DECLARATION

We hereby declare that the work in this report of the integrated project is our own except for quotations and summaries which have been fully acknowledged.

14 MARCH 2011

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We would like to take this opportunity to state our appreciation to our lecturers Dr. Manal Ismail, Assoc. Prof. Dr. Zahira Yaakob and Prof. Dr. Abdul Amir Hassan Kadhum by providing guidance and help based on the format and issues of this integrated project in detail. Without their guidance, it is impossible to finish this project.

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Thirdly, we would like to thank each other as a group member. All of us had given very best cooperation during the progress of completing our project. We worked as a team in order to complete our project successfully. Also thanks to our course mates for sharing information and knowledge on this project.

Next, we would also like to express our appreciation to the other groups which are our classmates as well because of their selfless sharing of knowledge and suggestions in solving the questions. Group discussions are always the most efficient way.

Lastly, we also wish to thank to those whom we did not mention here but had helped us directly or indirectly in accomplishing our project. Thank you.
ABSTRACT

We are assigning to do a research on how to produce the phenol. The main objective of our report is to design the production plant for phenol in industry. Besides, in this report we had include information on the product usage, demand, supply and production, future marketing potential, sources of raw materials, process description, process flow diagram, waste generation, environmental issues and safety precaution for the production process. We have also performed material balance and energy balance calculation at selected reactor, which is oxidation vessel. Phenol is also known as carbolic acid. Phenol can be form from cumene peroxidation process. The raw material in this process is cumene and oxygen. In this peroxidation process cumene is oxidizing first with present of oxygen into cumene peroxide and then decomposition process to form phenol and acetone. A process flow diagrams (PFD) which is for production of phenol had been included to provide clearer picture of the process. It is done by using engineering design software, Microsoft Visio. Based on research, phenol is supply from all over the world such as Asia, Western Europe, North America and others. In global market, phenol production and consumption increases year by year. This is because in future world the development of technology growth rapidly. Many engineering equipments are made from phenol such as electrical and electronic equipment, automobiles, sports safety equipment and reusable food. Hence, increases the demand of phenol. From the calculation of mass balance, we obtain $F_1$, mass flow rate in for cumene (66239.76 kg/h ), $F_2$ mass flow rate in for oxygen (5930.65 kg / h),$F_3$ mass flowrate out for mixture of cumene,oxygen and cumene hydroperoxide (73722.26 kg / h). From calculation of energy balance we obtain $Q$ heat transfer (-6710.005 kJ/s ). As a conclusion we can assume that the phenol production per year is 165.6 kmole / year. During the process with $Q$=-6710.005 kJ/s heat is being released during the process.
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<tr>
<td>A</td>
<td>Area</td>
</tr>
<tr>
<td>C&lt;sub&gt;j&lt;/sub&gt;</td>
<td>Concentration of component j</td>
</tr>
<tr>
<td>C&lt;sub&gt;p&lt;/sub&gt;</td>
<td>Specific heat capacity constant pressure</td>
</tr>
<tr>
<td>D</td>
<td>Diameter</td>
</tr>
<tr>
<td>F</td>
<td>Friction force</td>
</tr>
<tr>
<td>F&lt;sub&gt;f&lt;/sub&gt;</td>
<td>Friction loss in pipe due to the flow</td>
</tr>
<tr>
<td>f</td>
<td>Fanning factor</td>
</tr>
<tr>
<td>F&lt;sub&gt;i&lt;/sub&gt;</td>
<td>Total mass flow rate at inlet</td>
</tr>
<tr>
<td>F&lt;sub&gt;o&lt;/sub&gt;</td>
<td>Total mass flow rate at outlet</td>
</tr>
<tr>
<td>F&lt;sub&gt;ij&lt;/sub&gt;</td>
<td>Mass flow rate of component j at inlet</td>
</tr>
<tr>
<td>F&lt;sub&gt;oj&lt;/sub&gt;</td>
<td>Mass flow rate of component j at outlet</td>
</tr>
<tr>
<td>g</td>
<td>Gravitational force</td>
</tr>
<tr>
<td>H</td>
<td>Head</td>
</tr>
<tr>
<td>Δ&lt;sup&gt;^&lt;/sup&gt;H&lt;sub&gt;j&lt;/sub&gt;</td>
<td>Enthalpy change of component j</td>
</tr>
<tr>
<td>h&lt;sub&gt;c&lt;/sub&gt;</td>
<td>Friction loss due to sudden contraction</td>
</tr>
<tr>
<td>h&lt;sub&gt;ex&lt;/sub&gt;</td>
<td>Friction loss due to sudden enlargement</td>
</tr>
<tr>
<td>h&lt;sub&gt;f&lt;/sub&gt;</td>
<td>Friction loss for fittings and valves</td>
</tr>
<tr>
<td>k&lt;sub&gt;c&lt;/sub&gt;</td>
<td>Contraction-loss coefficient</td>
</tr>
<tr>
<td>k&lt;sub&gt;ex&lt;/sub&gt;</td>
<td>Expansion-loss coefficient</td>
</tr>
<tr>
<td>k&lt;sub&gt;f&lt;/sub&gt;</td>
<td>Loss factor for the fitting or valve</td>
</tr>
<tr>
<td>k&lt;sub&gt;j&lt;/sub&gt;</td>
<td>Specific reaction rate of component j</td>
</tr>
<tr>
<td>L</td>
<td>Length of pipe</td>
</tr>
<tr>
<td>m</td>
<td>Mass flow rate (kg/s)</td>
</tr>
<tr>
<td>M&lt;sub&gt;j&lt;/sub&gt;</td>
<td>Molecular weight of component j</td>
</tr>
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</table>
\( N_i \)  
Total molar flow rate at inlet

\( N_{Re} \)  
Reynolds Number

\( N_o \)  
Total molar flow rate at outlet

\( N_{ij} \)  
Mole flow rate of component j at inlet

\( N_{o,j} \)  
Mole flow rate of component j in outlet

\( N_D \)  
Degree of freedom

\( N_V \)  
Number of unknown

\( N_E \)  
Number of independent equation

\( P \)  
Pressure

\( P_{vp} \)  
Vapour pressure

\( Q \)  
Energy

\( r \)  
Rate of reaction

\( r'_j \)  
Rate of reaction of component j in heterogeneous reaction

\( u \)  
Velocity

\( W \)  
Weight of catalyst

\( W_p \)  
Shaft work delivered to pump

\( W_s \)  
Mechanical work

\( w_{o,j} \)  
Mass fraction of component j at outlet

\( X \)  
Conversion

\( x_{ij} \)  
Mole fraction of component j at inlet

\( x_{o,j} \)  
Mole fraction of component j at outlet

\( Z \)  
Elevation

\( \alpha_x \)  
Stoichiometric coefficient of component j

\( \rho \)  
Density

\( \mu \)  
Viscosity

\( \varepsilon \)  
Equivalent roughness for new pipes
### GLOSSARY

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<th>Term</th>
<th>Definition</th>
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<tr>
<td>Aromatic compound</td>
<td>A Hydrocarbon characterized by general alternating double and single bonds between carbons</td>
</tr>
<tr>
<td>Bond Cleavage</td>
<td>Process of splitting the chemical bonds</td>
</tr>
<tr>
<td>Catalyst</td>
<td>A substance that causes or accelerates a chemical reaction without itself being affected</td>
</tr>
<tr>
<td>Caprolactam</td>
<td>An organic compound with the formula (CH₂)₅C(O)NH and used in synthetic polymer</td>
</tr>
<tr>
<td>Cumene</td>
<td>Systematic name for isopropylbenzene</td>
</tr>
<tr>
<td>Distillation</td>
<td>A method of separating mixtures based on differences in their volatilities in a boiling liquid mixture</td>
</tr>
<tr>
<td>Effluent</td>
<td>An out flowing of water or gas from a natural body of water, or from a human-made structure</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>A measure of the total energy of a thermodynamic system</td>
</tr>
<tr>
<td>Epoxy resin</td>
<td>Thermosetting polymer formed from the reaction of an epoxide with polyamine</td>
</tr>
<tr>
<td>Fluid Mechanics</td>
<td>The study of fluids and the forces on them. (Fluids include liquids, gases, and plasmas.)</td>
</tr>
<tr>
<td>Term</td>
<td>Definition</td>
</tr>
<tr>
<td>----------------------</td>
<td>-------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Heterogeneous</td>
<td>Having more than one type represented</td>
</tr>
<tr>
<td>Homogeneous</td>
<td>Having the same uniform appearance and composition throughout</td>
</tr>
<tr>
<td>Limiting Reactant</td>
<td>The substance which is totally consumed when the chemical reaction is complete</td>
</tr>
<tr>
<td>Polycarbonate</td>
<td>A particular group of thermoplastic polymers. They are worked, moulded and thermoformed</td>
</tr>
<tr>
<td>Stoichiometry</td>
<td>A branch of chemistry that deals with the quantitative relationships that exist between the reactants and products in chemical reactions</td>
</tr>
<tr>
<td>Synthesis</td>
<td>The combining of the constituent elements of separate material or abstract entities into a single or unified entity (opposed to analysis).</td>
</tr>
<tr>
<td>Viscosity</td>
<td>Measure of the resistance of a fluid which is being deformed by either shear stress or tensile stress</td>
</tr>
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CHAPTER I

INTRODUCTION

1.1 PHENOL

Phenol, is an aromatic compound with an OH group bonded to the phenyl ring with chemical formula C₆H₅OH. Phenol is used in the production of disinfectants, dyes, pharmaceuticals, plastics, germicides, preservatives, synthetic resin, antiseptic, detergent and drug.

