipulating the feed rate via the control valve as below. A rise in column pressure for instance closes the valve to reduce the feed rate so that vacuum pressure is maintained.



Control of feed, high purity distillate composition, bottom



Cotrol of distillate rate, distillate composition, bottom composition.

Level controller are used to control fluid (liquid) levels in excess where two phases are in contact. LIC controls the liquid level at the bottom of the maleic column by interacting with the inlet valve of the phthalic anhydride column. A rise in bottom liquid level of maleic anhydride column opens the inlet valve to increase bottom flow rate thereby stabilizing the liquid level. This establishes a fascinating mutual interaction between the two columns.

CHAPTER TEN

10.0 Environmental Acceptability

In any plant design, safety forms an important consideration. It is vital that other chemical plant be designed in away to ensure the safest possible mode of operations. Safe operations ensure efficient operation, which is very important if the aim of designing and establishing process plant is to be achieved. Processes can be divided into those that are inherently safe and others from which the safety has been engineered in.

Inherently safe processes are those in which safe operations are embedded in the nature of the processes, the processes cause no or negligible danger all foreseeable circumstances. Clearly, the designer should always select a process that is inherently safe whenever it is practical and economic to do so. However, most chemical manufacturing processes are, to a greater or lesser extent, inherently unsafe and dangerous situations form the design values.

For a process, such as production of phthalic anhydride from the oxidation of o- xylene is risk of explosion. In such cases safety is "engineered in" the plant design. Engineered safety covers the provision in the design of control systems, alarms, trips, pressure relieve devices, automatic shut-down systems, duplication of key equipment services and fire fighting equipments, sprinkler systems and blast walls, to contain any fire or explosion.

In general, in design of a chemical process plant, the following are considered:

- Substitution: the processing route may be replaced with one using less hazardous material with non-toxic materials.
- Containment; in plant design, there must be the sound design of equipment and piping to avoid leaks. Also, the proper specification of equipment must be made.
- Ventilation: there must be provision of adequate ventilation system, use of open structure allows for goods ventilation.
- Disposal: the design should make provision of effective vent stacks to disperse materials vented scrubbers from pressure relief devices, or use vent scrubbers.
- Emergency equipment: the plant design must include escape routes, rescue equipment, respirators, safety showers and eye baths.

Along with adequate safety devices and measures, in addition, there should be good plant operating practice, which include:

- Proper maintenance of all plant equipment
- Adequate training of all plant personnel
- Proper labelling and written instrumentation in the handling, use and storage of the hazardous substances and the risks involved.
- Provision of protective clothing.
- Good housekeeping and personal hygiene.
- Regular medical check-ups on employees.
- Monitoring of the levels of emissios in the environments to check exposure levels.

10.1 ENVIRONMENTAL CONSIDERATION

All individuals and companies have a duty of care to their neighbours, and to the environment in general.

Vigilance is required in both the design and operation of process plant to ensure that legal standards are met and that harm is done to the environment.

- **Gaseous wastes**

Gaseous waste effluents, which contain toxic or noxious substances, will need treatment before discharge into the atmosphere. The practice of relying on dispersion from tall stacks is seldom entirely satisfactory. Gaseous pollutant can be removed by absorption or adsorption. Finely dispersed solids can be removed by scrubbing; using electrostatic precipitators while flammable gases can be burnt.

- **Noise**

Noise can cause a serious nuisance in the neighbourhood of a process plant. Apart from the main equipment, excessive noise can also be produced when venting through steam and other relief valves and from flare stacks. Such equipment should be fitted with silencers. Vendor's specification should be checked to ensure that equipment complies with statuary noise levels. Noisy equipment should, as far as practicable, be sited well away from the site boundary.

- **Visual impact**

Few people object to the fairyland appearance of a process plant illuminated at night, but it is different scene in daylight. Actually, there is little that can be done to change the appearance of a modern style plant, where most of the equipment and piping will be outside and in full view, but some steps can be taken to minimise the visual impact. Large equipment, such as storage tanks can be painted to blend in with or even contrast with the surroundings. Landscaping and screening by belts of trees can also help improve the overall appearance of the site.

