Modelling and Optimizing 2-Ethylhexanol Production from Propylene and Synthesis Gas, Using A Case Study of Aspen Hysys

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Abstract- 2-Ethylhexanol (2-EH) is a branched, eight-carbon alcohol with the molecular formula $C_8H_{18}O$. It is an eight-carbon alcohol that belongs to the family of branched alcohols. 2. Ethylhexanol is a colourless liquid that is soluble in organic solvents but insoluble in water. It also has a slight odour. By using ASPEN HYSYS as a case study, this research project aims to simulate and optimize the manufacture of 2-Ethylhexanol from propylene and synthesis gas. Using Aspen HYSYS chemical engineering software, a process plant was simulated to produce 5000 tons of 2-ethylhexanol annually using propylene and synthesis gas as feedstocks. To remove contaminants that could harm the rhodium catalyst used in the hydroformylation process, fresh propylene and syngas are treated. The plant needed to be optimized when the simulation was over, thus an optimizer that was included in the program and an optimizer spreadsheet containing the parameters were used. With this, an energy analysis was activated to calculate the amount of energy saved. The energy analyzer showed 2.45% energy savings once the first simulation results were made available, which provided a sense of the changes. The simulation results showed that the process can produce 2-ethylhexanol with a purity of 100% after optimizing.

I. INTRODUCTION

1.1 Background of Study

2-Ethylhexanol (2-EH) is a branched, eight-carbon alcohol with the molecular formula $C_8H_{18}O$. After the lighter alcohols (those with one to four carbons such as methanol or butanol) 2-Ethylhexanol is the most important synthetic alcohol (Mohammad *et al.,* 2020). 2-Ethylhexanol occurs naturally in food, as it is used as a flavour volatile and is approved as an indirect food additive by the U.S. Food and Drug Administration (FDA). A flavour volatile is a compound naturally present in a food or added by the manufacturer (Chongran *et al.,* 2023). 2-Ethylhexanol is an alcohol that is a colourless liquid at room temperature with a slightly floral odour or it is a clear, mobile and neutral liquid with a characteristic odour. It is miscible with most common organic solvents but its miscibility with water is very limited (Poulikidou *et al.,* 2017). 2-Ethylhexanol is an important organic chemical as it is used as a chemical intermediate and an alternative fuel. For example, its carboxylic acid esters such as dioctyl terephthalate (DOTP), dioctyl phthalate (DOP) and dioctyladipate (DOA) are widely used as plasticizers, especially in polyvinylchloride manufacturing. Other uses include the production of intermediates for acrylic surface coatings, diesel fuel and lube oil additives and surfactants. 2-Ethylhexanol is used as a pesticide-inert ingredient in pesticide formulations applied to growing crops, raw agricultural commodities (RAGs) or animals (Dennis and Elliot, 2012).

The industrial production of Ethylhexanol comprises of three reaction steps: propylene hydroformylation to n-butanal, n-butanal self-condensation to 2-ethyl-2-hexenal (2E2H) and 2-ethyl-2-hexenal hydrogenation to 2-Ethylhexanol. The hydrogenation of 2-ethyl-2-hexenal is composed of the following processes: crude hydrogenation and refined hydrogenation with the support of some catalysts like Cu or Ni (Raghda and Alaa, 2019). Today, nearly all2-Ethylhexanol is produced by catalytic hydro formylation of Propylene with Synthesis gas (Carbon monoxide and Hydrogen). The catalytic process now mostly uses Rhodium catalysts rather than the older cobalt hydro carbonyl catalysts (Reinhard and Hermann, 2014).

Optimization of a process is simply to maximize the production of 2-Ethylhexanol while minimizing the consumption of resources such as raw materials, energy, and catalysts. The optimization process involves the running of a simulation with various

input parameters and constraints to identify the optimal operating conditions that lead to the highest possible production of 2-Ethylhexanol while meeting the desired product specifications. This optimization will contribute to a more efficient and cost-effective production process. This is achieved by utilizing Aspen HYSYS and Aspen Optimizer.

Heat integration is a crucial aspect of the project, aiming to enhance the overall energy efficiency of the 2-Ethylhexanol production process. It involves the integration of heat exchangers and process streams to minimize heat losses and maximize heat recovery within the plant. Yu *et al.,* (2016) stated that using Aspen HYSYS will identify potential heat integration opportunities in the process, such as the recovery of waste heat from reaction steps, distillation columns, and other unit operations. The integration of heat exchangers will help transfer heat from hot streams to cold streams, reducing the need for additional energy inputs. In this work, the optimal heat exchanger network and heat integration scheme to improve the energy efficiency of the 2-Ethylhexanol production process will be determined as this will lead to lower operating costs and a more sustainable operation.

Energy recovery is identifying and implementing strategies to recover and reuse energy within the 2-Ethylhexanol production process. Energy recovery can be achieved through various methods, including process stream recycling, power generation from waste heat, and heat-to-power conversion technologies (Poulikidou *et al.,* 2017). The ultimate aim of energy recovery aspect is to minimize energy wastage and increase the overall energy efficiency of the production process. This not only contributes to cost savings but also reduces the environmental impact of the plant. By integrating optimization, heat integration, and energy recovery aspects into the project, the study aims to provide a comprehensive and sustainable approach for the efficient production of 2-Ethylhexanol from propylene and synthesis gas. Modelling and simulation play a crucial role in the design and optimization of chemical processes. Modelling involves creating mathematical representations of the chemical reactions and physical phenomena involved in the production of 2-Ethylhexanol. These models help to understand the underlying mechanisms, predict behaviour and identify potential bottlenecks or limitations in the production process (Mike, 2016). ASPEN HYSYS is a powerful simulation tool widely used in the industry for such purposes as it describes the reaction mechanism, the catalyst used, and the key process parameters that influence the conversion and selectivity of the reaction (Ikpaki *et al.,* 2021). Using simulation software like Aspen HYSYS, you can input the models and parameters to simulate the entire production process virtually. This allows for observation of the system's behaviour under various conditions, test different process configurations, and predict the process performance without conducting actual experiments (Ghaemi and Zerehsaz, 2018).

In this work, modelling, simulation, and optimization will be integrated to accelerate the development process, minimize experimental efforts and achieve a more reliable and efficient production of 2-Ethylhexanol.

2.1 Overview of Propylene

Propylene, also known as propene, with the relative molecular mass of 42.08 has its structural and molecular formula to be $H_2C{=}CH\text{-}CH_3$ and C_3H_6 respectively is an important organic compound in the petrochemical industry that is a gaseous hydrocarbon that belongs to the alkene group of compounds, characterized by a double bond between two carbon atoms. Propylene is derived from fossil fuels, primarily petroleum, through various refining and cracking processes. Propylene is one of the fastest growing petrochemicals driven primarily by the high growth rate of polypropylene and the consumption of propylene is 64% (Ahlgren *et al.,* 2015). Propylene is a crucial compound in the petrochemical industry, playing a significant role in the production of plastics, chemicals, fuels, and other materials that are widely used in our daily lives. Propylene is primarily produced as a by-product of the petroleum refining process and the cracking of hydrocarbon feed stocks, such as naphtha, gas oil, or propane. It can also be produced from other sources, such as coal, natural gas, or biomass. The largest application of propylene is in the production of polypropylene (PP), which is one of the most widely used plastics worldwide. PP is used in a variety of products, including packaging materials, textiles, automotive parts, and consumer goods (Hackl *et al.,* 2016). Propylene is a versatile building block for the production of various chemical intermediates, such as propylene oxide, acrylonitrile, cumene, and isopropanol. These intermediates are further processed to manufacture a wide range of

products, including polyurethanes, solvents, paints, adhesives, and synthetic fibres. Propylene can be used as a fuel for heating, cooking, and as a propellant in aerosol products. It is also a component in liquefied petroleum gas (LPG) and can be used as a substitute for propane in certain applications. Propylene is used as a refrigerant in certain systems due to its low boiling point and favourable thermodynamic properties (Zhang *et al.,* 2016). It is considered an environmentally friendly alternative to chlorofluorocarbons (CFCs) and hydro-chlorofluorocarbons (HCFCs), which contribute to ozone depletion and global warming. Propylene finds applications in various other industries, such as pharmaceuticals, cosmetics, detergents, lubricants, and rubber manufacturing. Propylene is flammable and should be handled with caution. It can form explosive mixtures with air and can be ignited by open flames, sparks, or electrical equipment. Proper storage, handling, and ventilation are necessary to ensure safe usage (Fujiwara *et al.,* 2019).