Molecular structure:

![Figure 1.1: Structural Formula of phenol](Sources: Wikipedia, ChemBlink, Wikimedia Commons)

1.2 CHEMICAL REACTION INVOLVE

Phenol is form initially from the basic raw material; benzene and propylene which in turn to produce cumene or the systematic name is isopropylbenzene. The cumene is further oxidised to become a cumene hydroperoxide before it is split into phenol and acetone as the product. The sulphonation route produced large quantities of waste, and more and thus being replaced by oxidation of cumene process.

The reaction between phenol and acetone would yield to the production of Bisphenol-A (BPA). It is used to manufacture polycarbonate and epoxy resin.

However, the process that we studied for the project is oxidation of cumene. The chemical reactions are shown by below.
\[ C_6H_5CH(CH_3)_2 (l) + O_2 (g) \rightarrow C_6H_5C(CH_3)_2OOH (l) \]  
\[ C_6H_5C(CH_3)_2OOH (l) \rightarrow C_6H_5OH + CH_3COCH_3 \]  

Figure 1.2: Reaction of the manufacture of phenol

- Reaction of benzene sulfonic acid with base
- Reaction of chlorobenzene with base
- Acidic oxidation of cumene
- Hydrolysis of diazonium salts

1.3 PHYSICAL PROPERTIES

Phenol is a caustic, poisonous, white crystalline solid at room temperature. The molecular weight and density of phenol are 94.11 g/mole and 1.07 g/cm\(^3\) respectively. Phenol is soluble in water is due to its ability to form hydrogen bonds with water.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Phenol</th>
</tr>
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<tr>
<td>Molecular formula</td>
<td>(C_6H_5O)</td>
</tr>
<tr>
<td>Molar mass</td>
<td>94.11 g mol(^{-1})</td>
</tr>
<tr>
<td>Appearance</td>
<td>White Crystalline Solid</td>
</tr>
<tr>
<td>Density</td>
<td>1.07 g/cm(^3)</td>
</tr>
<tr>
<td>Melting point</td>
<td>40.5 °C, 314 K</td>
</tr>
<tr>
<td>Boiling point</td>
<td>181.7 °C, 455 K</td>
</tr>
<tr>
<td>Solubility in water</td>
<td>8.3 g/100ml</td>
</tr>
<tr>
<td>Dipole moment</td>
<td>1.7 D</td>
</tr>
</tbody>
</table>

(Source: http://en.wikipedia.org/wiki/Phenol, Wikipedia)
CHAPTER II

RAW MATERIAL

2.1. SOURCES OF RAW MATERIAL

Cumene peroxidation process is a process involves the liquid phase air oxidation of cumene to cumene peroxide, which in turn is decomposed to phenol and acetone by the action of acid. During the cumene peroxidation process, there are two main raw materials used in this process which are cumene and oxygen.

Oxygen is a gas form fluid. Oxygen is colourless gas that can be found in the air. In the air there is 21% of oxygen contains while another 79% is nitrogen gas. Oxygen acts as an oxidizer. Table 2.1 shown the physical and chemical properties of oxygen.

Table 2.1: The physical and chemical properties of oxygen

<table>
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<tr>
<th>Physical Properties</th>
<th>Data</th>
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<tr>
<td>Synonyms</td>
<td>Oxygen</td>
</tr>
<tr>
<td>Chemical Formula</td>
<td>O₂</td>
</tr>
<tr>
<td>Physical State at room temperature</td>
<td>Gas</td>
</tr>
<tr>
<td>Odor</td>
<td>Odourless</td>
</tr>
<tr>
<td>Appearance</td>
<td>Colorless gas</td>
</tr>
<tr>
<td>Melting Point</td>
<td>219 °C</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>183°C</td>
</tr>
<tr>
<td>Critical Temperature</td>
<td>118°C</td>
</tr>
<tr>
<td>Relative Density</td>
<td>1.1 g/cm³</td>
</tr>
</tbody>
</table>
Cumene is an aromatic hydrocarbon. Cumene can be formed from the alkylation of benzene with the addition of propylene. Cumene is a liquid form fluid. Cumene is a colourless liquid. The systematic name for cumene is isopropyl benzene.

Table 2.2: The physical and chemical properties of cumene

<table>
<thead>
<tr>
<th>Physical Properties</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synonyms</td>
<td>Isopropyl benzene</td>
</tr>
<tr>
<td>Chemical Formula</td>
<td>C₆H₅CH(CH₃)₂</td>
</tr>
<tr>
<td>Physical State at room temperature</td>
<td>Liquid</td>
</tr>
<tr>
<td>Odor</td>
<td>Aromatic</td>
</tr>
<tr>
<td>Appearance</td>
<td>Colorless liquid</td>
</tr>
<tr>
<td>Melting Point</td>
<td>-</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>152°C</td>
</tr>
<tr>
<td>Critical Temperature</td>
<td>-</td>
</tr>
<tr>
<td>Relative Density</td>
<td>4.1 g/cm³ (vapour)</td>
</tr>
<tr>
<td>Molar mass</td>
<td>120.00 g/mol</td>
</tr>
<tr>
<td>Solubility mg/L water</td>
<td>Negligible solubility in cold water</td>
</tr>
<tr>
<td>Viscosity</td>
<td>0.7</td>
</tr>
</tbody>
</table>

Source: CITGO Petroleum Corporation *MSDS (Material Safety Data Sheet) Information.*
CHAPTER III

PRODUCT USAGE AND APPLICATION

3.1 PRODUCT USAGE FOR PHENOL

Figure 3.1: The uses of phenol

Source: *Dow Phenol: Properties, Usage, Storage and Handling*, The Dow Chemical Company

Based on the chart most of the phenol is used as a Bisphenol A (BPA). Bisphenol A is an industrial chemical used in the production of epoxy and polycarbonate plastic resins. Polycarbonate plastic resins are a lightweight, high-performance plastic that possesses a unique balance of toughness, high heat resistance, and very good electrical resistance.
Because of these features, polycarbonate is used in a wide variety of common products including digital media for example CDs and DVDs, sports safety equipment and reusable food. Epoxy resins have many uses including engineering applications such as electrical laminates for printed circuit boards, composites, paints and adhesives, as well as in a variety of protective coatings.

Second large usage of phenol is Phenol-formaldehyde (PF) resins which is 30%. A PF resin is commonly used as molding powders, laminates, adhesives, and coating resins. PF resins in powder form are molded into products such as telephone housings and electrical outlets or plugs. The other application of PF resins are high and low pressure laminates are used in the manufacture of panel boards, chemically resistant containers, boat hulls, airplane parts, luggage, brake linings and many others.

Next, the usage of phenol is caprolactam which contribute 8% of product usage. Caprolactam used in nylon 6 production to make carpet and rug yarns. Besides, caprolactam also used in resins. Caprolactam based resins are used in automotive and truck parts including rear-end license panels, louvers, mirror housings, and wheel covers. Others usage also contribute 18%. Lastly, alkyl phenol is one of the usages. The examples of alkylphenol are p-nonylphenol and p-dodecylphenol. Alkyl phenols are used as stabilizers or antioxidants in motor oil.
CHAPTER IV

ECONOMIC ISSUE

4.1. SUPPLY AND DEMAND OF PHENOL

4.1.1. DEMAND OF PHENOL

The phenol/acetone capacity expansion in the world has been brisk in recent years due to the strong demand for its derivatives such as Bisphenol A and phenolic resins. The largest single market for phenol is in the production of Bisphenol A (BPA), which is manufactured from phenol and acetone. About 40% of BPA is made up from phenol. According to SRI Consulting, world consumption of phenol for BPA is estimated to grow at a good average annual rate during 2009–2014. Increased demand and capacity for BPA will result in strong demand for phenol in these regions. Bisphenol A of Asian demand is expected to increase by 13% this year. The second-largest derivative market for phenol is phenol resins which are used in the moulding of heat-resistant components for household appliances, counter-top and flooring laminates, and foundry castings. From ICIS news, the global phenol market has been growing at an average of 5%/year and total demand will recover from 7.9m tonnes in 2009 to reach 10.6m tonnes by 2015. The phenol markets look especially promising in China since 2000.
Figure 4.1: Pie chart of worldwide demand of phenol

Figure 4.2: Pie chart of world consumption of phenol

(Source: HighBeam Research)

*the data is translated from words to pie chart form
Table 4.1: Demand of Phenol in Global Market

<table>
<thead>
<tr>
<th>Year</th>
<th>Supplied quantity (million tones / year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009</td>
<td>7.9</td>
</tr>
<tr>
<td>2010</td>
<td>8.3</td>
</tr>
<tr>
<td>2011</td>
<td>8.7</td>
</tr>
<tr>
<td>2012</td>
<td>9.1</td>
</tr>
<tr>
<td>2013</td>
<td>9.6</td>
</tr>
<tr>
<td>2014</td>
<td>10.1</td>
</tr>
<tr>
<td>2015</td>
<td>10.6</td>
</tr>
</tbody>
</table>

(Source: ICIS Market News)

*the data for 2011 to 2015 is the estimation data while the other is the data published by ICIS market research and some other site.