- **Emissions and controls**

Emissions from o-xylene storages are small and do not require control. The

Major contributor of emissions is the reactor and condenser effluent, which is vented from the condenser unit. Particulate matter and carbon dioxide make up half the emissions from the reactor. The most efficient (96%) system of controls is the combined usage of a water scrubber and thermal incinerator. A thermal incinerator alone is approximately 80% efficient in combustion of the pollutants.

Scrubbers have 99% efficiency in collecting particulate, but are partially ineffective in reducing carbon monoxide emissions. Cyclone can be used to control catalyst dust emissions with 90- 98% efficiency pre-treatment and distillation emissions particulates and hydrocarbons are normally processed through the water scrubber and / or incinerator used for the main processed stream,(reactor and condenser) or scrubbers alone, with the same efficiency percentages applying.

Product storage in the phase results in small amount of gaseous emissions. These gas streams can either be sent to the main process vent gas control devices or first processed through sublimation boxes or devices used to recover PAN. Flaking and bagging emissions are negligible, but can be sent to a cyclone for recovery of PAN dust. Exhaust from the cyclone present presents no problem.

CHAPTER ELEVEN

11.0 START UP AND SHUT DOWN PROCEDURE

Start up time may be defined as the time span between end of construction and the beginning of normal operations. Start up and shut down procedure must proceed safely and be flexible enough to be carried out in various ways. In other words, the start up and shut down of the phthalic plant should be such that it can be easily and safely operated. The operating limits of the plant should not be exceeded and dangerous mixtures must not be formed as a result of abnormal states of concentration, composition, temperature, phase, pressure, reactants and products.

It should be noted that some items of actions must be completed before even the start up of the plant in order to prepare the plant for the start up operation.

i. All scaffolds and temporary piping and supports should be removed.
ii. Lines and equipment should be flushed out.
iii. Pumps, motors/turbines and compressors should be run.
iv. Hydrostatic or pneumatic lines and equipment should be tested.
v. Laboratory and sampling schedule should be prepared.
vi. All instruments should be inspected and tested.

11.1 START UP PROCEDURES

For the phthalic plant designed, the following are the start up procedures:

i. The reactor should be heated up and maintained at their operating temperatures and pressures.
ii. The inlet and outlet valves of the reactors should be opened up.
iii. The compressor valve to supply air at a regulated pressure should be opened.
iv. All the inlet and outlet valves to the reactor should be shut as soon as the feed enters the reactor in order to achieve maximum conversion.
v. The outlet value of the reactor should be opened for the evacuation of the reactor contents.

vi. The outlet valve of the reactor should be locked before opening the inlet valve before further entering of the feed into the reactor.

11.2 SHUT DOWN PROCEDURES

The shut down procedures for the phthalic plant are as outlined below

i. The supply of the o- xylene to the vapourizer should be cut off.

ii. The air supply into the converter should also be cut off.

iii. All the purge valves should be opened to discharge unconverted reactants

11.2.1 EMERGENCY SHUT DOWN OF PLANT

Emergency shut down of plant is deemed necessary if there is abnormality, which might result in costly top (unwanted) event. This may be due to breakdown of any major equipment that is not easily replaceable. For example, if the o- xylene superheater has major problem or breakdown completely, there is no other option than to shut down thephthalic plant. Insufficient utility services may also necessitate emergency shut down of plant.

When there is emergency, the process trip system is designed to affect the emergency shut down of plant. Unit shut down is preferable; it would not affect production and quality because of the cost involved in starting up the whole unit.

A trip system carries out the appropriate activity on command from automatic actuation of the relay or other means. Such systems are closely associated to the shut down of plant when some units are operating on abnormal manner. The shut down can be designed to subdivide the plant into different segments. These segments include: operating utilities, pressure level, or volume of flammable material. Thus, it would be possible to reduce the volume of fluid that would be spilled in the event of pipe rupture.

