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Theme:

Optimization of Ethylene Oxide Production Using Sliding Mode Control

Realized by: Yahiaoui Moncef

Presented before the honored jury composed of:

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In the name of Allah the most gracious the most merciful the one and only true god.

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Yahiaoui Moncef

Dedication:

I would like to dedicate my work to the most important people in my life my family my mother Saida and my sister Insaf and to my late father Helal. I couldn't achieve a fraction of what I have achieved today without their support, and for that I would love to offer them my most heartfelt and sincere thank you, you mean the world to me.

I would also like to dedicate it to all my friends who are more like brothers to me, and who supported me the most second only to family.

Finally, I would like to dedicate it to all those who helped me achieve what I reached today.

Summery:

This thesis focuses on optimizing the production of ethylene oxide in a continuous stirred tank reactor (CSTR) using sliding mode control. It discusses the system modeling, controller design, simulation, and performance evaluation. The results show that sliding mode control is effective in improving production efficiency and selectivity. Sliding mode control parameters are also studied to reduce oscillations and enhance system stability. This research contributes to a better understanding of control techniques in chemical reactors and provides valuable insights for the optimization of ethylene oxide production processes.

Key words: sliding mode control, CSTR, ethylene oxide, optimization, non-linear system, ethylene.

Résume:

Cette thèse se concentre sur l'optimisation de la production d'oxyde d'éthylène dans un réacteur chimique bien agité en utilisant la commande par mode glissant. Elle aborde la modélisation du système, la conception du contrôleur, la simulation et l'évaluation des performances. Les résultats montrent que le contrôle en mode glissant est efficace pour améliorer l'efficacité de production et la sélectivité. Les paramètres de contrôle en mode glissant sont également étudiés pour réduire les oscillations et améliorer la stabilité du système. Cette recherche contribue à une meilleure compréhension des techniques de contrôle dans les réacteurs chimiques et fournit des perspectives précieuses pour l'optimisation des processus de production d'oxyde d'éthylène.

Mots clés : commande en mode glissant, RCTC, oxyde d'éthylène, optimisation, système non linéaire, éthylène.

ملخص

تركز هذه الرسالة على تحسين إنتاج أكسيد الإيثيلين في وحدة التفاعل المستمر باستخدام تحكم الانزلاق .تتناول الرسالة نمذجة النظام وتصميم المتحكم والمحاكاة وتقييم الأداء .تشير النتائج إلى أن تحكم الانزلاق فعال في تحسين كفاءة الإنتاج والانتقائية .يتم أيضًا دراسة معلمات تحكم الانزلاق لتقليل التذبذبات وتحسين استقرارية النظام .تسهم هذه الدراسة في فهم أفضل لتقنيات التحكم في المفاعلات الكيميائية وتقدم رؤى قيمة لتحسين عمليات إنتاج أكسيد الإيثيلين

.الكلمات المفتاحية: التحكم بوضع الانزلاق ، مفاعل مستمر الخلط، أكسيد الإيثيلين ، تحسين ، نظام غير خطي ، إيثيلين

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Introduction

Introduction:

Ethylene oxide (EO) plays a vital role in the ethylene-based chemical industry, serving as a key intermediate compound in the production of various derivatives. These derivatives, including ethylene glycol, surfactants, and ethanolamines, have diverse applications in numerous industries such as textiles, automotive, pharmaceuticals, and personal care products.

The commercial production of ethylene oxide has a rich history. It was first synthesized in 1859 through the reaction of ethylene chlorohydrin and aqueous potassium hydroxide. During World War I, commercial production of ethylene oxide began in Germany using the chlorohydrin process. However, in 1931, a breakthrough occurred with the development of the direct oxidation process, which involved the use of a silver catalyst to directly oxidize ethylene to ethylene oxide. This method quickly replaced the chlorohydrin process and continues to be the dominant technology in ethylene oxide production today.

The production process of ethylene oxide involves the controlled reaction between ethylene and oxygen on a silver catalyst surface. The challenge lies in achieving high selectivity towards ethylene oxide to minimize the consumption of ethylene, as ethylene is a significant cost factor in the production process. Optimization of the reaction conditions and control of process variables are crucial to enhance selectivity and improve overall efficiency.