4.1.2 SUPPLY OF PHENOL

Shell, Sunoco, Georgia Gulf, Dow, JLM and INEOS are the major producer in United State. Shell Chemical LP have a facility that is fully integrated from raw materials to end products gives Shell Chemical LP a significant advantage in operating as a low cost producer of phenol. However, INEOS Chemical is the world largest phenol producer. INEOS Chemical produce 540 kilo tonne per year to USA and 1330 kilo tonne per year to Europe while Sunoco produces over 590,000 t/a of phenol in its facility in Philadelphia, Penn, USA. Sunoco/UOP phenol technology is currently used in 11 plants worldwide having a total phenol capacity of more than 1,500,000 t/a. The capacity of phenol in China still cannot meet the demand thus many enterprises are plan to expand or construct the new units.
<table>
<thead>
<tr>
<th>Year</th>
<th>Supplied quantity (million tones / year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009</td>
<td>8.58</td>
</tr>
<tr>
<td>2010</td>
<td>9.09</td>
</tr>
<tr>
<td>2011</td>
<td>9.55</td>
</tr>
<tr>
<td>2012</td>
<td>10.12</td>
</tr>
<tr>
<td>2013</td>
<td>10.73</td>
</tr>
<tr>
<td>2014</td>
<td>11.37</td>
</tr>
<tr>
<td>2015</td>
<td>11.37</td>
</tr>
</tbody>
</table>

(Source: ICIS Market News)

Figure 4.3: Supply and demand of phenol from 2009 to 2015

(Source: ICIS Market News)
4.2. FUTURE MARKETING POTENTIAL OF PHENOL

Figure 4.4: Future Marketing Potential Of Phenol

x-axis: production per year(millions tones/year)
y-axis: year

From the figure 4.4 we have made a prediction for future market potential of phenol from years 2016 until 2020. We have made an extrapolation from the previous data for supply and demand of phenol from 2009 until 2015. From the graph we can see that, the demand and supply of phenol will increase by year. The supply graph is slightly higher than demand graph. Moreover the supply graph showed that steeper increase year by year. While the demand graph increases less steeper.
CHAPTER V

ENVIRONMENT ISSUE

5.1. WASTE GENERATION

Waste generation is quantity of materials or products that enter a waste stream before land filling, or recycling. In this process acetophenone is the side product while phenol is the major product. Sometimes the company sells their side product or uses it for another purpose. Next is Acidified wash water can be harmful to environment if we release it in the exceed limit. The table below shows the physical and chemical properties for acetophenone.

<table>
<thead>
<tr>
<th>Physical Properties</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synonyms</td>
<td>Ketone methyl phenyl</td>
</tr>
<tr>
<td>Chemical Formula</td>
<td>C₆H₅COCH</td>
</tr>
<tr>
<td>Physical State at room temperature</td>
<td>Liquid</td>
</tr>
<tr>
<td>Melting Point</td>
<td>19.7°C</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>201.7°C</td>
</tr>
<tr>
<td>Critical Temperature</td>
<td>-</td>
</tr>
<tr>
<td>Relative Density</td>
<td>4.1 g/cm³ (vapour)</td>
</tr>
<tr>
<td>Molar mass</td>
<td>120.16 g/mol</td>
</tr>
<tr>
<td>Solubility mg/L water</td>
<td>soluble in water, methanol, diethyl ether</td>
</tr>
<tr>
<td>Vicousity</td>
<td>-</td>
</tr>
</tbody>
</table>

Source: http://www.sciencelab.com/xMSDS-Acetophenone-9922778 MSDS (Material Safety Data Sheet) Information.
Acidified wash water is released from the separation process. The acidified water form is removed from the process. Table below shows the physical and chemical properties for acidified wash water.

Table 5.2: The physical and chemical properties for acidified wash water

<table>
<thead>
<tr>
<th>Physical Properties</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synonyms</td>
<td>Water</td>
</tr>
<tr>
<td>Chemical Formula</td>
<td>H₂O</td>
</tr>
<tr>
<td>Physical State at room temperature</td>
<td>Liquid</td>
</tr>
<tr>
<td>Odor</td>
<td>-</td>
</tr>
<tr>
<td>Appearance</td>
<td>Colourless liquid</td>
</tr>
<tr>
<td>Melting Point</td>
<td>0°C</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>100°C</td>
</tr>
<tr>
<td>Critical Temperature</td>
<td>-</td>
</tr>
<tr>
<td>Relative Density</td>
<td>1 g/cm³ (vapour)</td>
</tr>
<tr>
<td>Molar mass</td>
<td>18.00 g/mol</td>
</tr>
<tr>
<td>Solubility mg/L water</td>
<td>Infinite</td>
</tr>
<tr>
<td>Vicousity</td>
<td>8.90 × 10⁻⁴ Pa·s</td>
</tr>
<tr>
<td>pH</td>
<td>3.0</td>
</tr>
</tbody>
</table>

Source :GE Power & Water MSDS (Material Safety Data Sheet) Information.

Lastly, acetone is also one of the waste generations in this process. Acetone is form during acetone fractionation process. Acetone is a colorless liquid with pungent smell. The table below shows the physical and chemical properties for acetone.

Table 5.3: The physical and chemical properties for acetone

<table>
<thead>
<tr>
<th>Physical Properties</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synonyms</td>
<td>2-propanone</td>
</tr>
<tr>
<td>Chemical Formula</td>
<td>C₃H₆O</td>
</tr>
<tr>
<td>Physical State at room temperature</td>
<td>Liquid</td>
</tr>
<tr>
<td>Odor</td>
<td>Pungent smell</td>
</tr>
<tr>
<td>Appearance</td>
<td>Colourless liquid</td>
</tr>
<tr>
<td>------------------</td>
<td>-----------------------------------</td>
</tr>
<tr>
<td>Melting Point</td>
<td>-95.3°C</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>56.2°C</td>
</tr>
<tr>
<td>Critical Temperature</td>
<td>235°C</td>
</tr>
<tr>
<td>Relative Density</td>
<td>0.7925 g/cm³</td>
</tr>
<tr>
<td>Molar mass</td>
<td>58.08g/mol</td>
</tr>
<tr>
<td>Solubility mg/L water</td>
<td>soluble in cold water and hot water</td>
</tr>
<tr>
<td>Vicousity</td>
<td>0.4013 mPa·s at 0°C</td>
</tr>
<tr>
<td></td>
<td>0.3311 mPa·s at 20°C</td>
</tr>
<tr>
<td></td>
<td>0.2562 mPa·s at 50°C</td>
</tr>
</tbody>
</table>


5.2 ENVIRONMENTAL ISSUES

Leading to the phenol production plant, there is acidified wash water has been eliminate during the process. This waste generation will lower water pH due to acid precipitation and deposition usually through precipitation. This process disrupts ecosystem nutrient flows and may kill freshwater fish and plants dependent on more neutral or alkaline conditions.

Next, the air pollution cause by emission of hazardous substance such as acetophenon from this plant has been one of the issues. Air pollution happen when there is emission of hazardous substance in exceed limit. Air pollution can cause the possibility of children living within them to develop asthma, pneumonia and other lower respiratory infections.

Lastly, the latest issues in Malaysian government banned the use of milk bottles containing bisphenol A. Bisphenol A contains toxic substance that use to made milk bottles for babies. Bisphenol A is one of phenol’s product usages. Bisphenol A is
an endocrine disruptor, which can mimic the body's own hormones and may lead to negative health effects.

5.3 RELEVANT ENVIRONMENTAL ACT

Environmental act that is related to this process is Environmental Quality Act 1974. These environmental quality acts have their regulation to make sure the plant will not discharge or use harmful or hazardous materials. The waste generation discharges for this pulp mill are following the environmental quality (sewage and industrial effluents) regulations 1979. There are list of environmental quality (sewage and industrial effluents) regulations:-

1. Prohibition against new and altered sources of effluent discharge
2. Requirement and approval of plans.
3. Prohibition of discharge of effluent containing certain substances.
5. Parameter limits of effluent to be discharged into inland waters.

Table 5.4 showed parameter limits of effluent to be discharged into inland waters. It is also one of the regulations for environmental quality (sewage and industrial effluents).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Standard</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH value</td>
<td>5.5 - 9.0</td>
</tr>
<tr>
<td>COD (mg/L)</td>
<td>100</td>
</tr>
<tr>
<td>BOD$_{5@20}$°C (mg/L)</td>
<td>50</td>
</tr>
<tr>
<td>Suspended Solids (mg/L)</td>
<td>100</td>
</tr>
</tbody>
</table>

Source: Anon. 2006. MSDS (Material Safety Data Sheet) Information.
5.4. **EXPOSURE LIMIT**

Exposure limit is a legal limit for exposure to a chemical substance. These limits are generally discretionary and every country defines its own limits, resulting in a lack of widely accepted standards. The exposure limits of raw materials and waste are stated in table 5.5.

<table>
<thead>
<tr>
<th>Chemical Substance</th>
<th>Exposure limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cumene</td>
<td>0.2 ppm</td>
</tr>
<tr>
<td>Oxygen</td>
<td>&gt;21% concentration of air</td>
</tr>
</tbody>
</table>

**Table 5.5: Exposure limits of raw materials**

Source: *MSDS (Material Safety Data Sheet) Information.*

5.5 **SAFETY PRECAUTION**

In this cumene process the raw materials are oxygen and cumene. Oxygen will become a hazardous substance if we are exposed to it in the exceeded limit around more than 21% air in atmosphere. The plant must use only properly specified equipment, which is suitable for this product, its supply pressure and temperature. Keep away from ignition sources (including static discharges). Apart from that, peoples that working with oxygen are advise not to smoke while handling product.