This system must be reliable and respond only when required, so as to avoid unnecessary shut down of plant and also when necessary they must not fail. The trip setting should be designed to incorporate safety.

11.2.2 START UP AFTER EMERGENCY SHUT DOWN

When the trip system is being designed, each start up must be undertaken with care. It is necessary to consider what happens when the trip system occurs and when the trip system condition is removed. The necessary actions are planned for all those cases, which cannot be foreseen.

In addition, during the start up after emergency shut down,

i. Undesirable or toxic materials under pressure should be removed during the start up.

ii. Non-conforming specification process materials should be recycled.

iii. Air and undesirable materials or chemicals used for cleaning system should be removed.

iv. The controls and set points should be checked and adjusted.

v. It should be ensured that everything is in good order before the start up.

CHAPTER TWELVE

12.0 SITE FOR PLANT LOCATION

The location of the phthalic plant can have a crucial effect on the profitability of the phthalic 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 phthalic. 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.For a material produced in bulk quantities such as the formaldehyde 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.

- **RAW MATERIALS**

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

- **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 to 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.

- **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.

- **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 auxillary services needed in the operation of any production process. These services will normally be supplied from a central facility; and will include:

a. **Steam for process heating:** - The steams required for the process are generated in the Tube boilers using most economic fuel.
b. **Cooling water:** - Natural and forced draft cooling towers are generally used to provide the cooling water required on site.
c. **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.
d. **Effluent disposal facilities:** - facilities must be provided for the effective disposal of the effluent without any public nuisance.

12.2 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.

12.3 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.

12.4 AVAILABILITY OF SUITABLE LAND (SITE CONSIDERATIONS)

Sufficient suitable land is 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.

12.5 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.

12.6 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.

12.7 AVAILABILITY OF RAW MATERIALS

The major raw material in the production of phthalic is the o-xylene and air. Looking at it very well, the major source of this major raw material, phathalic is the petrochemical industries such as the refineries. In addition, considering the situations in the country, Nigeria, today, it is obvious the refineries functioning well are in the area of River State. So, siting the phthalic plant in the suburb of Eleme in Port Harcourt is siting the plant close the source of the raw material.

12.8 TRANSPORT

Regarding the transport facilities, Eleme is close to seaport and a waterway. Besides, it is close to a major airport (that is, Port Harcourt 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. Another advantage is that Eleme has good road network.

$$C_2 = C_1 \times \left(\frac{S_2}{S_1} \right)^n \qquad \text{(Sinnot, 2005)}$$

where

C_1 = "capital cost of the project with capacity"

C_2 = "capital cost of the project with capacity"

n = "index number"

CHAPTER THIRTEEN

Economic Analysis

In carrying the cost analysis calculations, the cost of an existing zeolite plant was obtained; the capacity of this existing plant was compared with the capacity of this design project in order to scale the cost of the existing plant down to meet the capacity of this design work.

The cost of the plant to be constructed by Borden Chemical in Edmonton, Alberta was obtained on the internet in the news issued by the company announcing to the world about the construction of the new plant.

From the simulation carried by Edingar in SuperPro, it was discovered that the cost of the new plant to be constructed is $90,000,000 and the capacity of this plant is 1 million pounds per annum

In other words, to proceed with the cost analysis of this design project, the basis parameter is the cost of plant of $90,000,000 with the capacity of 1 million pounds per annum.

It should be noted that this cost is the current cost, as such, there is no need looking for any cost index in order to scale up the cost to the current year. This is because the cost given by Edingar (Edingar, 2007) is the cost of the plant in the year 2007, which is the present year.

CALCULATION OF FIXED CAPITAL INVESTMENT

The fixed capital investment of this design project will be estimated from the capital investment of the plant constructed by Borden Chemical this year.