2.1.1 Physicochemical Properties of Propylene

The physicochemical properties of propylene and its overview are;

i. Boiling and Melting Points: The boiling point of propylene is -47.7°C (-53.9°F), which means it readily vaporizes at relatively low temperatures. The melting point of propylene is -185.2°C (-301.4°F), indicating that it is a solid at extremely low temperatures.
ii. Physical State: At room temperature and atmospheric pressure, propylene exists as a colourless gas. It has a slightly sweet odour, similar to gasoline. However, it can also be liquefied under moderate pressure, allowing for ease of storage and transportation. Its molecular weight is 42.08 g/mol (Albanese, 2023).
iii. Density: The density of propylene gas is about 0.493g/cm³ at 25°C (77°F). In its liquid state, the density of propylene is approximately 0.626 g/cm³.
iv. Solubility: Propylene is sparingly soluble in water. It has a low solubility due to its nonpolar nature, meaning it does not readily mix with polar solvents like water. However, it is more soluble in organic solvents such as ethanol and acetone.
v. Vapour Pressure: Propylene has a relatively high vapour pressure, meaning it easily evaporates into the air. At room temperature, its vapour pressure is approximately 502.5mmHg (Han *et al.,* 2021).
vi. Flammability: Propylene is highly flammable and can ignite easily. Its lower flammability limit (LFL) is 2.1% by volume in air, while the upper flammability limit (UFL) is 11.4%. These limits indicate the range of concentrations in air where propylene can form flammable mixtures.
vii. Chemical Reactivity: Propylene is an unsaturated hydrocarbon, containing a double bond between two carbon atoms. This double bond makes propylene more reactive than its saturated counterpart, propane. It can undergo addition reactions, such as hydrogenation or halogenation, to form various derivatives (Both *et al.,* 2016).
viii. Stability: Propylene is relatively stable under normal conditions. It is not prone to decomposition or degradation at typical temperatures and pressures. However, it may undergo reactions under specific conditions, such as in the presence of catalysts or under high temperatures.
ix. Toxicity: Propylene is generally considered to have low toxicity. It is not known to be carcinogenic or mutagenic to humans. However, it is important to handle propylene with caution as it is flammable, and its combustion products, such as carbon monoxide and carbon dioxide, can be harmful if inhaled in high concentrations (Hreczuch *et al.,* 2016).

2.2 Synthesis Gas

The concept of synthesis gas can be traced back to the late 18th century when researchers began experimenting with the production of gases by heating various organic materials. In the late 18th century, researchers like Alessandro Volta and Philippe Lebon discovered that heating organic materials such as wood, coal, and oil in the absence of oxygen produced flammable gases (Chen and Smith, 2017). These early experiments led to the development of several gasification processes, including wood gasification and coal gasification, which involved heating these materials to produce gases like hydrogen, carbon monoxide, and methane. In the early 19th century, the Industrial Revolution

sparked increased interest in gasification as a means of producing fuel for lighting, heating, and industrial processes (Ghaemi, 2018). Coal gasification became particularly popular during this period, with the first practical coal gas plant built in England in 1813 by Frederick Winsor. Coal gasification involved the heating of coal in a controlled environment, producing a mixture of hydrogen, carbon monoxide, methane, and other gases, which could be used as fuel. In the early 20th century, the focus shifted to the production of synthetic fuels from coal, especially during times of fuel shortages such as World War I and World War II. Germany, in particular, developed large-scale coal gasification plants to produce synthetic fuels like gasoline, diesel, and aviation fuel (Ku *et al.,* 2017). The Fischer-Tropsch process, developed by German scientists Franz Fischer and Hans Tropsch in the 1920s, allowed for the synthesis of liquid hydrocarbons from coal-derived Synthesis Gas, which played a crucial role in the German war effort. In the mid-20th century, natural gas became the dominant fuel source, and the interest in synthesis gas declined. However, the oil crises of the 1970s led to renewed interest in alternative energy sources, including Synthesis Gas (Li *et al.,* 2016). Today, synthesis gas is primarily produced from natural gas and biomass through various processes such as steam methane reforming, partial oxidation, and biomass gasification. Over the centuries, the understanding and utilization of synthesis gas have evolved significantly, driven by the need for alternative energy sources and the development of more efficient and environmentally friendly processes. Its versatility and potential as a clean energy source continue to make it a subject of interest for researchers and engineers today (Raghda and Alaa, 2019).

2.2.1 Properties of Synthesis Gas

Synthesis gas, often abbreviated as Syn Gas, is a versatile fuel and chemical intermediate that is produced through the gasification or reforming of carbonaceous materials such as coal, natural gas, petroleum, biomass, or other carbon-containing feed stocks. It is a mixture of carbon monoxide (CO), hydrogen (H_2), and other minor gases, with CO and H_2 being the primary components. Synthesis Gas has several properties that make it valuable for various applications (Arvidsson *et al.,* 2016). Here are some key properties of synthesis gas:

i. Composition: Synthesis Gas typically consists of carbon monoxide (CO) and hydrogen (H_2) as the major constituents. The molar ratio of CO to H_2 can vary depending on the production process and feedstock used. The ratio of CO to H_2 is often referred to as the "Synthesis Gas ratio" and is an important parameter for specific applications.

ii. Heating Value: Synthesis Gas has a relatively high heating value, which refers to the amount of heat released when the gas is combusted. The heating value is influenced by the composition of the Synthesis Gas and can vary depending on the production method and feedstock. The higher heating value of Synthesis Gas ranges from about 10 to 30 mega joules per cubic meter (MJ/m^3) or 250 to 750 British thermal units per standard cubic foot (BTU/scf).

iii. Flammability: Synthesis Gas is highly flammable and can be used as a fuel in various applications. It can be combusted directly in gas turbines, internal combustion engines, or boilers to generate heat or electricity. The flammability limits of Synthesis Gas, which indicate the range of concentrations where it can sustain combustion, depend on the composition of the gas but typically range between 6% and 75% volume concentrations (Bocque *et al.,* 2016).

iv. Energy Density: Synthesis Gas has a relatively low energy density compared to liquid or solid fuels. However, its high heating value compensates for this, making it suitable for a wide range of applications. The energy density of synthesis gas is typically expressed in mega joules per cubic meter (MJ/m^3) or British thermal units per standard cubic foot (BTU/scf).

v. Carbon Monoxide Toxicity: Carbon monoxide (CO) is a component of synthesis gas and is highly toxic to humans and animals. It is odourless, colourless, and tasteless, making it difficult to detect without specialized equipment. Proper handling, ventilation, and safety measures are essential when working with Synthesis Gas to prevent exposure to high levels of carbon monoxide.

vi. Synthesis Gas Ratio: The ratio of carbon monoxide (CO) to hydrogen (H_2) in synthesis gas, known as the synthesis gas

ratio, can influence its suitability for different applications. A higher CO content is often desirable for chemical synthesis processes, while a higher H_2 content is advantageous for fuel production and energy applications.

vii. Impurities: Synthesis Gas may contain impurities depending on the feedstock and gasification/reforming process used. Common impurities include sulphur compounds, nitrogen compounds, trace metals, particulates, and tars. These impurities need to be removed or treated before the synthesis gas can be used in specific applications, such as fuel cells or downstream chemical processes (Chang *et al.,* 2022).

viii. Synthesis Gas Clean-up: To make Synthesis Gas suitable for various applications, such as catalytic reactions or fuel cells, it often requires cleaning or conditioning. Synthesis Gas clean-up involves removing impurities, adjusting the synthesis gas ratio, and controlling the temperature and pressure to meet the requirements of specific processes.

ix. Versatility: Synthesis Gas is a highly versatile fuel and chemical feedstock. It can be used as a fuel for power generation, heating.

x. Density: The density of Synthesis Gas varies depending on its composition. It is generally lighter than air, with a density ranging from 0.6 to 1.2 kilograms per cubic meter (kg/m^3). The density decreases with an increase in the hydrogen content of the synthesis gas.

xi. Boiling Points: The boiling points of CO and H_2 are relatively low. Carbon monoxide has a boiling point of -191.5℃ (-312.7℉), while hydrogen boils at -252.9 ℃ (-423.2 ℉). These low boiling points make it easier to separate and purify the components of synthesis gas (Muller *et al.,* 2018).