Cumene is also listed as a hazardous chemical substance. It is a flammable liquid because it release vapour at or below ambient temperature. Its vapour can cause a flash fire when mixed with air in certain proportions and exposed to an ignition source. Therefore, when handling this material, if there is spill or leak of pipe people work in this plant must keep the containers closed and do not handle or store near heat. Those

Acetophenon is very hazardous in case of eye contact (irritant). It is also hazardous in case of skin contact (irritant). It is slightly hazardous in case of ingestion, of inhalation.
Inflammation of the eye is characterized by redness, watering, and itching. Peoples that have been in charge for handling this material should keep it away from heat and sources of ignition. They also should not ingest the materials. If ingested, seek medical advice immediately and show the container or the label.
CHAPTER VI

PROCESS FLOW DIAGRAM

6.1. PROCESS DESCRIPTION
In this production process, purified cumene is used as raw material input and is mixed with recycle Cumene in the main feed stream. It is feed to the oxidation vessel which the condition is maintained at 110-115 °C and pH range of 6.0 to 8.0. In the vessel, the mixture from the feed is exposed to compressed air until 20-25% of the Cumene has converted into Cumene Hydroperoxide. This is the stoichiometry equation of the reaction.

\[
C_6H_5CH(CH_3)_2 + O_2 \rightarrow C_6H_5C(CH_3)_2OOH
\]

The crude mixture from the oxidizer is concentrated up to 80% before entering the reactor where the Cumene Hydroperoxide is cleavage to phenol and acetone. The reaction is carried out in mild temperature and pressure around 70 °C and atmospheric pressure. Small amount of sulphuric acid is added to the reactor as the reaction takes place.

\[
C_6H_5C(CH_3)_2OOH \rightarrow C_6H_5OH + CH_3COCH_3
\]

After that, the stream is directed to the separation processes. First of all, the stream is washed with water and Acetone is removed overhead in the first column. The mixture is then further purified by going through steps of distillation. For the first distillation column, the unreacted Cumene is transferred to the recycle stream. The Cumene is purified before it is sent back to the feed stream. The purification of Cumene is done by catalytic hydrogenation of Methyl Styrene to Cumene, by careful fractionation where methyl styrene is available as by-product of the reaction.
The reaction of Phenol required 2 step of reaction. The first reaction is the production of Cumene Hydroperoxide by two raw materials, which is Cumene and Oxygen. The reaction occurs at tank T101, which is oxidizing tower. The reactions occur in the condition of temperature 110-115 °C and pH is at range of 6.0 to 8.0. Then, the intermediate product; Cumene Hydroperoxide will be used as the reactant in second reactor, R101. Type of reactor that will be used is Continuous Stirred Tank Reactor (CSTR). It about 90% conversions occurs in the cleavage process to form Phenol and Acetone. The next unit operation is the separation process where all of the side product and waste will be separate to get the main product: Phenol.

6.2. PROCESS FLOW DIAGRAM

Process flow diagram for the production of Phenol in figure 6.1

6.3. BLOCK DIAGRAM

Figure 6.2 below show the block diagram for the production of phenol.

![Block diagram for the process of Phenol](image)
CHAPTER VII

MATERIAL AND ENERGY BALANCE

7.1. MATERIAL BALANCE

The first reactor is chosen for the calculation of the mass balance. The reactor 1 involves the reaction between Cumene and Oxygen to produce Cumene Peroxide. These are the reaction that involves in the first reactor.

In this reaction it shows that 1 kmole of $\text{C}_6\text{H}_5\text{CH(CH}_3\text{)}_2$ and 1 kmole of $\text{O}_2$ will produce 1 kmole of $\text{C}_6\text{H}_5\text{C(CH}_3\text{)}_2\text{OOH}$. After that, the Cumene Hydroperoxide make a cleavage process by a reaction with catalyst Sulphuric Acids (H$_2$SO$_4$) and produce Phenol and Acetone in reactor number 2. Based on the reaction equation, 1 kmole of $\text{C}_6\text{H}_5\text{C(CH}_3\text{)}_2\text{OOH}$ will cleavage 1 kmole of $\text{C}_6\text{H}_5\text{OH}$ and 1 kmole of $\text{CH}_3\text{COCH}_3$.

Based on the principles of mass balance equation, mass is neither created nor destroyed but it can change in physical and chemical state. Total mass of feed into the reactor are equal to the mass of product out of reactor with the total accumulation of mass inside the reactor.

Rate of mass input = Rate of mass output + Rate of mass accumulation

Since that the reaction is steady flow process, so total mass in is equal to total mass out of the reactor.

Rate of mass input = Rate of mass output

These are the given data from the literature review:-

1. Phenol production per year =136363.64 tonnes / year
   
   = 15.56663 tonnes / h

   = 15566.63 kg / h

   = 165.6 kmole / h
2. Fraction composition for the product mixture of Cumene hydroperoxide acids in reactor 1.
   \[ X_{3\text{cumene}} = 0.6 \]
   \[ X_{3\text{cumene hydroperoxide}} = 0.3 \]
   \[ X_{3\text{oxygen}} = 0.1 \]

3. Conversion factor:
   \[ X_{\text{reactor 2}} = 90\% \]

To find the total number of molar flow rate to the feed in reactor 1, firstly find the total flow rate output of the reactor by calculate the total flow rate of reactor 2 (reaction between Cumene Hydroperoxide and Sulphuric Acids to produce Phenol and Acetone).

   - Molecule Balance on reactor 2 (acidifier).

1. Phenol Balance:
   \[ N_3X_{3\text{phenol}} = N_4X_{4\text{phenol}} - ar_2 \]
   \[ N_4X_{4\text{phenol}} = 165.6 \text{ kmole / h} \]
   \[ a = 1 \]
   \[ 0 = N_4X_{4\text{phenol}} - r_2 \]
   \[ r_2 = 165.6 \text{ Kmole / h} \]

2. Acetone Balance:
   \[ N_3X_{3\text{acetone}} = N_4X_{4\text{acetone}} - ar_2 \]
   \[ N_4X_{4\text{acetone}} = 165.6 \text{ kmole / h} \]

3. Cumene Peroxide Balance:
   \[ N_3X_{3\text{cumene hydroperoxide}} = -ar_2 / X_{\text{reactor 2}} \]
   \[ = -(-1)(165.6) / (0.9) \]
   \[ = 184 \text{ kmole / h} \]

4. Total number of mole in feed reactor 2, \( N_3 \)
   \[ N_3X_{3\text{cumene hydroperoxide}} = 184 \text{ kmole / h} \]
   \[ X_{3\text{cumene hydroperoxide}} = 0.3 \]
   \[ N_3 \times 0.3 = 184 \text{ kmole / h} \]
   \[ N_3 = 613.3 \text{ kmole / h} \]
5. Finding mass flow rate for feed in reactor 2.

\[ F_3 = N_3 X_{3\text{cumene}} (M_{\text{cumene}}) + N_3 X_{3\text{cumene hydroperoxide}} (M_{\text{cumene hydroperoxide}}) + N_3 X_{3\text{oxygen}} (M_{\text{oxygen}}) \]

\[ = (613.33) (0.6) (120) + (613.33) (0.3) (150) + (613.33) (0.1) (32) \]

\[ = 73722.26 \text{ kg / h} \]

From this value, it shows that the reactor 2 required \textbf{73722.26 kg / h} feed mixture of Cumene hydroperoxide, Cumene and Oxygen to produce \textbf{15566.63 kg / h} of Phenol at the conversion of 90% of Cumene Peroxide at reactor 2.

- Molecule Balance on reactor 1:
  1. Cumene hydroperoxide Balance:
     \[ N_1 X_{1\text{cumene hydroperoxide}} = N_3 X_{3\text{cumene hydroperoxide}} - ar_1 \]
     \[ 0 = 184 \text{ kmole / h} - ar_1 \]
     \[ r_1 = 184 \text{ kmole / h} \]
  2. Cumene Balance:
     \[ N_1 X_{1\text{cumene}} = N_3 X_{3\text{cumene}} - ar_1 \]
     \[ X_{1\text{cumene}} = 1 \text{ (100% purity feed of Cumene)} \]
     \[ N_1 X_{1\text{cumene}} = (613.33) (0.6) - (-1) (184) \]
     \[ = 551.998 \text{ kmole / h} \]
  3. Oxygen Balance:
     \[ N_2 X_{2\text{oxygen}} = N_3 X_{3\text{oxygen}} - ar_1 \]
     \[ X_{2\text{oxygen}} = 1 \text{ (100% purity feed of Oxygen)} \]
     \[ N_2 X_{2\text{oxygen}} = (613.33) (0.1) - (-1) (184) \]
     \[ = 185.33 \text{ kmole / h} \]
     \[ F_1 = (N_1 X_{1\text{cumene}}) (M_{\text{cumene}}) = (551.998) (120) = 66239.76 \text{ kg / h} \]
     \[ F_2 = (N_2 X_{2\text{oxygen}}) (M_{\text{oxygen}}) = (245.33) (32) = 5930.65 \text{ kg / h} \]
     \[ \text{Total mass flow rate} = F_1 + F_2 \]
     \[ = 66239.76 + 5930.65 \]
     \[ = 74090.42 \text{ kg / h} \]
Based on the calculation above, the total mass flow rate required in the feed stream of Cumene and Oxygen is about \( \textbf{74090.42} \text{ kg/h} \) to produce \( \textbf{74200} \text{ kg/h} \).