Now, denoting the fixed capital investment of the Borden plant by C_1, and the fixed capital investment of this design project by C_2 also the capacity of the capacity of the Borden plant by S_1 and the capacity of this design work by S_2, we have that,

$$C_2 = C_1 \times \left(\frac{S_2}{S_1}\right)^n \quad \text{(Sinnot, 2005)}$$

$$\text{attainment} \equiv 92\%$$

$$\text{annum} \equiv \text{attainment} \times 365 \times \text{day}$$

$$\text{annum} = 336 \times \text{day}$$

Conversion Factor (CF): $CF = 128$

where

C_1 = "capital cost of the Borden Chemical project"

C_2 = "capital cost of the this project "

n = "index number"

S_1 = "capacity of Borden Chemical project"

S_1 = "capacity of this project"

Now,

$C_1 = 20 \times 10^6 \times CF \times \text{Naira}$

$n = 0.6$

$$S_1 = 1 \times 10^6 \times \frac{\text{lb}}{\text{annum}}$$

$$S_1 = 56.283 \frac{\text{kg}}{\text{m}^3} \times \frac{\text{m}^3}{\text{hr}}$$

$$V = 400000 \times \frac{\text{lb}}{\text{annum}}$$

$$V = 181.437 \times \frac{\text{tonne}}{\text{annum}}$$

$S_2 = V$ $\qquad$ $S_2 = 4 \times 10^5 \times \dfrac{\text{lb}}{\text{annum}}$

$$C_2 = C_1 \times \left(\frac{S_2}{S_1}\right)^n$$

becomes

$$C_2 = 90\times 10^6 \times \left(\frac{2.107\times 10^7}{20\times 10^6} \right)^{0.6}$$

$$C_2 = 1.477\times 10^9 \times \text{Naira}$$

So, the fixed capital investment (FCI) for the production of 25 L/day of Bio-ethaol Plant from Jatropha Oil is equal to

$$C_2 = 1.477\times 10^9 \times \text{Naira}$$

Now, making

$$FCI = C_2$$

$$FCI = 1.477\times 10^9 \times \text{Naira}$$

CALCULATON OF TOTAL INVESTMENT COST

DIRECT COST

PURCHASED EQUIPMENT COST (PEC)

The purchased equipment cost (PEC) was found to be 15-40% of the fixed capital investment (FCI). Now, taking the purchased equipment cost (PEC) to be 17% of fixed capital investment (FCI), then

$$PEC = 17\% \times FCI$$

$$PEC = \frac{17}{100} \times 1.254\times 10^{10}$$

$$PEC = 2.511\times 10^8 \times \text{Naira}$$

INSTALLATION COST

The installation cost (IC) was found to be 35-45% of the purchased equipment cost (PEC). Now, taking the installation cost (IC) to be 37% of the purchased equipment cost (PEC), then

$$IC = 37\% \times PEC$$

$$IC = \frac{37}{100} \times 2.131 \times 10^9$$

$$IC = 9.292 \times 10^7 \times \text{Naira}$$

INSTRUMENTATION AND CONTROL INSTALLATION COST

The instrumentation and control installation cost was found to be 6-30% of the purchased equipment cost (PEC). Now taking the instrumentation and control installation cost (IC) to be 15% of purchased equipment cost (PEC), then

$$ICIC = 15\% \times PEC$$

$$ICIC = \frac{15}{100} \times 2.131 \times 10^9$$

$$ICIC = 3.767 \times 10^7 \times \text{Naira}$$

PIPING INSTALLATION COST

The piping installation cost (PIC) was found to be 10-80% of the purchased equipment cost (PEC). Now taking the piping installation cost (IC) to be 18% of purchased equipment cost (PEC), then

$$PIC = 18\% \times PEC$$

PIC = $4.521 \times 10^7 \times$ Naira

ELECTRICAL INSTALLATION COST

The electrical installation cost (EIC) was found to be 10-40% of the purchased equipment cost (PEC). Now taking the electrical installation cost (IC) to be 15% of purchased equipment cost (PEC), then