2.2.3 Applications of Synthesis Gas

The application of syngas, also known as synthesis gas, is wide-ranging and encompasses various sectors including energy production, chemicals manufacturing, and transportation. Its versatility and potential as a feedstock have led to numerous practical applications (Poulikidou *et al.,* 2019).

i. Power Generation: Syngas can be used as a fuel in gas turbines or internal combustion engines to generate electricity. It offers flexibility by allowing the use of different feedstocks, reducing reliance on fossil fuels, and facilitating the transition to cleaner energy sources.

ii. Chemicals and Fertilizer Production: Syngas serves as a crucial precursor in the production of a wide range of chemicals. Through various chemical reactions, syngas can be converted into methanol, ammonia, synthetic natural gas (SNG), and other valuable compounds. These chemicals are essential for manufacturing plastics, solvents, fertilizers, and other industrial products.

iii. Synthetic Fuels: Syngas can be converted into liquid fuels through a process called Fischer-Tropsch synthesis. This enables the production of synthetic hydrocarbons, such as synthetic diesel or gasoline, which can be used as drop-in replacements for conventional fossil fuels. Synthetic fuels derived from syngas can help reduce carbon emissions and provide an alternative to petroleum-based fuels.

iv. Hydrogen Production: Syngas is an important source of hydrogen, a clean and versatile energy carrier. Hydrogen produced from syngas can be used in fuel cells for electricity generation, as a feedstock in various chemical processes, or as a potential fuel for hydrogen-powered vehicles (Obringer *et al.,* 2023).

v. Waste Treatment and Recycling: Syngas can be generated from waste materials through gasification, offering an efficient and environmentally friendly method for waste treatment. By converting waste into syngas, it is possible to recover energy and valuable by-products while minimizing the environmental impact of waste disposal.

vi. Carbon Capture and Storage (CCS): Syngas production can be integrated with carbon capture technologies to mitigate greenhouse gas emissions. By capturing and storing carbon dioxide (CO_2) generated during the gasification process, syngas production can become a cleaner and more sustainable energy option (Subagjo and Gunawan, 2019).

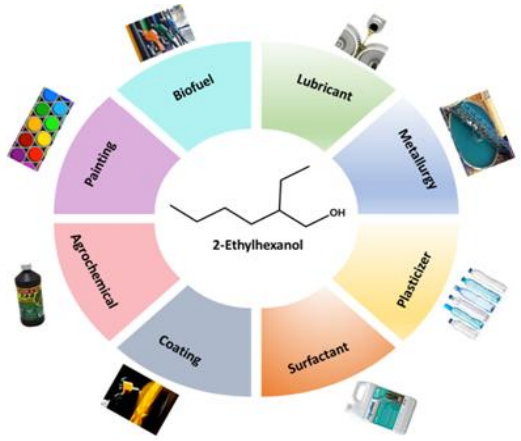

Figure 2.1: Applications of 2-ethylhexanol in different fields.

2.3 2-Ethylhexanol

2-Ethylhexanol is a chemical compound with the molecular formula $C_8H_{18}O$ and the structural formula CH_3 $(CH_2)3CH$ (C_2H_5) CH_2OH. It is an eight-carbon alcohol that belongs to the family of branched alcohols. 2-Ethylhexanol is a colourless liquid with a mild odour and is insoluble in water but soluble in organic solvents (Zhang *et al.,* 2016).

2-Ethylhexanol was first discovered and synthesized in the early 20th century. It was primarily derived from the reaction of n-butyraldehyde and ethylmagnesium bromide, resulting in the formation of 2-ethylhexyl magnesium bromide. This compound was then subjected to hydrolysis to obtain 2-ethylhexanol. The industrial production of 2-ethylhexanol began in the mid-20th century. It is typically produced through the aldol reaction, where n-butyraldehyde is condensed with isobutyraldehyde, followed by hydrogenation. The resulting product is a mixture of isomers, including 2-ethylhexanol. Like many organic compounds, 2-ethylhexanol should be handled with care. It is flammable and may emit toxic fumes when heated or exposed to flames. It can cause eye and skin irritation upon direct contact. Proper safety measures, including the use of protective equipment, should be employed when working with 2-ethylhexanol (Hackl *et al.,* 2016).

2.3.1 Physicochemical Properties of 2-Ethylhexanol

Here are the physicochemical properties of 2-ethylhexanol:

i. Molecular Weight: The molecular weight of 2-ethylhexanol is approximately 130.23g/mol.
ii. Physical State: 2-Ethylhexanol exists as a liquid at room temperature and atmospheric pressure.
iii. Melting Point: The melting point of 2-ethylhexanol is around -78.2°C (-108.8°F). This is the temperature at which the solid form of the compound starts to melt and convert into a liquid.
iv. Boiling Point: The boiling point of 2-ethylhexanol is approximately 183-186°C (361-367°F). This is the temperature at which the liquid form of the compound starts to vaporize and convert into a gas.
v. Density: The density of 2-ethylhexanol is about 0.832 g/cm³ at 20°C (68°F). Density is the mass of a substance per unit volume and is an important property for determining the behaviour of a substance in various conditions.
vi. Solubility: 2-Ethylhexanol is slightly soluble in water, with an estimated solubility of about 1.1 g per 100 mm of water at 25°C (77°F). It is more soluble in organic solvents such as ethanol, acetone, and benzene.
vii. Vapour Pressure: The vapour pressure of 2-ethylhexanol is relatively low. At 20°C (68°F), the estimated vapour pressure is around 0.03 mmHg. Vapour pressure is the pressure exerted by the vapour of a substance when it is in equilibrium with its liquid phase.
viii. Refractive Index: The refractive index of 2-ethylhexanol is approximately 1.431 at 20°C (68°F). The refractive index is a measure of how much light is bent or refracted when passing through a substance.
ix. Flash Point: The flash point of 2-ethylhexanol is approximately 86°C (187°F). This is the lowest temperature at which the vapour of a substance can ignite in the presence of an ignition source.
x. Viscosity: 2-Ethylhexanol exhibits a relatively low viscosity, which means it flows easily. The estimated viscosity of 2-ethylhexanol at 20°C (68°F) is about 4.28Cp (Asmaa *et al.,* 2022).