### 7.2. ENERGY BALANCE

Cumene Peroxidation Process is the process where the raw material, cumene and oxygen gas that is 100% purity is react. The product form is cumene hydroperoxide. The calculation of the energy balance is done in the first reactor.

\[
\text{C}_6\text{H}_5\text{CH(CH}_3\text{)_2} (l) + \text{O}_2 (g) \rightarrow \text{C}_6\text{H}_5\text{C(CH}_3\text{)_2OOH (l)}
\]

\[C_p = A + BT + CT^2 + DT^3 \text{(J/mol.K)}\]

<table>
<thead>
<tr>
<th>( \text{C}_6\text{H}_5\text{CH(CH}_3\text{)_2} )</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>139.2\times10^{-3}</td>
<td>53.76\times10^{-5}</td>
<td>-39.79\times10^{-8}</td>
<td>120.5\times10^{-12}</td>
<td></td>
</tr>
<tr>
<td>\text{O}_2</td>
<td>29.1\times10^{-3}</td>
<td>1.158\times10^{-5}</td>
<td>-0.6706\times10^{-8}</td>
<td>1.311\times10^{-12}</td>
</tr>
<tr>
<td>\text{C}_6\text{H}_5\text{C(CH}_3\text{)_2} \text{OOH}</td>
<td>1.345\times10^{5}</td>
<td>3.8060\times10^{2}</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Source: Perry’s Chemical Engineer’s Handbook, Perry, R.H. and Elementary Chemical Process

<table>
<thead>
<tr>
<th>( \text{C}_6\text{H}_5\text{CH(CH}_3\text{)_2} )</th>
<th>( \Delta H^\circ \text{(kJ/mol)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>\text{O}_2</td>
<td>0</td>
</tr>
<tr>
<td>\text{C}_6\text{H}_5\text{C(CH}_3\text{)_2} \text{OOH}</td>
<td>-149.67</td>
</tr>
</tbody>
</table>

Source: National Institute of Standards and Technology

Equation for Energy Balance:

\[ Q = \Delta H_{\text{out}} - \Delta H_{\text{in}} + r\Delta H^\circ_f \]
Where,

\[ Q = \text{Heat absorbed or heat released in the reactor} \]
\[ \Delta H_{\text{out}} = \text{Change of enthalpy in the system out} \]
\[ \Delta H_{\text{in}} = \text{Change of enthalpy in the system in} \]
\[ r = \text{Rate of reaction} \]
\[ \Delta H^o_r = \text{Heat of formation at 298.15 K} \]

Enthalpy change for the component

\[ \Delta H = \int_{T_1}^{T_2} C_p dT \]
\[ \Delta H = A(T_2 - T_1) + B(T_2^2 - T_1^2)/2 + C(T_2^3 - T_1^3)/3 + D(T_2^4 - T_1^4)/4 \]

where,
\[ T_1 = \text{Reference Temperature (298.15 K)} \]
\[ T_2 = \text{Input / Output Temperature} \]

Enthalpy change for the inflow,

\[ T_1 = 110^\circ \text{C} = 383.15 \text{ K} \]

For Cumene:

\[ \Delta H = \int_{298.15}^{383.15} C_p \, dT \]
\[ = (139.2 \times 10^{-3})(383.15-298.15) + (53.76 \times 10^{-5})(383.15^2-298.15^2)/2 + (-39.79 \times 10^{-8})(383.15^3-298.15^3)/3 + (120.5 \times 10^{-12})(383.15^4-298.15^4)/4 \]
\[ = 11.832 + 15.566 + (-3.945) + 0.411 \]
\[ = 23.864 \text{ kJ/mol} \]

For Oxygen:

\[ \Delta H = \int_{298.15}^{383.15} C_p \, dT \]
\[ = (29.1 \times 10^{-3})(383.15-298.15) + (1.158 \times 10^{-5})(383.15^2-298.15^2)/2 + (-0.6076 \times 10^{-8})(383.15^3-298.15^3)/3 + (1.311 \times 10^{-12})(383.15^4-298.15^4)/4 \]
\[ = 2.4735 + 0.3353 + (-0.06024) + 0.0044736 \]
\[ = 2.75303 \text{ kJ/mol} \]
Enthalpy change for outflow,

\[ T_2 = 115^\circ C = 388.15 \text{ K} \]

For Cumene Hydroperoxide,

\[ \Delta H = \int_{298.15}^{388.15} Cp \, dT \]

\[ = (1.345 \times 10^5)(388.15-298.15) + (3.8060 \times 10^5)(388.15^2 - 298.15^2) / 2 \]

\[ = 1210500 + 11754260.1 \]

\[ = 23859260.1 \text{ J/mol} \]

For Cumene:

\[ \Delta H = \int_{298.15}^{388.15} Cp \, dT \]

\[ = (139.2 \times 10^{-3})(388.15 - 298.15) + (5.76 \times 10^{-5})(388.15^2 - 298.15^2) / 2 + (-39.79 \times 10^{-8})(388.15^3 - 298.15^3)/3 + (120.5 \times 10^{-12})(388.15^4 - 298.15^4)/4 \]

\[ = 12.528 + 16.603 + (-4.241) + 0.446 \]

\[ = 25.336 \text{ kJ/mol} \]

For Oxygen,

\[ \Delta H = \int_{298.15}^{388.15} Cp \, dT \]

\[ = (29.1 \times 10^{-3})(388.15 - 298.15) + (1.158 \times 10^{-5})(388.15^2 - 298.15^2) / 2 + (-0.6076 \times 10^{-8})(388.15^3 - 298.15^3) / 3 + (1.311 \times 10^{-12})(388.15^4 - 298.15^4) / 4 \]

\[ = 2.619 + 0.358 + (-0.06024) + (-0.065) + (4.85 \times 10^{-3}) \]

\[ = 2.917 \text{ kJ/mol} \]

For overall enthalpy at inflow, \( \Delta H_{in} \),

\[ \Delta H_{in} = (\Delta H_{iCumene} \times N_{iCumene}) + (\Delta H_{iOxygen} \times N_{iOxygen}) \]

\[ = (23.864 \text{ kJ/mol} \times 551998 \text{ mol/h}) + (2.75303 \text{ kJ/mol} \times 185333 \text{ mol/h}) \]

\[ = 13683099.32 \text{ kJ/h} \]

For overall enthalpy at outflow, \( \Delta H_{out} \),

\[ \Delta H_{out} = (\Delta H_{oCumene Hydroperoxide} \times N_{oCumene hydroperoxide}) + (\Delta H_{oCumene} \times N_{iCumene}) + (\Delta H_{oOxygen} \times N_{iOxygen}) \]
\[ (23859.2601 \text{ kJ/kmol} \times 613330 \text{ mol/h}) + (25.336 \text{ kJ/mol} \times 367998 \text{ mol/h}) + \\
(2.917 \text{ kJ/mol} \times 61333 \text{ mol/h}) \\
= 9503960.298 \text{ kJ/h} \]

For Heat of formation, \( H_f^o \)

\[
H_f^o = \sum \Delta H_f^o_{\text{product}} - \sum \Delta H_f^o_{\text{reactant}} \\
= [-149.67 \text{ kJ/mol}] - [(-41.1 \text{ kJ/mol}) + 0 \text{ kJ/mol}] \\
= -108.57 \text{ kJ/mol} 
\]

From the overall energy balance equation,

\[
Q = \Delta H_{\text{out}} - \Delta H_{\text{in}} + r\Delta H_f^o \\
= 69753.978 \text{kJ/h} - 66.011 \text{kJ/h} + (184000 \text{ mol/h} \times -108.57 \text{kJ/mol}) \\
= -24156019.02 \text{kJ/hr} \\
= 24156019.02 \text{kJ/h} \times (1 \text{h/3600s}) \\
= -6710.005 \text{ kJ/s} 
\]

### 7.3 iCON® SIMULATION ON MATERIAL AND ENERGY BALANCES

In order to perform material and energy balance using iCON®, we have drawn conversion reactor and the respective input and output streams using standard symbols in the software. Figure 5.7 shows the diagram we have drawn in iCON®.
7.4 ERROR CALCULATION OF MATERIAL BALANCE
The table 7.3 below shows the comparison of material balance calculation between manual calculation and iCON®.

<table>
<thead>
<tr>
<th>Mass flow rate</th>
<th>Manual calculation (kmole hr$^{-1}$)</th>
<th>iCON® (kmole hr$^{-1}$)</th>
<th>Percentage error(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream 1</td>
<td>551.998</td>
<td>551.12</td>
<td>0.16</td>
</tr>
<tr>
<td>Stream 2</td>
<td>185.330</td>
<td>185.34</td>
<td>0.0054</td>
</tr>
<tr>
<td>Stream 3</td>
<td>613.33</td>
<td>614.00</td>
<td>0.11</td>
</tr>
</tbody>
</table>

Error calculation of mass flow rate of stream 1

\[
\text{Error} = \left| \frac{(551.998) - (551.12)}{551.98} \right| \times 100\% = 0.16\%
\]

Error calculation of mass flow rate of stream 2

\[
\text{Error} = \left| \frac{(185.330) - (185.340)}{185.330} \right| \times 100\% = 0.0054\%
\]

Error calculation of mass flow rate of stream 3

\[
\text{Error} = \left| \frac{(613.33) - (614.00)}{613.33} \right| \times 100\% = 0.11\%
\]

7.5 ERROR CALCULATION OF ENERGY BALANCE
The table 7.4 shows the results comparison of energy balance between manual calculation and iCON®.
### Table 7.4: Comparison of energy balance between manual and iCON® calculation

<table>
<thead>
<tr>
<th>Heat flow</th>
<th>Manual calculation (kJ/s)</th>
<th>iCON® (kJ/s)</th>
<th>Percentage error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactor 1</td>
<td>-6710.005</td>
<td>-6855.608</td>
<td></td>
</tr>
</tbody>
</table>

**Error calculation of reactor 1 energy balance**

\[
\text{Error} = \left| \frac{-6710.005 - (-6855.608)}{-6710.005} \right| \times 100\% \\
= 2.17\% 
\]
8.1 REACTOR DETERMINATION

Choosing a suitable reactor is the most important part before the reaction will be done in the real plant. It is important, especially in designing an industrial process. Furthermore, factors such as reaction conversion rate, phase reaction, and the condition of the process should be taken in selecting the type of reactor as well as designing the reactors.

The production of phenol required a multiple reaction, that is called a series reaction. Series reaction is reaction where the reactant forms an intermediate product, which will react further to form another product. The first reactor (oxidation column) consist of the reaction between Cumene and Oxygen gas to form Cumene Hydroperoxide. In this reaction, reactor that will be chosen is Plug Flow Reactor (PFR) because the reaction consists of the gas-liquid phase reaction.

For the second reactor, that is the place where the main product is being produce, which is Phenol. This process consist the reaction between Cumene Hydroperoxide with Sulphuric acids. Sulphuric acids act as catalyst of this reaction. Since that reaction is in the liquid phase and the catalyst involve also at liquid phase so that the reactor that have been choose for the second process is Continuous-Stirred Tank Reactor (CSTR). CSTR or called as vat, backmix reactor is usually primarily used for liquid phase reactions. It is normally operates at steady state and is assumed to be a perfectly mixed. Consequently, there is no time dependence or position dependence of the temperature, the concentration, or the reaction inside the CSTR.
Thus, the temperature and the concentration in the exit stream are modelled as being the same as those inside to the CSTR.