EIC = $15\% \times$ PEC

EIC = $3.767 \times 10^7 \times$ Naira

BUILDING PROCESS AND AUXILLIARY COST

The building process and auxilliary cost (BPAC) was found to be 10-70% of the purchased equipment cost (PEC). Now taking the building process and auxilliary cost (BPAC) to be 11% of purchased equipment cost (PEC), then

BPAC = $11\% \times$ PEC

BPAC = $2.763 \times 10^7 \times$ Naira

SERVICE FACILITIES COST

The service facilities cost (SFC) was found to be 30-80% of the purchased equipment cost (PEC). Now taking the service facilities cost (SFC) to be 31% of purchased equipment cost (PEC), then

SFC = $31\% \times$ PEC

SFC = $7.786 \times 10^7 \times$ Naira

YARD IMPROVEMENT COST

The yard improvement cost (YIC) was found to be 10-50% of the purchased equipment cost (PEC). Now taking the yard improvement cost (YIC) to be 15% of purchased equipment cost (PEC), then

$$YIC = 15\% \times PEC$$

$$YIC = 3.767 \times 10^7 \times \text{Naira}$$

COST OF LAND

The cost of land (LC) was found to be 4-8% of the purchased equipment cost (PEC). Now, taking the cost of land (LC) to be 5% of the purchased equipment cost (PEC), then

$$LC = 5\% \times PEC$$

$$LC = 1.256 \times 10^7 \times \text{Naira}$$

All the costs calculated so far are referred to as the direct costs. So, the total direct cost can be computed as the sum of all the various costs above. That is, denoting total direct cost by TDC,

$$TDC = PEC + IC + ICIC + PIC + EIC + BPAC + SFC + YIC + LC$$

$$TDC = 6.203 \times 10^8 \times \text{Naira}$$

INDIRECT COSTS

The indirect costs, which are the costs that are neither directly involved in the material and labour of actual installation nor in the complete facility. They include the costs calculated below.

ENGINEERING AND SUPERVISION COST

The engineering and supervision cost (ESC) was found to be 5-30% of the total direct cost (TDC). Now, taking the engineering and supervision cost (ESC) to be 15% of the total direct cost (TDC), then

ESC = 6% × TDC

ESC = 3.722×10^7 × Naira

CONSTRUCTION EXPENSES

The construction expenses (CE) were found to be 10% of the total direct cost (TDC). Now, this means that the construction expenses (CE) is 10% of the total direct cost (TDC), then

CE = 10% × TDC

CE = 6.203×10^7 × Naira

CONTRACTORS' FEE

The contractors' fee (CF) was found to be 2-7% of the total direct cost (TDC). Now taking the contractors' fee (CF) to be 3.5% of the total direct cost (TDC), then

CF = 3.5% × TDC

CF = 2.171×10^7 × Naira

CONTINGENCY FEE

The contingency fee (COF) was found to be 8-20% of the total direct cost (TDC). Now, taking the contingency fee (COF) to be 11% of the total direct cost (TDC), then

$$COF = 11\% \times TDC$$

$$COF = \frac{11}{100} \times 5.264 \times 10^9$$

$$COF = 6.824 \times 10^7 \times \text{Naira}$$

All the costs after the direct costs are known to be part of the indirect costs. The total indirect costs is thus given as

$$TIC = ESC + CE + CF + COF$$

$$TIC = 1.892 \times 10^8 \times \text{Naira}$$

FIXED CAPITAL INVESTMENT

Fixed capital investment is given as the sum of the direct and indirect costs. That is, denoting the fixed capital investment by FCI,

$$FCI = TDC + TIC$$

$$FCI = 8.095 \times 10^8 \times \text{Naira}$$

WORKING CAPITAL INVESTMENT

The working capital investment cost (WCIC) was found to be 10-20% of the fixed capital investment (FCI). Now taking the working capital investment cost (WCIC) is 11% of the fixed capital investment (FCI), then