In this study, our focus is on simulating the ethylene oxide production process in a continuous stirred tank reactor (CSTR) using MATLAB. The objective is to optimize the consumption of ethylene while maximizing the selectivity of ethylene oxide over carbon dioxide and water. Through the use of advanced control strategies, such as sliding mode control, we aim to regulate key process variables, such as the cooling jacket temperature and C_2H_4 availability, to achieve optimal production rates and maintain product quality.

By simulating the reactor and implementing advanced control techniques, we expect to gain valuable insights into the behavior of the system and develop effective control strategies to optimize ethylene oxide production. This research contributes to the ongoing efforts in the chemical industry to improve process efficiency, reduce costs, and minimize the environmental impact of ethylene oxide production.

In the first chapter we talk about the generalities of ethylene oxide its uses and dangers, then we jump to the reactor and the catalyst used , after that we move on to learning about sliding

mode control , in the next chapter we simulate the system and optimize it and discuss our results, finally we have a conclusion to finish off our study.

Chapter I

Ethylene-oxide

Chapter I: Ethylene-oxide:

Ethylene oxide also known as the smallest oxirane is a small organic molecule with the chemical formula C_2H_4O, which consists of two carbon atoms, four hydrogen atoms, and one oxygen atom. It is a highly reactive gas that readily reacts with other substances due to its highly strained and easily openable ring, making it useful in many industrial applications. Ethylene oxide is produced by the oxidation of ethylene, a hydrocarbon gas, in the presence of a catalyst. This reaction results in the formation of ethylene oxide and water.

Ethylene oxide is commonly used in the production of various chemicals, such as ethylene glycols, ethanolamines, and polyethylene glycols. Ethylene glycols are used as antifreeze agents, solvents, and in the production of polyester fibers and resins. Ethanolamines are used in the production of detergents, soaps, and personal care products. Polyethylene glycols are used as surfactants, lubricants, and in the production of various pharmaceuticals.

One of the most significant uses of ethylene oxide is as a sterilizing agent for medical equipment and supplies. Ethylene oxide is capable of killing bacteria, viruses, and other microorganisms, making it a critical tool in the healthcare industry. Medical devices and supplies that cannot be sterilized using traditional methods, such as high-temperature steam sterilization, can be sterilized using ethylene oxide gas.

However, ethylene oxide is also a hazardous substance that poses significant risks to human health and the environment. Exposure to ethylene oxide can cause irritation to the eyes, skin, and respiratory system, and long-term exposure can lead to cancer and other serious health problems. Ethylene oxide is also a flammable gas that can ignite easily, making it a significant fire and explosion hazard.

Due to its hazardous properties, the handling, transportation, and use of ethylene oxide are subject to strict safety regulations and guidelines to minimize the risk of exposure to humans and the environment. These safety measures include the use of personal protective equipment, proper ventilation, and the implementation of appropriate engineering controls to prevent leaks and spills.

Chapter I Ethylene-oxide

I.1.Historical overview:

The history of ethylene oxide (EO) production dates back to 1859 when the French chemist, Charles Adolphe Wurtz, first synthesized it by heating ethylene chlorohydrin with potassium hydroxide. However, it was not until 1914 that the industrial production of EO began. In the early days, the chlorohydrin process was used for the production of EO, which involved the reaction of ethylene with hypochlorous acid to form ethylene chlorohydrin followed by its treatment with alkali to obtain EO.

The direct oxidation of ethylene to EO was discovered by the German chemist Paul Schlack in 1931. This process involved the reaction of ethylene with air over a silver catalyst to form EO and carbon dioxide. The direct oxidation process gradually replaced the chlorohydrin process due to its higher efficiency and lower cost.

During World War II, EO was used as a fumigant for disinfecting military equipment and supplies. After the war, the demand for EO increased due to its use in the production of ethylene glycol for antifreeze and polyester fibers. In the 1950s, EO was also used in the production of detergents and other surfactants.