![Figure 8.1: Continuously-Stirred tank reactor.](image)

### 8.2. GENERAL MOLE BALANCE EQUATIONS.

This is the equation for the general mole balance for the CSTR. Since that this is the continuously flow reaction, so this balance equation will used molar flow rate as the parameter.

\[
\begin{bmatrix}
\text{Molar flow rate of species } j_{\text{In at } V} \\
\text{Molar flow rate of species } j_{\text{Out at } (V + \Delta V)}
\end{bmatrix} - \begin{bmatrix}
\text{Molar rate of Generation of species } j_{\text{within } \Delta V}
\end{bmatrix} + \begin{bmatrix}
\text{Molar rate of Accumulation of species } j_{\text{within } \Delta V}
\end{bmatrix} = \begin{bmatrix}
\text{Molar rate of Accumulation of species } j_{\text{within } \Delta V}
\end{bmatrix}
\]

*Molar flow rate in } - \text{Molar flow rate out} + \text{Molar Generation} = \text{Molar Accumulation}*

The general molar flow rate for the continuous reaction:

\[
F_{j0} - F_j + \int_0^V r_j dV = \frac{dN_j}{dt}
\]

It is applied to the second reactor, CSTR. For this overall reaction, we assumed that the first step reaction is very fast such that the overall reaction rate is not affected to the overall reaction. It just considered the second reaction, which is CSTR.
The reaction applied to a CSTR operated at steady state, that is the condition do not change with time:

\[ \frac{dN_j}{dt} = 0 \]

For CSTR, it assumed that the condition inlet is equal to the exit of the reactor. It means that there are no spatial variation in the rate of the reaction or perfectly mixing.

\[ \int_0^V \eta \, dV = \eta V \]

So, it takes the familiar form known as the design equation for a CSTR for a species A:

\[ F_{Ao} - F_A = -r_A V \]

The volume necessary for CSTR to reduce the entering flow rate of species A from \( F_{Ao} \) to \( F_A \) when species A is disappearing at a rate, \(-r_A\).

\[ V_{CSTR} = \frac{F_{Ao} - F_A}{-r_A} \]

### 8.3. KINEMATIC RATE EXPRESSION

The rate law is defined as the product of the concentration of the individual species to the raise of power of the species. This is the example for the rate law expression in term of concentration.

\[ -r_A = k_A C_A^\alpha C_B^\beta \]

The rate of reaction, \(-r_A\) is the number of moles of A reacting or disappearing per unit time per unit volume. \(-r_A\) is always determined based on the experimental observation.

The rate law also depend on the power law. The power law is related with the reaction order. Again, the order of reaction depend to the experimental observation. The order of reaction is the power index to which the concentration are raised based on the kinetic rate laws. The reaction is \(\alpha\) order with respect to reactant A and \(\beta\) order with respect to the reactant B. The overall order of the reaction rate, \(n\), is
\[ n = \alpha + \beta \]

For the second reaction at CSTR, the overall stoichiometric reaction involved to the production of phenol and acetone.

\[
\text{C}_6\text{H}_5\text{C(CH}_3\text{)}_2\text{OOH} \rightarrow \text{C}_6\text{H}_5\text{OH} + \text{CH}_3\text{COCH}_3
\]

1 Kmole of cumenehydroperoxide ≡ 1kmole of phenol ≡ 1kmole of acetone

Let:

\[
\text{C}_6\text{H}_5\text{C(CH}_3\text{)}_2\text{OOH} = A
\]

\[
\text{C}_6\text{H}_5\text{OH} = B
\]

\[
\text{CH}_3\text{COCH}_3 = C
\]

Therefore, the chemical equation in term of alphabetical form:

A→ B + C

Net rates of reaction:

\[
r_A = r_A
\]

\[
r_B = r_B
\]

\[
r_C = r_C
\]

The reaction stoichiometric form is:

\[
\frac{r_A}{-1} = \frac{r_B}{1} = \frac{r_C}{1}
\]

The rate of reaction of each of the species:

Cumene Hydroperoxide:

\[
r_A = -k_A C_A^\alpha
\]

Phenol:

\[
r_B = \frac{1}{-1} r_A = -r_A = k_A C_A^\alpha
\]

Acetone:

\[
r_C = \frac{1}{-1} r_A = -r_A = k_A C_A^\alpha
\]

So, the design equation for the CSTR to produce Phenol:

\[
V = \frac{F_{AO} - F_A}{k_A C_A^\alpha}
\]
8.4. STOICHIOMETRY TABLE FOR CSTR.

Let species A stand for Cumene Hydroperoxide, B for Phenol and C for Acetone.

<table>
<thead>
<tr>
<th>Species</th>
<th>Feed Rate To reactor</th>
<th>Change Within Reactor</th>
<th>Effluent Rate From Reactor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cumene Peroxide (A)</td>
<td>$F_{AO}$</td>
<td>$-F_{AO}X$</td>
<td>$F_{A}=F_{AO}(1-X)$</td>
</tr>
<tr>
<td>Phenol (B)</td>
<td>$F_{BO} = \Theta_{B}F_{AO}$</td>
<td>$-F_{AO}X$</td>
<td>$F_{B}=F_{AO}(\Theta_{B}-X)$</td>
</tr>
<tr>
<td>Acetone (C)</td>
<td>$F_{CO} = \Theta_{C}F_{AO}$</td>
<td>$F_{AO}X$</td>
<td>$F_{C}=F_{AO}(\Theta_{C}+X)$</td>
</tr>
<tr>
<td>Total</td>
<td>$F_{TO}$</td>
<td></td>
<td>$F_{T}=F_{TO} - F_{AO}X$</td>
</tr>
</tbody>
</table>

Where \( \Theta_{B} = \frac{F_{BO}}{F_{AO}} \), \( \Theta_{C} = \frac{F_{CO}}{F_{AO}} \)

For liquids, volume change with the reaction is negligible when no phase changes are taking place. Consequently, we can take \( \nu = \nu_{0} \)

Then, the concentration in term of conversion is:

\[
C_{A} = \frac{F_{AO}}{\nu_{0}} (1-X) = C_{AO} (1-X)
\]

<table>
<thead>
<tr>
<th>Species</th>
<th>In term of flow rate</th>
<th>In term of concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cumene Hydroperoxide</td>
<td>$F_{A}=F_{AO}(1-X)$</td>
<td>$C_{A}=C_{AO}(1-X)$</td>
</tr>
<tr>
<td>Phenol</td>
<td>$F_{B}=F_{AO}(\Theta_{B}-X)$</td>
<td>$C_{B}=C_{AO}(\Theta_{B}-X)$</td>
</tr>
<tr>
<td>Acetone</td>
<td>$F_{C}=F_{AO}(\Theta_{C}+X)$</td>
<td>$C_{C}=C_{AO}(\Theta_{C}+X)$</td>
</tr>
</tbody>
</table>
8.5. CATALYST

A catalyst is a substance that affects the rate of a reaction but emerges from the process unchanged. A catalyst usually changes a reaction rate by promoting a different molecular path for the reaction. A catalyst can either accelerate or slow down the formation of the particular product species. A catalyst changes only the rate of a reaction and it does not affect the equilibrium.

In this process, Sulphuric Acids are used as the catalyst for the cleavage of Cumene Hydroperoxide into Phenol and Acetone. It is homogeneous catalysis that concern process in which a catalyst is in solution with at least one of the reactants.
9.1 BALANCED STOICHIOMETRY EQUATION

The balanced stoichiometric equations of the production of phenol process are shown as below:

\[ C_6H_5CH(CH_3) _2 (l) + O_2 (g) \rightarrow C_6H_5C(CH_3) _2 OOH (l) \] \hspace{1cm} \text{(1)}

\[ C_6H_5C(CH_3) _2 OOH (l) \rightarrow C_6H_5OH + CH_3COCH_3 \] \hspace{1cm} \text{(2)}

9.2 BY-PRODUCT OF THE PROCESS AND SEPARATION METHOD

9.2.1 Introduction

Distillation is a purification technique in which compounds with different boiling points can be separated by controlled heating. The performance of the distillation column is based on feed condition, state of feed, composition of feed and internal liquid and fluid flow condition. During the reaction to produce phenol, the byproducts, acetone and acetophenone are produced and a few of separation methods are used to get rid of the byproduct.

9.2.2 Separation method

Fractional distillation is used for the mixture whose boiling points are similar. Acetone is passed through the fractional distillation column which operated at 65°C. The boiling point of acetone is 56.7°C thus it will be volatile. Vacuum distillation is distillation at a reduced pressure. It is used to distill compounds that have a high boiling point or any compound
which might undergo decomposition on heating at atmospheric pressure. Since the boiling point of a compound is lower at a lower external pressure, the compound will not have to be heated to high temperature in order for it to boil. The vacuum is provided either by a water aspirator or by a mechanical pump. The unreacted cumene is discharged to the purifying column after pass through the vacuum distillation column. The methylstyrene is distilled off from the distillation column 1. Cumene can be purified by catalytic hydrogenation of methylstyrene. The cumene stream which contains methylstyrene can be supplied to a hydrogenation reactor, hydrogenated over a two-bed nickel and noble metal catalyst system to produce pure cumene. The cumene stream can be recycled as a feed stream. The extracting agent, diethylene, is fed to the extraction distillation column. The pure phenol is coming off from the head of the extraction column and acetophenone is drawn out as a side stream.