$\text{WCIC} = 11\% \times \text{FCI}$

$\text{WCIC} = 8.905 \times 10^7 \times \text{Naira}$

TOTAL CAPITAL INVESTMENT

The total capital investment is given as the sum the fixed capital and working capital investments. That is, denoting the total capital investment by TCI

$\text{TCI} = \text{FCI} + \text{WCIC}$

$\text{TCI} = 8.986 \times 10^8 \times \text{Naira}$

ESTIMATION OF TOTAL PRODUCTION COST (TPC)

FIXED CHARGES

DEPRECIATION

The depreciation (Dep) was found to be 10% of the fixed capital investment (FCI). Now, making the depreciation (Dep) to be 10% of the fixed capital investment (FCI), then,

$\text{Dep} = 10\% \times \text{FCI}$

$\text{Dep} = 8.095 \times 10^7 \times \text{Naira}$

LOCAL TAXES

The local taxes (LT) was found to be 1-2% of the fixed capital investment (FCI). Now taking the local taxes (LT) to be 1.5% of the fixed capital investment (FCI), then

$\text{LT} = 1.5\% \times \text{FCI}$

$LT = 1.214\times 10^{7} \times \text{Naira}$

INSURANCE

The insurance (Ins) was found to be 0.4-1% of the fixed capital investment (FCI). Now, taking the insurance (Ins) is 0.7% of the fixed capital investment (FCI), then

$Ins = 0.7\% \times FCI$

$Ins = 5.667\times 10^{6} \times \text{Naira}$

RENT

The rent (Rent) was found to be 8-12% of the fixed capital investment (FCI). Now,

taking the rent (Rent) to be 9% of the fixed capital investment (FCI), then

$Rent = 9\% \times FCI$

$Rent = 7.286\times 10^{7} \times \text{Naira}$

Therefore, the total production costs which is the sum of the depreciation, local taxes, insurances and rent is equl to

$TPC = Dep + LT + Ins + Ren$

$TPC = 1.716\times 10^{8} \times \text{Naira}$

DIRECT PRODUCTION COSTS

RAW MATERIAL

The cost of raw material (RMC) was found to be 10-50% of the total production cost (TPC). Now,taking the cost of raw material (RMC) is 15% of the total production cost (TPC), then

$RMC = 15\% \times TPC$

$RMC = 2.574 \times 10^7 \times$ Naira

OPERATING LABOUR

The cost of operating labour (OLC) was found to be 10-20% of the total production cost (TPC). Now, taking the cost of operating labour (OLC) to be 13% of the total production cost (TPC), then

$OLC = 13\% \times TPC$

$OLC = 2.231 \times 10^7 \times$ Naira

DIRECT SUPERVISORY AND ELECTRIC LABOUR COST

The direct supervisory and electric labour cost (DSELC) was found to be 10-25% of the operating labour cost (OLC). Now, taking the direct supervisory and electric labour cost (DSELC) is 13% of the operating labour cost (OLC), then

$DSELC = 13\% \times OLC$

$DSELC = 2.9 \times 10^6 \times$ Naira

COST OF UTILITIES

The cost of utilities (UC) was found to be 10-20% of the total production cost (TPC). Now, taking the cost of utilities (UC) is 13% of the total production cost (TPC), then

$UC = 13\% \times TPC$

$UC = 2.231 \times 10^7 \times$ Naira

MAINTENANCE COST

The maintenance cost (MC) was found to be 2-10% of the fixed capital investment (FCI). Now, taking the maintenance (MC) to be 5% of the fixed capital investment (FCI), then

$MC = 5\% \times FCI$

$MC = 4.048 \times 10^7 \times$ Naira

OPERATING SUPPLIES COST

The operating supply cost (OSC) is found to be 10-20% of the maintenance cost (MC). Now, taking the operating supply cost (OSC) to be 11% of the maintenance cost (MC), then