2.3.2 Uses of 2-Ethylhexanol

i. Plasticizers: One of the primary applications of 2-ethylhexanol is as a raw material for the production of plasticizers. It is a key ingredient in the manufacturing of phthalate esters, such as di-2-ethylhexyl phthalate (DEHP). Plasticizers are added to polymers

and resins to improve their flexibility, durability, and processability. They are widely used in the production of PVC (polyvinyl chloride) products, including cables, vinyl flooring, automotive parts, and medical devices.

ii. Solvents: 2-Ethylhexanol is used as a solvent in various applications. It can dissolve a wide range of substances, including oils, resins, waxes, and dyes. Its solvency properties make it useful in industries such as paints, coatings, inks, adhesives, and cleaning agents.

iii. Chemical Intermediates: 2-Ethylhexanol serves as an important intermediate in the synthesis of other chemicals. It is used in the production of various compounds, including esters, acrylates, and ethoxylates. For example, it is a precursor in the manufacturing of 2-ethylhexyl acrylate (2-EHA), which finds applications in adhesives, paints, and textiles (Yu *et al.,* 2018).

iv. Fragrances and Flavours: Due to its mild odour and compatibility with other fragrance ingredients, 2-ethylhexanol is utilized in the production of fragrances and flavours. It acts as a diluent or carrier for the aroma compounds and helps enhance their stability and diffusion.

v. Emollients and Personal Care Products: 2-Ethylhexanol is employed in the formulation of personal care products, particularly in the production of emollients and moisturizers. It imparts a smooth, non-greasy feel and helps in the absorption of cosmetic products into the skin.

vi. Fuel Additives: In some cases, 2-ethylhexanol is used as an additive in fuel formulations, primarily in diesel fuels. It can enhance the lubricity and improve the flow properties of diesel, which can help reduce wear on fuel system components (Chongran *et al.,* 2023).

vii. Agrochemicals: 2-Ethylhexanol can be utilized in the production of pesticides and herbicides. It can act as a solvent or a component in pesticide formulations to improve their efficacy and stability.

viii. Lubricants: 2-Ethylhexanol can be used as a lubricant additive to enhance the performance of oils and greases. It improves lubricity, reduces friction, and provides better resistance to oxidation and corrosion.

ix. Herbicides: Some herbicide formulations incorporate 2-Ethylhexanol as a co-formulant or an additive to improve the efficacy and spreading properties of the active ingredients (Ikpaki *et al.,* 2021).

2.4 Pathways of 2-Ethylhexanol Production

There are three pathways of production;

2.4.1 2-Ethylhexanol Production through Biomass Fermentation and Ethanol

The ethanol- based 2- EH production route is based on a cellulosic ethanol production process, followed by acetaldehyde production and conversion to crotonaldehyde, n- butyraldehyde and finally aldolization and hydrogenation to 2-Ethylhexanol.

The process description is as follows:

i. Production of Acetaldehyde: The first step is to produce acetaldehyde. Acetaldehyde can be obtained through various methods, but one common method is the oxidation of ethanol. Ethanol is oxidized using a suitable catalyst, such as a silver-based catalyst, to produce acetaldehyde as shown in Equation 2.1.

$$2C_2H_5OH + O_2 \rightarrow 2CH_3CHO + 2H_2O$$

Equation 2.1

ii. Aldol Condensation: In the next step, acetaldehyde undergoes aldol condensation. This reaction involves the self-condensation of acetaldehyde to form crotonaldehydeas shown in Equation 2.2.

$$2CH_3CHO \rightarrow CH_3CH=CHCHO + H_2O$$

Equation 2.2

iii. Hydrogenation of Crotonaldehyde: The crotonaldehyde produced in the previous step is hydrogenated to produce 2-ethylhexanol. This reaction requires a hydrogen source and a suitable catalyst, typically a metal catalyst such as nickel or palladium as shown in Equation 2.3.

$$CH_3CH=CHCHO + 6H_2 \rightarrow CH_3(CH_2)_4CH(OH)CH_3$$

Equation 2.3

iv. Purification and Refining: After the hydrogenation step, the crude 2-ethylhexanol is obtained. However, it may contain impurities and other by-products.

Therefore, purification and refining processes are carried out to obtain a pure form of 2-ethylhexanol. This typically involves distillation and other separation techniques to remove impurities and isolate the desired product.

v. Further Processing: The purified 2-ethylhexanol can undergo further processing steps depending on its intended use. It can be used directly or undergo additional reactions to produce other chemicals or derivatives (Chrongen *et al.,* 2023).

vi.

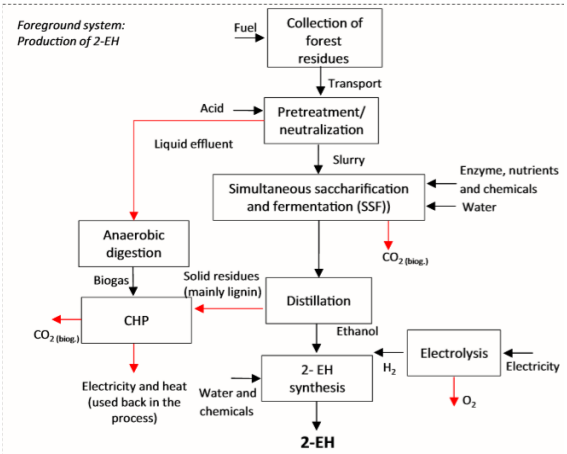

Figure 2.2: 2- Ethylhexanol Production Pathway through Biomass Fermentation and Ethanol as Intermediate Chemical (Poulikidou *et al.,* 2019).

2.4.2 2-Ethylhexanol Production through ABE Fermentation and Butanol

The 2-EH production pathway through Guerbet condensation of n- butanol is based on published data for corn stover- based acetone- butanol- ethanol (ABE) fermentation. However, this process has been adjusted to account for forest residues as feedstock using published data for both corn stover and forest ethanol.

The process description is as follows:

i. Feedstock Preparation: Biomass or feedstock (such as agricultural residues) is collected and prepared for the fermentation process.

ii. Fermentation: The feedstock is subjected to ABE fermentation using Clostridium bacteria. Fermentation takes place in a bioreactor under controlled conditions of temperature and pressure. Bacteria convert the sugars in the feedstock into acetone, butanol, and ethanol through metabolic processes.

iii. Product Recovery: The fermentation broth containing acetone, butanol, and ethanol is collected after the fermentation process.

iv. Separation: Solid-liquid separation methods, such as centrifugation or filtration, are employed to separate the biomass from the broth.

v. Distillation: The separated fermentation broth undergoes a multistage distillation process. Acetone, butanol, and ethanol are separated based on their boiling points. The desired product, butanol, is isolated as the main fraction during distillation.

vi. 2-Ethylhexanol Synthesis: The separated butanol is then subjected to a chemical conversion process to produce 2-ethylhexanol. Catalytic dehydrogenation or oxo-process are commonly used methods for this conversion. The reaction conditions involve specific temperature and pressure ranges suitable for the reaction to proceed.

vii. Purification and Refining: The synthesized 2-ethylhexanol is further purified to remove impurities and byproducts. Additional distillation or purification steps are performed to obtain a high-purity 2-ethylhexanol product.

viii. Final Product: The purified 2-ethylhexanol is collected and stored for various industrial applications, including plasticizers, solvents, and chemical intermediates.

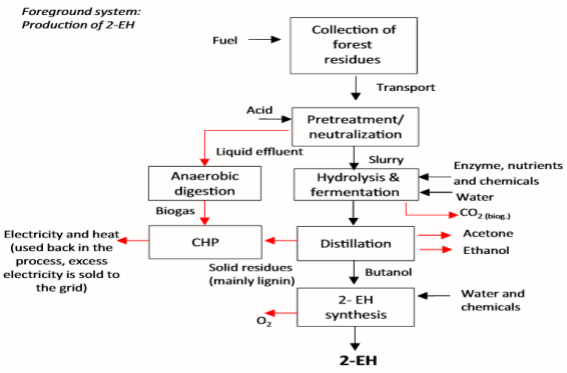

Figure 2.3: 2- Ethylhexanol Production Pathway through ABE Fermentation, Obtaining Butanol as Intermediate Chemical (Poulikidou *et al.,* 2019).