![Figure 9.1: Short path vacuum distillation apparatus with vertical condenser](image)

### 9.3 QUALITY AND STANDARD

Phenol also known as carbolic acid is a caustic, poisonous, white crystalline compound, $\text{C}_6\text{H}_5\text{OH}$, derived from benzene. It is widely used in resins, plastics, and pharmaceuticals and in dilute form as a disinfectant and antiseptic. The molecular weight and density of phenol are 94.11g/mole and 1.07g/cm$^3$ respectively.

By using the process we studied, 21.3% of phenol, 47.2% of cumene, 33.1% of acetone, 7.9% of oxygen and 2.3% of cumene peroxide will be produced. Table 9.1 show the percentage of composition of the product.
Table 9.1 Percentage of composition of phenol production

<table>
<thead>
<tr>
<th>COMPOUND (wt %)</th>
<th>%COMPOSITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phenol</td>
<td>21.3</td>
</tr>
<tr>
<td>Cumene</td>
<td>47.2</td>
</tr>
<tr>
<td>Oxygen</td>
<td>7.9</td>
</tr>
<tr>
<td>Acetone</td>
<td>21.3</td>
</tr>
<tr>
<td>Cumene peroxide</td>
<td>2.3</td>
</tr>
</tbody>
</table>
CHAPTER X

TRANSPORT PHENOMENON 1

10.1 Introduction

From the process flow diagram of the production of phenol, the pump which delivers the products from the cleavage reactor (R-101) along stream 5 to the washing tower (T-102) is chosen to be analyzed.

Here is some data acquired from the previous streams which is needed for our calculation:

Assumptions made:
1. We are taking the properties of the component with highest composition, cumene properties as the properties of the stream in our calculations.

Density of fluid in stream 5: \( \rho = 845 \text{ kg/m}^3 \)

Viscosity of fluid in stream 5: \( \mu = 0.621 \times 10^{-3} \text{ Pa.s} \)

Volumetric flow rate along stream 5: \( \dot{V} = \frac{\dot{m}}{\rho} \)

\[
\frac{\dot{V}}{} = \frac{20.58 \text{ kg/s}}{845 \text{ kg/m}^3} = 0.024 \text{ m}^3/s
\]

Given \( \dot{V} = A_f \times v_f ; \) where \( A = \pi \left( \frac{D}{2} \right)^2 \)

We choose to use 8 inch nominal pipe size, schedule 40 for this section, hence, the inside diameter, \( D = 0.2027 \text{ m} \). The cross-sectional area,

\[
A = \pi \left( \frac{0.2027}{2} \right)^2
\]
\[ A = 0.0323 \, m^2 \]

We know that,
\[ \dot{V} = 0.024 \, m^3/s; \quad \text{where } \dot{V} = A \times \dot{v} \]

Hence, \[ \dot{v} = \frac{\dot{V}}{A} \]

\[ \dot{v} = \frac{0.024 \, m^3/s}{0.0323 \, m^2} \]

\[ \dot{v} = 0.743 m/s \]

Hence, Reynolds Number of the flow:
\[ N_{Re} = \frac{D \dot{v} \rho}{\mu} \]

\[ N_{Re} = \frac{0.2027 \, m \times 0.743 \, m/s \times 845 \, kg/m^3}{0.621 \times 10^{-3} \, kg/m\, s} \]

\[ N_{Re} = 204931 \]

Since \( N_{Re} > 4000 \), it is a turbulent flow.

10.2 Friction loss calculation

Assumptions made:
1. The friction produced by the pump is negligible.
2. The pipe size is exactly the same along the pipe.
3. The volumetric flow rate is constant along the flow.
4. Pump efficiency is assumed as 80%.

10.2.1 Mechanical Energy Balance

The mechanical energy balance equation:

\[
\frac{1}{2\alpha} (v_{2av}^2 - v_{1av}^2) + g(z_2 - z_1) + \frac{P_2 - P_1}{\rho} + \sum F + W_z = 0
\]

Eliminating kinetic energy, since the flow rate is assumed constant, \( v_{2av}^2 - v_{1av}^2 = 0 \);

Hence,

\[
g(z_2 - z_1) + \frac{P_2 - P_1}{\rho} + \sum F + W_z = 0
\]

(1)

where \( \sum F = (4f \frac{AL}{D} + K_{ce} + K_e + K_f) \frac{v^2}{2} \)

So, we need to calculate total friction losses, \( \sum F \) in order to perform mechanical energy balance calculation.

10.2.2 Friction losses along pipe of stream 5

i. Contraction loss at reactor exit;

\[
\frac{A_5}{A_{R-101}} \text{ is assumed zero as the diameter of the reactor is large compared to diameter of the pipe.}
\]

For turbulent flow, \( \alpha = 1.0 \)

\[
K_c = 0.55 \left(1 - \frac{A_5}{A_{R-101}}\right)
\]

\[
K_c = 0.55 (1 - 0) = 0.55
\]

\[
h_c = K_c \frac{v^2}{2\alpha}
\]

\[
= 0.55 \times \frac{0.743^2}{2(1.0)} = 0.152 \text{ J/kg}
\]

ii. Friction in the straight pipe;
Same pipe size from the reactor to the washing tower;

\[ N_{Re} = 204931 \]

\[ D = 0.2027 \text{ m} \]

\[ v = 0.743 \text{ m/s} \]

Using commercial steel pipe roughness; \( \varepsilon = 0.000046 \text{ m} \)

Relative roughness, \( \frac{\varepsilon}{D} = \frac{0.000046}{0.2027} = 0.000227 \)

From Moody chart, fanning friction factor, \( f = 0.00375 \)

Total length of pipe connecting reactor and washing tower;

\[ \Delta L = 1 + 2 + 5 + 1 = 9 \text{ m} \]

\[ F_f = 4 \ f \ \frac{\Delta L \ v^2}{D} \]

\[ = 4 \times 0.00375 \times \frac{9}{0.2027} \times \frac{0.743^2}{2} \]

\[ = 0.184 \text{ J/kg} \]

iii. Friction in 3 elbows (90°);

Numbers of velocity heads, \( K_f = 0.75 \)

\[ h_f = 3 \ K_f \ \frac{v^2}{2} \]

\[ = 3 \times 0.75 \times \frac{0.743^2}{2} = 0.621 \text{ J/kg} \]

iv. Expansion loss at washing tower inlet;

\[ \frac{A_s}{A_{R-101}} \] is assumed zero as the diameter of the reactor is large compared to diameter of the pipe.

For turbulent flow, \( \alpha = 1.0 \)

\[ K_{es} = \left(1 - \frac{A_s}{A_{E1}}\right)^2 = (1 - 0)^2 = 1.0 \]
\[ h_{ex} = K_{ex} \frac{v^2}{2} = 1.0 \times \frac{0.743^2}{2} = 0.276 \text{ J/kg} \]

Hence, total friction loss:

\[ \sum F = \left(4 f \frac{\Delta L}{D} + K_{ex} + K_e + K_f \right) \frac{v^2}{2} \]

\[ \sum F = 0.152 + 0.184 + 0.621 + 0.276 \]

\[ = 1.233 \text{ J/kg} \]

Substituting \( \sum F = 1.233 \text{ J/kg} \) into material balance equation (1) in section 10.2.1:

\[ g(z_2 - z_1) + \frac{P_2 - P_1}{\rho} + \sum F + W_s = 0 \]

\[ 9.81(5 - 1) + \frac{(151.988 - 101.325) \times 10^3}{845} + 1.233 + W_s = 0 \]

\[ W_s = -100.43 \text{ J/kg} \]

We know that \( W_s = -\eta W_p \):

Assuming the efficiency of the pump is 80%,

\[ W_p = -\frac{W_s}{\eta} = \frac{100.43}{0.8} = 125.54 \text{ J/kg} \]

Hence, pump power, \( P = \dot{m} W_p \)

\[ = 20.58 \text{ kg/s} \times 125.54 \text{ J/kg} \]

\[ = 2.584 \text{ kW} \]

10.3 Performance rating of pump
Figure 10.1: unit operation involves pump at the second reactor

Assumptions made:
1. The position of the pump is taken as the reference point.
2. \( Z_1 \) is the reference height from the reactor to the pump.
3. \( Z_2 \) is the reference height from the washing tower to the pump.
4. Pump efficiency is assumed as 80%.

### 10.3.1 Suction Head Calculation

Let A denote the outlet from the reactor,

\[
Z_A = +1 \text{ m} \\
\alpha = 1.0 \\
\rho = 845 \text{ kg/m}^3 \\
u_A = v = 0.743 \text{ m/s} \\
\]

\[
H_A = \frac{P_A}{\rho} + g Z_A + \frac{\alpha u_A^2}{2} \\
H_A = \frac{101325}{845} + 9.81 \times 1 + \frac{1.0 \times 0.743^2}{2} \\
= 130 \text{ m}^2/\text{s}^2
\]

### 10.3.2 Discharge Head Calculation

Let B denotes the inlet stream of the washing tower,

\[
Z_B = +5 \text{ m} \\
\alpha = 1.0 \\
\rho = 845 \text{ kg/m}^3 \\
u_B = v = 0.743 \text{ m/s} \\
\]

\[
H_B = \frac{P_B}{\rho} + g Z_B + \frac{\alpha u_B^2}{2} \\
H_B = \frac{151988 \times 10^3}{845} + 9.81 \times 5 + \frac{1.0 \times 0.743^2}{2} \\
= 130 \text{ m}^2/\text{s}^2
\]
\[ S = 229.19 \text{ } m^2/s^2 \]

### 10.3.3 Pump Fluid Power Calculation

Total Head, \( \Delta H = H_B - H_A \)

\[ \Delta H = 229.19 - 130 \]

\[ \Delta H = 99.19 \text{ } m^2/s^2 \]

Total Head in unit length, \( \frac{\Delta H}{g} = \frac{99.19 \text{ } m^2/s^2}{9.81 \text{ } m/s^2} \)

\[ = 10.1 \text{ } m \]