$OSC = 11\% \times MC$

$OSC = 4.452 \times 10^6 \times$ Naira

LABORATORY CHARGES

The laboratory charges (LabC) was found to be 10-20% of the operating labour cost (OLC). Now, assuming that the laboratory charges (LabC) is 13% of the operating labour cost (OLC), then

$LabC = 13\% \times OLC$

$LabC = 2.9 \times 10^6 \times$ Naira

PATENT AND ROYALTIES

The patent and royalties (PR) was found to be 2-6% of the total production cost (TPC). Now, taking the patent and royalties (PR) to be 3% of the total production cost (TPC), then

PR = 3% × TPC

PR = 5.149×10^6 × Naira

PLANT OVERHEAD COST

The plant overhead cost (OvC) was found to be 50-70% of the sum of operating labour (OLC), operating supplies (OSC) and maintenance cost (MC). Now, taking the plant overhead cost (OvC) is 53% of the sum of operating labour (OLC), operating supplies (OSC) and maintenance cost (MC), then

OvC = 53% × (OLC + OSC + MC)

OvC = 3.564×10^7 × Naira

GENERAL EXPENSES

ADMINISTRATIVE COST

The administrative cost (AC) was found to be 10-60% of the operating labour cost (OLC). Now, taking the administrative cost (AC) to be 15% of the operating labour cost (OLC), then

AC = 15% × OLC

AC = 3.347×10^6 × Naira

DISTRIBUTION AND SELLING PRICE

The distribution and selling price (DSP) was found to be 2-30% of the total production cost (TPC). Now, taking the distribution and selling price (DSP) to be 3% of the total production cost (TPC), then

DSP = 3% × TPC

DSP = $5.149 \times 10^6 \times$ Naira

RESEARCH AND DEVELOPMENT COST

The research and development cost (RDC) was found to be 3% of the total production

cost (TPC). Now, since research and development cost (RDC) is 3% of the total production

cost (TPC), then

RDC = 3% × TPC

RDC = $5.149 \times 10^6 \times$ Naira

So, the general expenses (GE) is given as the sum of the administrative cost, distribution and selling price and research and development cost. That is,

GE = AC + DSP + RDC

GE = $1.364 \times 10^7 \times$ Naira

TOTAL PRODUCT COST

The total product cost (TPC) is given as the sum of the maintenance cost and the general expenses. That is

TProdC = MC + GE

TProdC = $5.412 \times 10^7 \times$ Naira

Further, **the total expenditure,** which is given as the sum of raw material, factory labour, depreciation and overhead, is equal to

TE = RMC + OLC + Dep + OvC

$TE = 1.646 \times 10^{8} \times Naira$

REVENUE EXPECTATIONS

On the basis that the plant is working for 347 days per year, that is, in this case, the cost price is calculated as thus;

that is, making $annum = 336 \times day$

$Amount\_Per\_Annum = V$

$$Amount\_Per\_Annum = 4.002 \times 10^{5} \times \frac{lb}{annum}$$

$$Price\_of\_Phthalic\_Anhydride = 650 \times \frac{Naira}{lb}$$

Having known the cost price, the selling price can now be set. Setting the selling price to be 60 naira/L, that is,

$Profit = Amount\_Per\_Annum \times Price\_of\_Phthalic\_Anhydri$

$$Profit = 2.602 \times 10^{8} \times \frac{Naira}{annum}$$

$TI = Profi$

$TI = 2.602 \times 10^{8} \times Naira$

Gross income (GI) is the difference between the total income and the total expenditure (TE). That is