2.5 Oxo-Process Route of Production of 2-Ethylhexanol

The Oxo process is a chemical route for the production of 2-ethylhexanol (2-EH), which is an important industrial chemical used in the

manufacturing of various products, including plasticizers, solvents, and synthetic lubricants. The Oxo process involves the hydroformylation of propylene followed by hydrogenation.

The step-by-step process description is as follows:

i. Oxo Reactor (Hydro-formylation): The first step of the process is Hydro-formylation (Oxo reaction) from which the main product is n-butyraldehyde. The reactor operates at 130^0C and 350bars. The reactor residence time is 1-2 hours. The feeds to the reactor are synthesis gas (CO/H_2 mixture) and propylene in the molar ratio 2:1. The catalyst used is Cobalt Carbonyl in the solution (0.1-1.0 wt% Cobalt concentration). The synthesis gas may contain several percent methane which acts as an inert in the reactor. Traces of water introduced with the synthesis gas are not harmful. Impurities such as hydrogen sulfide and triethylamine should be carefully excluded, however to prevent reaction with the active cobalt complex to form catalytically inactive complexes.
   Oxygen should be excluded from the system, during the start-up phase when the active catalyst concentration is being established. Oxygen has been shown to inhibit cobalt hydrocabonyl formation, but once the system is operating, concentration up to 2% can be tolerated CO2 acts in the same manner as oxygen, with concentration up to 4% permissible.
   Polymer grade (99^+ %) pure propylene may be fed. Propylene feed should be vaporized & fed into the reactor as a gas. Designing for propylene conversions of greater than 95% per pass will minimize propylene losses in the blow down vent stream.
   The main reaction products are n- and iso butyraldehyde in the ratio of 4:1, the former being the required product for subsequent conversion to 2-Ethylthexanol. Within the reactor, however 6% of n-butyrablahyle product is reduced to n-butanol, 4% of isobytyraldehylde product is reduced to iso-butanol & other reactions occur to a small extent yielding molecular weight compounds (heavy ends) to the extent of 1% by weight of the butyraldehyde/butanol mixture at the reactor exit.

ii. Separation: In the separator, which follows the Oxo-reactor, the catalyst solution is separated from the oxo-raw product & recycled to the Oxo reactor.

iii. Stripper: In the stripper, the unconverted propylene is removed from the Oxo-product using fresh synthesis gas. This synthesis gas is recycled to the Oxo reactor.

iv. Distillation Column (1) Alcohol/Aldehyde Separation: The Oxo-product from the stripper passes to a distillation column, which gives a top product of mixed butyraldehyde & the bottom product alcohols.

v. Distillation Column (2) n- and iso Butyraldehyde Separation: The butyraldehydes are passed into a 2nd distillation column which separates the two butyraldehydes into an iso-butyraldehyde (top) stream containing 1.3% moles nbutyraldehyde & an n-butyraldehyde (bottom) stream containing 1.2% mole is butyraldehyde.

vi. Aldolization: The n-butyraldehyde stream passes on into an Aldolization reactor. In the Aldolization reactor, n-butyraldehyde reacts very quickly to give 2-Ethylhexanal. 2% w/w aqueous NaOH is employed as the standard industrial catalyst. The conversion efficiency is 90%. The temperature is 80-130^0C & pressure 3-10 atmospheres. The Aldolization reactor may be a mixing pump, a packed column or a stirring vessel.

vii. Second Separation: The product from the Aldolization reactor passes on to a separator where 2-Ethyhexanol is separated and then sent to a hydrogenation unit.

viii. Hydrogeneration: The 2-Ethylhexanal is reduced to 2-Ethylhexanol by hydrogen in the presence of a Raney Nickel Catalyst with a 99% conversion rate. The selectivity attained is greater than 99%. In the subsequent stages 99.8% of 2-Ethyl hexanol is recovered at a purity of 99% by weight (Poulikidou *et al.,* 2019).

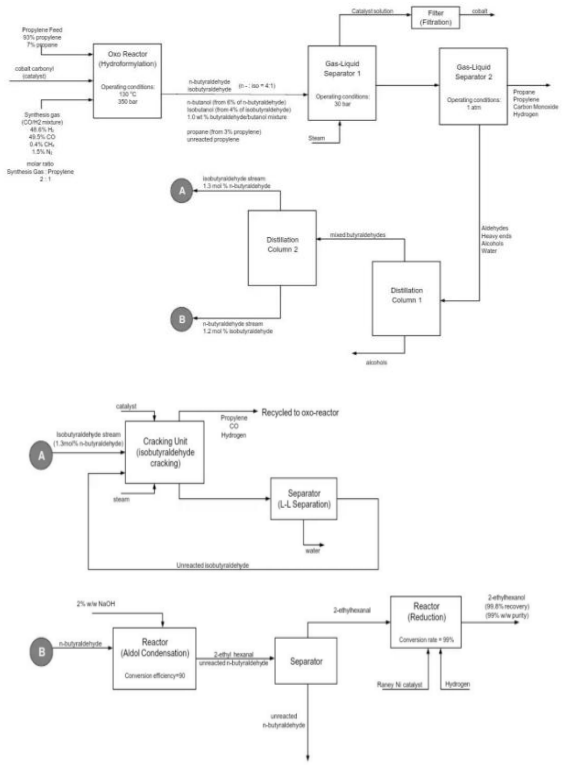

Figure 2.4: Process Flow Diagram of Hydroformulation Process (Asmaa *et al*.,2022).

2.5.1 Advantages of the Oxo-Process Route

The oxo-process route is commonly used to produce 2-ethylhexanol because it offers an efficient and economical method for its synthesis. The limitations of producing 2-ethylhexanol from ethanol and ABE fermentation in comparison to the oxo route are:

Ethanol Route

i. Energy Intensive: Dehydration of ethanol requires energy-intensive processes to remove water and produce ethylene. This can impact the overall energy efficiency of the process.
ii. Raw Material Cost: Ethanol itself can be a costly feedstock, especially if it's used in large quantities for chemical synthesis rather than other applications like fuel.
iii. Limited Carbon Chain Length: The ethanol route typically produces smaller carbon chain alcohols, which may need additional processing to produce 2-ethylhexanol with a longer carbon chain.

ABE Fermentation Route

i. Productivity and Yields: ABE fermentation can have lower product yields compared to other routes. Clostridium bacteria used in the fermentation might produce a mix of acetone, butanol, and ethanol in varying ratios, making it less efficient for specifically targeting 2-ethylhexanol production.
ii. Process Complexity: ABE fermentation involves multiple steps, including fermentation, product recovery, and purification, making the overall process complex and potentially costlier.
iii. Strain Sensitivity: The performance of Clostridium bacteria is sensitive to process conditions, which can lead to variations in product quality and yield.

Oxo Route

i. Versatility in Feedstocks: The oxo route offers more flexibility in feedstock selection, including various olefins derived from crude oil or natural gas, which are more readily available and less dependent on agricultural cycles.
ii. Higher Yields and Purity: The oxo process is designed to specifically target the desired aldehyde (2-ethylhexanal) with higher selectivity and yield compared to other routes, resulting in better purity for downstream conversion to 2-ethylhexanol.
iii. Controlled Reaction: The oxo process provides better control over reaction conditions, temperature, and pressure, which can lead to improved efficiency and consistency in product quality.
iv. Economic Feasibility: While the oxo process might require initial investment in catalysts and equipment, its overall efficiency, product purity, and versatility often make it a more economically feasible option (Chongran *et al.,* 2023).

2.6 Simulation and Optimization

The simulation and optimization process focuses on the modelling and simulation of the production process of 2-ethylhexanol from propylene and synthesis gas. This process involves a series of chemical reactions and separation steps to obtain the desired product by using Aspen Hysys software to create a comprehensive process flow diagram (PFD) and simulate the entire production process.

2.6.1 Simulation

The production of 2-ethylhexanol from propylene and synthesis gas involves a series of reactions and unit operations. The main reactions include the hydroformylation of propylene to produce butyraldehyde, which is then hydrogenated to form 2-ethylhexanol. The process flow diagram (PFD) comprises of reactors, distillation columns, heat exchangers, and other essential equipment (Ghaemi and Zerehsaz, 2018).