We know that;

Total Head, \( \Delta H = 99.19 \text{ } m^2/s^2 \)

Mass flow rate, \( \dot{m} = 20.58 \text{ } kg/s \)

Fluid Power, \( P_f = \dot{m} \Delta H \)

\[ = 20.58 \text{ } kg/s \times 99.19 \text{ } m^2/s^2 \]

\[ = 2.041 \text{ } kW \]

### 10.3.4 Net Positive Suction Head (NPSH) Calculation

![Diagram](image)

Figure 10.1: unit operation involves pump at the second reactor

\[ p_1 = 101325 \text{ } Pa \quad \rho = 845 \text{ } kg/m^3 \]
\[ Z_i = +1 \text{ m} \quad \quad \nu = 0.743 \text{ m/s} \]

Friction loss in suction line to the pump, \( \Sigma F \):

i. Contraction loss at reactor exit;
\[
\alpha = 1.0
\]
\[
K_c = 0.55 \left(1 - 0\right) = 0.55
\]
\[
h_c = \frac{K_c \nu^2}{2\alpha}
\]
\[
h_c = 0.55 \times \frac{0.743^2}{2(1.0)} = 0.152 \text{ J/kg}
\]

ii. Friction along straight pipe of suction line;
\[
\Delta L = 1 + 2 = 3 \text{ m}
\]
\[
F_f = 4 f \frac{\Delta L \nu^2}{D \frac{2}{2}}
\]
\[
= 4 \times 0.00375 \times \frac{3}{0.2027} \times \frac{0.743^2}{2}
\]
\[
= 0.0613 \text{ J/kg}
\]

iii. Friction in elbow (90\(^\circ\));
Numbers of velocity heads, \( K_f = 0.75 \)
\[
h_f = \frac{K_f \nu^2}{2}
\]
\[
= 0.75 \times \frac{0.743^2}{2} = 0.207 \text{ J/kg}
\]

Hence, total friction loss in suction line, \( \Sigma F \) is,
\[
\Sigma F = h_c + F_f + h_f
\]
\[
\Sigma F = 0.152 + 0.0613 + 0.207
\]
\[
\Sigma F = 0.4203 \text{ J/kg}
\]
Table 10.1 vapour pressure of components in stream 5

<table>
<thead>
<tr>
<th>Components</th>
<th>Mole fraction</th>
<th>Vapour pressure (kPa)</th>
<th>Partial pressure (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cumene</td>
<td>0.472</td>
<td>4.667</td>
<td>2.203</td>
</tr>
<tr>
<td>Phenol</td>
<td>0.213</td>
<td>0.467</td>
<td>0.099</td>
</tr>
<tr>
<td>Acetone</td>
<td>0.213</td>
<td>24.000</td>
<td>5.112</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0.079</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Cumene hydroperoxide</td>
<td>0.023</td>
<td>18.665</td>
<td>0.429</td>
</tr>
</tbody>
</table>

\[ p_{vp} = 2.203 + 0.099 + 5.112 + 0.429 \]
\[ = 7.843 \text{kPa} \]

Net Positive Suction Head that will be available, \((NPSH)_A\) at the pump suction:

\[
g(NPSH)_A = \frac{p_1}{\rho} - \frac{p_{vp}}{\rho} + gz_1 - \frac{v^2}{2} - \Sigma F
\]
\[
= \frac{101325}{845} - \frac{7.843 \times 10^3}{845} + 9.81 \times 5 - \frac{0.743^2}{2} - 0.4203
\]
\[ = 158.98 \text{ m}^2/\text{s}^2 \]

\[
(NPSH)_A = \frac{158.98 \text{ m}^2/\text{s}^2}{9.81 \text{ m/s}^2}
\]

\[
(NPSH)_A = 16.21 \text{m}
\]

### 10.3.5 Pump Performance Curve

Table 10.2 Data-data calculated by HYSYS in plotting pump performance curve

<table>
<thead>
<tr>
<th>Volumetric Flow Rate ((m^3/h))</th>
<th>Total Head (m)</th>
<th>((NPSH)_A ) ((m))</th>
<th>Efficiency (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>10.1122</td>
<td>16.23</td>
<td>0</td>
</tr>
<tr>
<td>3.38</td>
<td>10.1083</td>
<td>16.55</td>
<td>20</td>
</tr>
<tr>
<td>7.82</td>
<td>10.1055</td>
<td>16.78</td>
<td>37</td>
</tr>
<tr>
<td>-------</td>
<td>---------</td>
<td>--------</td>
<td>-------</td>
</tr>
<tr>
<td>12.07</td>
<td>10.1017</td>
<td>17.27</td>
<td>53</td>
</tr>
<tr>
<td>16.02</td>
<td>10.0974</td>
<td>17.88</td>
<td>69</td>
</tr>
<tr>
<td>19.57</td>
<td>10.0929</td>
<td>18.35</td>
<td>80</td>
</tr>
<tr>
<td>23.71</td>
<td>10.0892</td>
<td>18.72</td>
<td>85</td>
</tr>
<tr>
<td>27.16</td>
<td>10.0869</td>
<td>19.26</td>
<td>82</td>
</tr>
<tr>
<td>31.20</td>
<td>10.0828</td>
<td>19.68</td>
<td>65</td>
</tr>
<tr>
<td>35.01</td>
<td>10.0791</td>
<td>19.75</td>
<td>40</td>
</tr>
</tbody>
</table>

**Figure 10.2** Pump performance curve plot using data from iCON®

10.4 iCON® calculation

10.4.1 Introduction

For analysis of the pump, iCON® calculation is carried out to compare the results with our manual calculation. By using iCON®, the total head, fluid power and \((NPSH)_A\) of the pump are determined. Consequently, comparison results between manual and iCON® calculation is used to confirm the consistency and accuracy of our manual calculation.

10.4.2 Calculation of Pump

For this analysis, the inlet temperature is same with the reaction temperature, which is 70°C. Meanwhile, the inlet pressure is at atmospheric pressure, \(P = 101325 Pa\) and the outlet
pressure is assumed to be $151988 \text{ Pa}$. After the efficiency of the pump is set to 80%, iCON® calculation of the pump is then run. We are interested in the results of total head and pump power. Finally, the result of iCON® calculation is compared with the result of manual calculation.

![Figure 7.2: iCON® Calculation of Pump](image)

**Figure 10.3:** iCON simulator to the unit operation of pump

<table>
<thead>
<tr>
<th>Table 10.3 Comparison of Manual Calculation and iCON® Calculation of Pump</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manual Calculation</td>
</tr>
<tr>
<td>Total Head, $\Delta H$ ($m$)</td>
</tr>
<tr>
<td>Pump Power, $P_f$ ($kW$)</td>
</tr>
</tbody>
</table>

According to table 10.3, we found out that the percentages of error of total head and pump power are quite significant. However, the occurrence of errors is due to some mistakes and differences between the data sources. Firstly, assumptions are made in order to simplify our manual calculation. For instance, the relative height of the reactor in the suction line to the pump, $Z_1$ and the relative height of the evaporator in the discharge line from the pump, $Z_2$ is assumed to be at 1m and 5m respectively. This may contribute to error because the values of $Z_1$ and $Z_2$ in the iCON® calculation cannot be set accordingly. Furthermore, the efficiency of the pump is set to be 80% in iCON® calculation which is an approximate
It is because the actual efficiency of the pump may not be ideally have 80% efficiency. Besides that, the error percentage of the total head is partly contributed by the liquid density of components in stream 5. The density in manual calculation is assumed same as the major component, cumene but the density used in iCON® is based on the data input in iCON®.

10.5 COMPUTATIONAL FLUID DYNAMIC (CFD)

Computational Fluid Dynamics (CFD) is the science of predicting fluid flow, heat transfer, mass transfer, chemical reactions and related phenomena by solving the mathematical equations which govern these processes using a numerical process. The main application of CFD is as an engineering method, to provide data that is complementary to theoretical and experimental data. The result of CFD analyses is also used in conceptual studies of new designs, detailed product development, troubleshooting and redesign.

Figure 10.4: Typical CFD presentation for heat exchanger
CHAPTER XI

CONCLUSION

The process that we studied for the production of phenol is oxidation of cumene process. Cumene is used as the raw material for this process. First of all, cumene is feed into the oxidation vessel and some dilute soda ash solution is added to maintain the pH. The mixer is exposed to compressed air until the cumene has converted into cumene peroxide. The cumene peroxide is cleaved to phenol and acetone. Sulphuric acid as the catalyst has been added to the reactor while reactions take place. In order to separate the main product which is the phenol and the by-product which is the acetone, we have to use the method of distillation. Distillation is a method of separating mixtures based on differences in their volatilities in a boiling liquid mixture. Besides, the friction losses and performance rating of a pump and a compressor also apply in this project.

After analysis properties of phenol, we found that there are many side effects if we expose to phenol such as irritation, corneal damage or blindness in humans. It is not only hazardous to our health but also harmful to the environment. A good management of the by-products and waste that produced is needed to make sure the environment is being protected.

Demand of the phenol is increasing year by year from 2009 to 2015. From last year data, estimation had been made until year 2015 which shown an increase quantity from 7.9m tonnes in 2009 to reach 10.6m tonnes by 2015.
REFERENCES


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http://www.shell.com/home/content/chemicals/products_services/our_products/phenol_acetone_nonene/phenol/product_overview/ [6 March 2011]


APPENDIX

APPENDIX A  MSDS ACIDIFIED WATER
APPENDIX B  MSDS ACETONE
APPENDIX C  MSDS ACETOPHENONE
APPENDIX D  CUMENE
APPENDIX E  CUMENE HYDROPEROXIDE
APPENDIX F  PHENOL
APPENDIX G  MALAYSIA ENVIRONMENTAL LAW
APPENDIX H  ICON SIMULATION