$GI = TI - TE$

$GI = 9.551 \times 10^{7} \times Naira$

The total income above is the income before tax. Giving that tax is 30% of the total income, that is, $\text{Tax} = 30\% \times \text{GI}$

$$\text{Tax} = 30\% \times \text{GI}$$

$$\text{Tax} = 2.865 \times 10^{7} \times \text{Naira}$$

Net profit (NP) is thus obtained as the difference between the gross income (GI) and the tax (Tax). That is,

$$\text{NP} = \text{GI} - \text{Tax}$$

$$\text{NP} = 6.686 \times 10^{7} \times \text{Naira}$$

Rate of return (RR) is given as

$$\text{Rate\_of\_return} = \frac{\text{Net\_profit}}{\text{Total\_capital\_investment}} \times 100$$

So, symbolically,

$$\text{ROR} = \frac{\text{NP}}{\text{TCI}} \times 100 \times \%$$

$$\text{ROR} = 7.44 \times \%$$

CASH FLOW

Cash flow is given as the difference between the amount earned and the amount expended. That

$$\text{Cash\_Flow} = \text{TI} - \text{TProdC}$$

$$\text{Cash\_Flow} = 2.06 \times 10^{8} \times \text{Naira}$$

PAY BACK PERIOD

The pay back period (PBP) is the time required after the start of the project to pay off the initial investment from income. It is given as the reciprocal of the rate of return (ROR).

That is,

$$\text{PBP} = \frac{1}{\text{ROR}} \times \text{yr}$$

$$\text{PBP} = 13 \times \text{yr}$$

DISCOUNTED CASH FLOW (TIME VALUE OF MONEY)

The discounted cash flow is used in this project to obtain the Net Present Value of the cash flow in year n. The net cash flow in each year of the project is brought to its "present worth" at the start of the project by discounting it at some chosen compound interest rate.

The formula for the net present worth (NPW) of cash flow in year n is given as

$$\text{NPW} = \sum_{i=1}^{n} \frac{\text{Cash\_Flow}}{(1+r)^{n}}$$

Now, for this project, $r = \text{ROR}$ $n = 1$

Therefore,

$$\text{NPW} = \sum_{i=1}^{n} \frac{\text{Cash\_Flow}}{(1+r)^{n}}$$

$$\text{NPW} = 1.918 \times 10^{8} \times \text{Naira}$$

DISCOUNTED CASH FLOW RATE OF RETURN

The discounted cash flow is given as is the interest rate that will make the condition given as

$$\mathrm{DCF} = \sum_{i=1}^{n} \frac{\mathrm{Cash\_Flow}}{(1+r)^{n}} = 0$$

Using trial-and-error calculations as suggested by Sinnot R. K. (Coulson and Richardson's Chemical Engineering, 3rd Edition, pg 277,

$i = 54.15\times\%$ $\quad\quad n = 2($

$\mathrm{DCFRR} = r$ $\quad\quad \mathrm{DCFRR} = 54.15\times\%$

$$\mathrm{DCF} = \sum_{i=1}^{n} \frac{\mathrm{Cash\_Flov}}{(1+r)^{n}}$$

$\mathrm{DCF} = 7.18\times 10^{5}\times \mathrm{Nair}$

That is to say that the Discounted Cash Flow Rate of Return (DCFRR) is equal to

DCFRR $= 54.15\times\%$.

RETURN ON INVESTMENT

This is calculated as given thus.

Return on investment (ROI) is given by the expression.

$$\mathbf{ROI} = \frac{\mathrm{Total\_profit\_less\_depreciati}}{\mathrm{Total\_investment}}$$

That is,

$$\mathrm{ROI} = \frac{\mathrm{TI-Dep}}{\mathrm{TCI}}\times 100\times\%$$

$\mathrm{ROI} = 20\times\%$

CHAPTER FOURTEEN

14.0 CONCLUSION AND RECOMMENDATION

14.1 CONCLUSION

From the result of this project which showed that the total capital investment was ₦898600000, the overall production cost was ₦54120000, the net profit was ₦ 66860000 at a selling price of ₦650 Per pound and the payback period 13 years. It can be concluded that the design of a plant to produce 400,000lb/yr of phthalic anhydride is economically viable.

14.2 RECOMMENDATIONS

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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