Aspen Hysys a powerful process simulation tool is employed to model the production process. The software allows us to define reaction kinetics, thermodynamics, and various operating conditions. The process flow diagram (PFD) is constructed by assembling the necessary unit operations and connecting them in a logical sequence. Reactors are configured with the appropriate reaction kinetics, and distillation columns are designed to separate the products from by-products and unreacted feed. Key parameters such as reaction rates, heat transfer coefficients, and equilibrium constants are specified based on available literature or experimental data. Assumptions are made regarding ideal behaviour, pressure drop calculations, and other factors to simplify the simulation while maintaining reasonable accuracy. The simulation generates results such as product yields, concentrations, temperatures, pressures, and flow rates. These results are compared with experimental data from literature or previous studies to validate the simulation's accuracy. Any discrepancies are analyzed and explained based on the assumptions and simplifications made during the simulation (Ikpaki *et al.,* 2021).

2.6.2 Optimization

The history of optimization processes showcases a progression from traditional methods to modern techniques with a focus on maximizing yield, improving quality, and implementing sustainable practices. In recent decades, there has been increased interest in optimizing chemical processes to improve yield, quality, and efficiency. Optimization involves studying and optimizing parameters such as solvent type, solvent-to-solid ratio, temperature, extraction time, and pre-treatment methods. These parameters are adjusted to maximize oil yield, minimize degradation and enhance the bioactive compound profile of the product (Mariano *et al.,* 2017).

2.6.3 Methods of Optimization

Most optimization methods entail the application of statistical software to optimize the control variables (extraction time, sample weight, solvent volume, nature of solvent, seeds' variability, and particle size, etc.) that seek to reduce cost and increase performance while at the same time minimizing deterioration of the quality of the product as much as possible. Design-Expert is a widely used software tool that is specifically designed for experimental design and analysis, including optimization. It is developed by Stat-Ease, Inc. and provides a user-friendly interface for designing experiments, analyzing data, and optimizing processes. Design-Expert offers a range of features and tools for experimental design, including factorial designs, response surface designs (such as central composite design and Box-Behnken design), mixture designs, and more. It allows users to define experimental factors, their levels, and constraints, and generates an optimized experimental design based on the selected design criteria (Divine and Anuanwen, 2020).

Response Surface Methodology (RSM) uses a number of mathematical and statistical techniques which are employed to model and analyze problems in two or more process variables that have an influence on the intended response and the objective is to identify the optimal operating conditions for a system under study. Amongst the many RSM designs available, the central composite design (CCD) and the Box-Behnken design (BBD) have been popularly used for chemical processes (Subroto *et al.,* 2014).

2.7 Process Integration and Pinch Technology

Process integration is a systematic approach that aims to optimize the design and operation of chemical processes by maximizing resource utilization, energy efficiency, and overall process performance. It involves combining different process units and streams in a way that minimizes waste, energy consumption, and environmental impact. During the production of 2-ethylhexanol from propylene and synthesis gas, process integration plays a crucial role in optimizing the entire production process. The goal is to minimize energy consumption, improve heat recovery, and enhance resource efficiency by integrating different units and streams (Ghaemi and Zerehsaz, 2018). Process integration techniques can be applied to identify opportunities for heat and mass exchange, process synergies, and potential process

modifications. For example, heat exchangers can be strategically placed to recover heat from high-temperature streams and supply it to those requiring heat. By optimizing the integration of various process units, the overall energy consumption of the production process can be reduced, leading to economic and environmental benefits (Ikpaki *et al.,* 2021).

Pinch Technology is a subset of process integration that focuses specifically on energy optimization in chemical processes. It involves identifying the "pinch point," which is the point where the hot and cold utility requirements of a process come closest together. Pinch Technology seeks to minimize the temperature difference across the pinch point, thereby reducing the need for external utilities and improving energy efficiency. Pinch Technology is a valuable tool for optimizing the energy consumption of the 2-ethylhexanol production process. By analyzing the heat exchange opportunities and the temperature profiles of the process streams, pinch analysis can identify the optimal placement of heat exchangers and the integration of heat recovery networks (Iman *et al.,* 2018). In the case of 2-ethylhexanol synthesis, pinch analysis can help determine the minimum hot and cold utility requirements, as well as the optimal approach temperatures for heat exchangers. By designing the process to operate as closely as possible to the pinch point, the overall energy consumption can be minimized, leading to reduced operating costs and improved process sustainability. In this work, process Integration and pinch technology provide powerful methods to enhance the efficiency and sustainability of the 2-ethylhexanol production process. By optimizing heat and mass exchange, minimizing energy consumption, and identifying synergies between process units, these techniques contribute to a more efficient and environmentally friendly production process (Poulikidou *et al.,* 2019).
recovery were not detected but all these will be in this present work.

3.1 Material

This research project was centered on the simulation design of the 2-Ethylhexanol Production Plant from propylene and synthesis gas, hence the material that were used to achieve the research objective include:

i. Aspen HYSYS Version 11.0
ii. Aspen Optimization Tool
iii. Aspen Energy Analyzer
iv. Material Property Data Sheet

3.2 Methods

Chemical process design and simulation are carried out using computer software called the Aspen HYSYS simulator. It has unit operating modules, libraries of chemical components, thermodynamic calculation techniques, user-defined units, and a pseudo-FORTRAN programmer specifically for hydrocarbon components. Case studies and steady state mass and energy balance computations may be performed using it.

The following stages may be used to define a standard simulation the process: The data input comprises of the following: (1) a process flow diagram made up of chosen unit operations connected by streams; an appropriate thermodynamic method from the current thermodynamic method libraries, user-defined methods, or CAPE (Computer-Aided Process Engineering)-OPEN resources; and the selection of components and their properties (from current component libraries or the thermodynamic data manager, TDM). This stage entailed adding the relevant components—whether they were mixtures or pure chemicals—to the process along with their related characteristics, which could be calculated further; (2) process simulation, which involved simulating the process using the originally estimated parameters. Step one involved determining the feasibility of the process; step two involved process optimisation to find the optimal set of processing conditions to achieve a desired result, like the maximum amount of 2-ethylhexanol subject to certain property constraints; and step three involved energy process analysis using a parametric case study.

3.2.1 Composition for Simulation

Table 3.1 displays the composition of the components utilized in the plant simulation, along with their respective types. This includes the presence of 2-ethylhexenal, a compound whose structure was constructed using a structure builder tool. The compound's properties were determined based on the UNIFAC structure incorporated in the software, which is specifically designed for hypothetical hydrocarbon compounds.

Table 3. 1 Composition Used in the Simulation

Components	Type
Propene	Pure Component
H2O	Pure Component
2-ethylhexenal*	User Defined Hypothetical Component
2-ETH	Pure Component
i-Butanol	Pure Component
1-Butanol	Pure Component
n-Butanal	Pure Component
tert-Butanol	Pure Component
i-Butanal	Pure Component
Propanal	Pure Component
Nitrogen	Pure Component
Methane	Pure Component
CO	Pure Component
Hydrogen	Pure Component
Propane	Pure Component

3.2.2 Selection of Fluid Package

The use of UNIQUAC fluid packages in Aspen HYSYS software is preferred for modelling the manufacture of 2-ethylhexanol due to its capability to accurately represent phase equilibria in liquid mixtures that deviate from ideal behaviour. UNIQUAC, abbreviation for universal quasi chemical, is an activity coefficient model that considers the effects of mixing on entropy and enthalpy contributions. UNIQUAC is capable of handling systems including both polar and non-polar components, as well as systems containing electrolytes and azeotropes. UNIQUAC serves as the basis for the group contribution technique UNIFAC, which may predict the model's parameters based on the molecular structure of the components (Zhao, 2016).

Ikpaki et al. (2021) used the UNIFAC fluid package for the alkali-catalyzed process of 2-ethylhexanol synthesis, whilst the UNIQUAC fluid package was utilised in Aspen HYSYS for the heterogeneous-catalyzed process. These findings indicate that the UNIQUAC fluid package is better suited for the heterogeneous-catalyzed process, which entails the presence of a solid catalyst and a liquid phase reaction. The UNIQUAC fluid package can account for the non-ideal behavior of the liquid mixture and the interactions between the reactants and the catalyst.

3.2.3 Reactions Involved in the Simulation

Table 3. 2 Reaction and Type of Reaction Used in the Simulation

Reaction	Type of Reaction
Hydroformylation	Kinetic
Aldol Condensation	Kinetic
Hydrogenation-1	Kinetic
Hydrogenation-2	Kinetic

3.3 Process Description

The present simulation approaches 2-Ethylhexanol (2-EH) production from propylene and syngas. The process under analysis comprises three major sections: (1) Propylene Hydroformylation; (2) EHAL Formation; and (3) EHAL Hydrogenation.

3.3.1 Propylene Hydroformylation

Fresh propylene and syngas are treated to eliminate impurities that might poison the rhodium catalyst utilised in the hydroformylation process, which yields n-butyraldehyde (NBAL) and iso-butyraldehyde (IBAL) as products. The reactor (CSTR-100) output is degassed, and unreacted gaseous reactants return to the reactor via a Vent Gas Compressor (K-100), while a liquid stream is channelled to two absorber columns running alternately for catalyst regeneration from a gas stream that is supplied to a C3 Stripper (T-100). This stripper recovers propylene, which is transported to the C3 Absorber (T-101) and subsequently returned to hydroformylation, while an aldehyde stream is directed to a distillation column (T-102) to separate the NBAL from the IBAL, recycling the NBAL in the hydroformylation reactor.

3.3.2 EHAL Formation

The IBAL is supplied to the Aldol Condensation Reactor (PFR-100) together with a caustic soda solution, where 2-ethyl-hexenal (EHAL) or isobutyraldehyde is produced. The resultant mixture is transferred to the Reactive Column (T-103) to strip out unreacted NBAL, which is returned to the reactor. The bottom stream from the reactive column is transported to the heat exchanger (E-103) before being mixed with pure hydrogen before going to the hydrogenation reaction zones.

3.3.3 EHAL Hydrogenation

The mixed stream of pure hydrogen and 2-ethyl-hexenal (EHAL) is sent to two hydrogenation zones

(PFR-101, 102), where it reacts with hydrogen in the presence of heterogeneous catalysts (copper and nickel) to produce 2-ethyl-hexanol. The product stream is routed via a column (T-104) to remove light ends while obtaining 2-EH from the bottom.

3.4 Kinetic Data Used for the Simulation

There is limited kinetic data available for the production of 2-ethylhexanol from propylene and synthesis gas. However, some kinetic data can be inferred from the kinetic data for the following reactions:

- Hydroformylation of propylene to isobutyraldehyde
- Aldol condensation of isobutyraldehyde to 2-ethylhexanal
- Hydrogenation of 2-ethylhexanal to 2-ethylhexanol

3.4 Process Optimization and Energy Analysis

After the simulation completed, the plant needed to be optimised; consequently, an optimiser built into the programme was employed, along with an optimizer spreadsheet displaying the parameters. With this, an energy analysis was activated to calculate the amount of energy saved.

IV. RESULTS AND DISCUSSION

4.1 Process Simulation

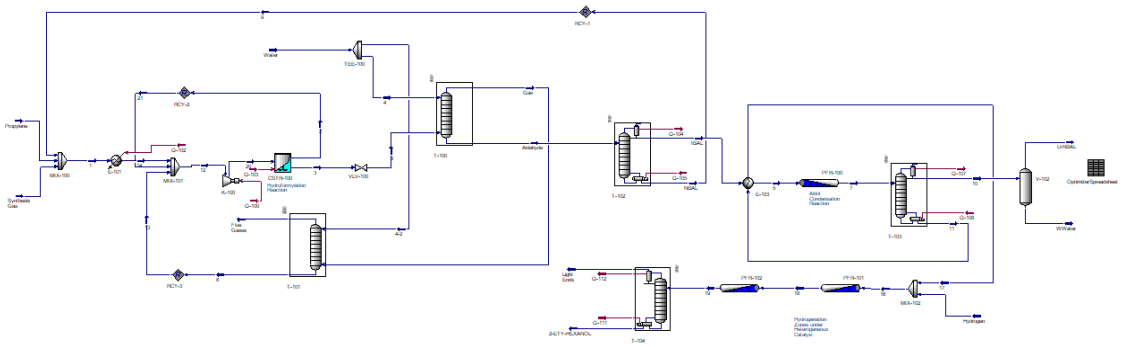

Figure 4. 1 Process Flow Diagram of 2-ETH Production Plant from Propylene and Synthesis Gas.

Synthesis gas stream contain 48.6% H_2, 49.5% CO, 0.4% CH_4 and 1.5% N_2. Synthesis gas to propylene feed to the hydroformylation reactor was 2:1, where the propylene stream contained 93% propylene and 7% of propene.

The hydroformylation followed two catalytic routes:
(1) the reaction of propylene and H_2 to propane (0.4723 act. Conversion% of propylene and 57.05 reaction extent).

$$\underset{Propylene}{CH_3CH{=}CH_2} + \underset{Hydrogen}{H_2} \rightarrow \underset{Propane}{CH_3CH_2CH_3}$$

(2) the reaction of propylene, CO, and H_2 to iso-butyraldehyde and n-butyraldehyde (18.82 act. Conversion% of propylene and 757.8 reaction extent).

$$\underset{Propylene}{CH_3CH{=}CH_2} + \underset{Carbon-monoxide}{CO} + \underset{Hydrogen}{H_2} \rightarrow \underset{Iso\ butyraldehyde}{CH_3CH_2CH_2CHO} + \underset{n-butyraldehyde}{CH_3CH_2CHO}$$

Bernas et al., (2008) conducted kinetic modelling of propene hydroformylation with Rh/TPP and Rh/CHDPP catalysts with activation energy and pre-exponential factor of 68100 kJ/mol and 171000 $m^3mol^{-2}s^{-1}$, which was used in the process at a control pressure and temperature of 350 bar and 165ºC, which is consistent with the patent presented by Beadle et al., (2008) for hydroformylation reactions using rhodium-based catalysts and typically operate at pressures from 50 to 350 bar, preferably 150 or 250 to 350 bar, and optimum temperatures ranging from 120oC to 190ºC, preferably 165ºC to 185ºC to prevent decomposition of the catalyst (Xie, 2013).

The biphasic aldol condensation of n-butyraldehyde (nBAL), catalysed by an aqueous sodium hydroxide solution, yields 2-ethylhexanal prior to the final reaction, with 3.634% conversion and 8.805 extent of reaction for the first reaction and 99.99% conversion and 95.87 extent of reaction for iso-butyraldehyde for the first and second reaction respectively.

$$1.242 Isobutyraldehyde + Hydrogen \rightarrow 1 - butanol \quad (1)$$

$$2.483 Isobutyradelhyde \rightarrow 2 - ethylhexenal + Water \quad (2)$$

In this simulation process, the temperature condition was set to operate at 110oC which was consistent to the intrinsic reaction rate was obtained in the

industrially relevant range 110–150oC and 0.76–1.9 M NaOH of biphasic aldol condensation with average values of the activation energy and the pre-exponential factor were determined to be 56388kJ/mol and 171200000 $m^3mol^{-2}s^{-1}$, respectively (Lee et al., 2013).

The hydrogenation of 2-ethylhexenal is the final step in the production of 2-ethylhexanol, which is an important chemical intermediate and solvent. The hydrogenation reaction converts the aldehyde group of 2-ethylhexenal into the alcohol group of 2-ethylhexanol using hydrogen gas and a metal catalyst, such as nickel and copper, respectively. Liu et al., (2017) The reaction is usually performed at high temperature and pressure to achieve high conversion and selectivity of 100 and 99.1%, respectively, when the reaction was carried out at 240°C for 7 h within the range of the simulated results at the first and second hydrogenation reactors at 280ºC and 403ºC, respectively. The product 2-ethylhexanol can be separated from the catalyst and the unreacted 2-ethylhexenal by distillation and purification. This process is usually carried out by forcing hydrogen to the point of saturation in a high-pressure container into the aldehyde to be reduced in the presence of a catalyst (Nadine, 2022) in the liquid phase.

$$2-ethylhexenal + 2Hydrogen \rightarrow 2-ethylhexanol \quad (3)$$

The reaction described above followed the kinetic data provided by an experimental study by Virgana et al., (2019) of 3.9498 m3mol-2s-1 and activation energy of 58.39 kJ/mol by the reaction extent of 52.42 after 58% conversion was achieved for the first reactor, while a reaction extent of 56.90 and 151.2% conversion of 2-ethylhexanal was achieved for the second reactor.

4.2 Process Optimization and Energy Analyzer

The energy analyzer showed 2.45% energy savings once the first simulation results were made available, which provided a sense of the changes shown in figure 4.3. The energy savings increased to 6.8% when the modification was carried out in accordance with the suggestion to replace the cooler and heater with a heat exchanger. Figure 4.4 illustrates the significant increase in energy savings that occurred at 8% when optimisation was implemented. Specifically, the temperature inlet into the hydroformylation reactor was optimised from 1463ºC to 1469ºC, and the pressure of the aldol condensation reactor was increased from 35 bar to 70 bar, all while maintaining a temperature below 100ºC. The optimised settings that were taken from the simulation programme are shown in Figure 4.2.

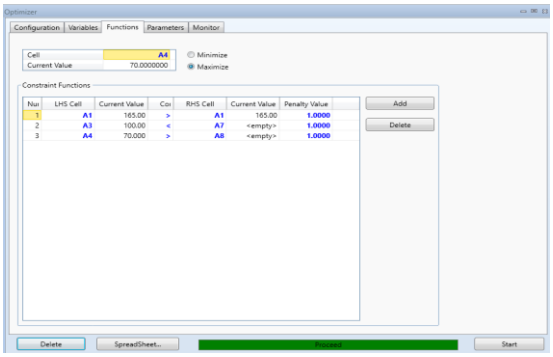

Figure 4. 2 Optimizer Function of 2-ethylhexanol Production Plant

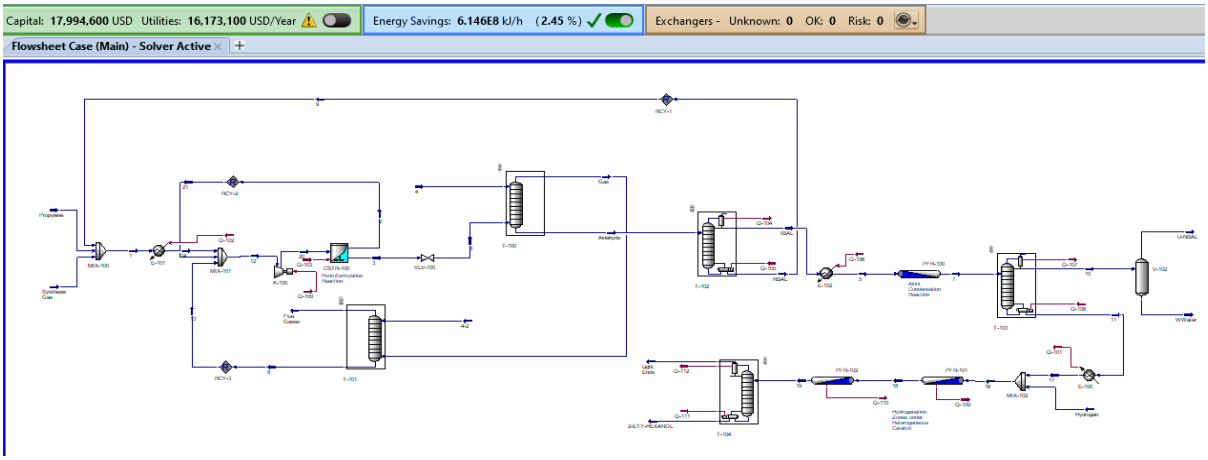

Figure 4. 3 PFD before Optimization

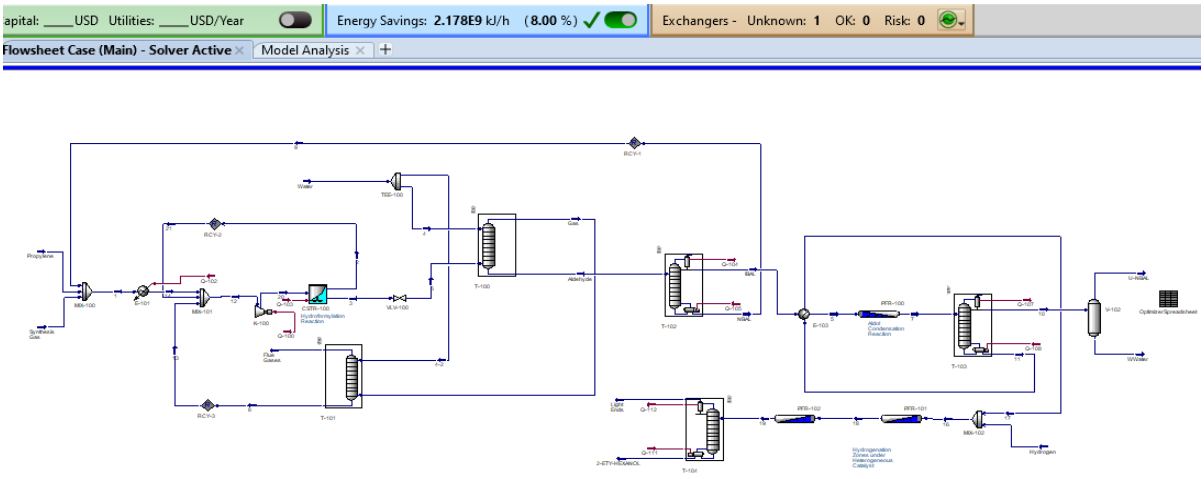

Figure 4. 4 PFD after Optimization

CONCLUSION

The production of 2-ethylhexanol from synthesis gas and propylene is a three-step process that involves the hydroformylation of propylene to n-butyraldehyde and i-butyraldehyde, followed by the aldol condensation and hydrogenation of 2-ethylhexanal to 2-ethylhexanol. The process was simulated at steady state using UNIQUAC fluid package, which is a thermodynamic model that can predict the phase equilibrium and the physical properties of the system. The simulation results showed that the process can produce 2-ethylhexanol with a purity of 100%. The process was also optimized by varying the operating parameters, such as the temperature, pressure, and tank volume of the hydroformylation reactor, to achieve the maximum conversion, selectivity, and energy efficiency. The optimization results showed that the process can save energy by 8% compared to the base case, by reducing the heating and cooling duties of the reactors and the distillation columns. The process was also evaluated for its economic feasibility and environmental impact, by estimating the capital and operating costs. The evaluation results showed that the process can be profitable and sustainable. The process can also be integrated with other processes, such as the production of propylene from propane and the production of synthesis gas from natural gas, to form a complete plant for the production of 2-ethylhexanol from natural gas. The production of 2-ethylhexanol from synthesis gas and propylene is a promising technology that can provide a valuable chemical intermediate and solvent for various applications, such as plasticizers, lubricants, and coatings.

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