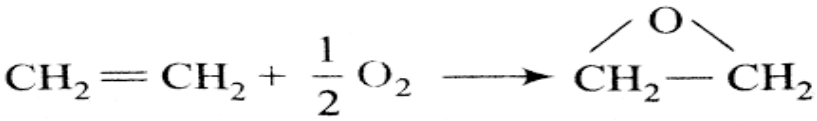
Today, the initial direct oxidation commercial process for EO was pioneered by Carbide and Carbon Chemicals Corp., now known as Union Carbide Corp., in the United States. Their first plant based on the use of air was established in 1937. The Scientific Design (SD) air-based process was introduced in 1953, which led to the replacement of the chlorohydrin process by the late 1950s. In 1958, Shell Development introduced the first oxygen-based process for direct oxidation of ethylene. Subsequently, SD/Halcon (1969), Nippon Shokubai (1976), and Union Carbide (1976) commercialized the oxygen-based process. The production process has undergone several improvements and modifications over the years, including the development of new catalysts, improved reactor designs, and the use of computerized control systems. According to the International Energy Agency (IEA), the world consumption of ethylene oxide (EO) was approximately 25 million tonnes in 2019. The major consuming regions were Asia, Europe, and North America, accounting for about 80% of global demand. The largest consumer was China, followed by the United States and Europe.

I.2. Chemical composition of ethylene-oxide:

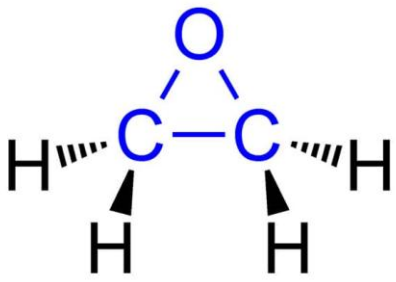
The chemical composition of ethylene oxide (EO) is C_2H_4O, which means it consists of two carbon atoms, four hydrogen atoms, and one oxygen atom. It is an organic compound that is a cyclic ether, meaning it contains an oxygen atom in a cyclic ring structure.

EO has a simple molecular structure consisting of a three-atom chain, with an oxygen atom at the center and two carbon atoms on either side. The molecule is polar, with the oxygen atom being more electronegative than the carbon and hydrogen atoms, giving it a partial negative charge on the oxygen atom and partial positive charges on the carbon and hydrogen atoms.

The formation of ethylene oxide (EO) involves the reaction of ethylene (C_2H_4) with oxygen (O2) in the presence of a catalyst. The overall reaction equation is:



This equation represents a simplified reaction, as the actual reaction is a complex process involving several intermediate species and reactions.



I.3.Uses of ethylene-oxide:

Ethylene oxide is very reactive because its highly strained ring can be opened easily, and is thus one of the most versatile chemical inter-mediates[1], therefor it is used in a huge number of industries such as:

Figure 1. Various uses of EO in industrial fields[2]

-Production of ethylene glycols: EO is primarily used in the production of ethylene glycols, which are used in the manufacture of a wide range of products such as antifreeze, coolants, solvents, resins, and textiles.

-Production of surfactants: EO is also used in the production of surfactants, which are compounds that lower the surface tension between two liquids or between a liquid and a solid. Surfactants are used in a variety of applications such as detergents, soaps, shampoos, and cosmetics.

-Production of ethanolamines: EO is used in the production of ethanolamines, which are used in the manufacture of herbicides, detergents, and personal care products.

-Sterilization: EO is used as a sterilant in the medical and food industries. It is particularly effective in sterilizing heat-sensitive equipment and materials such as plastics, fabrics, and electronics. [3]

-Fumigant: EO is used as a fumigant to control pests in stored grains, fruits, and vegetables. [4]

-Chemical intermediate: EO is used as a chemical intermediate in the production of a wide range of chemicals such as glycol ethers, polyethylene glycols, and other organic compounds.

-Pharmaceuticals: EO is used in the production of some pharmaceuticals as a reagent and a starting material.

-Textile Industry: EO is used in the textile industry for the production of non-woven fabrics, which are used in a variety of applications such as disposable medical products, filtration media, and geotextiles.
-Oil and Gas Industry: EO is used in the oil and gas industry for the production of chemicals used in drilling and production operations, as well as for the sterilization of equipment and pipelines.

-Personal Care Products: EO is used in the production of personal care products such as shampoos, body washes, and soaps, as well as in the production of cosmetics and fragrances.

-Water Treatment: EO is used in the treatment of water and wastewater to control microbial growth and to disinfect water. It is also used to sterilize equipment and piping used in the treatment process.

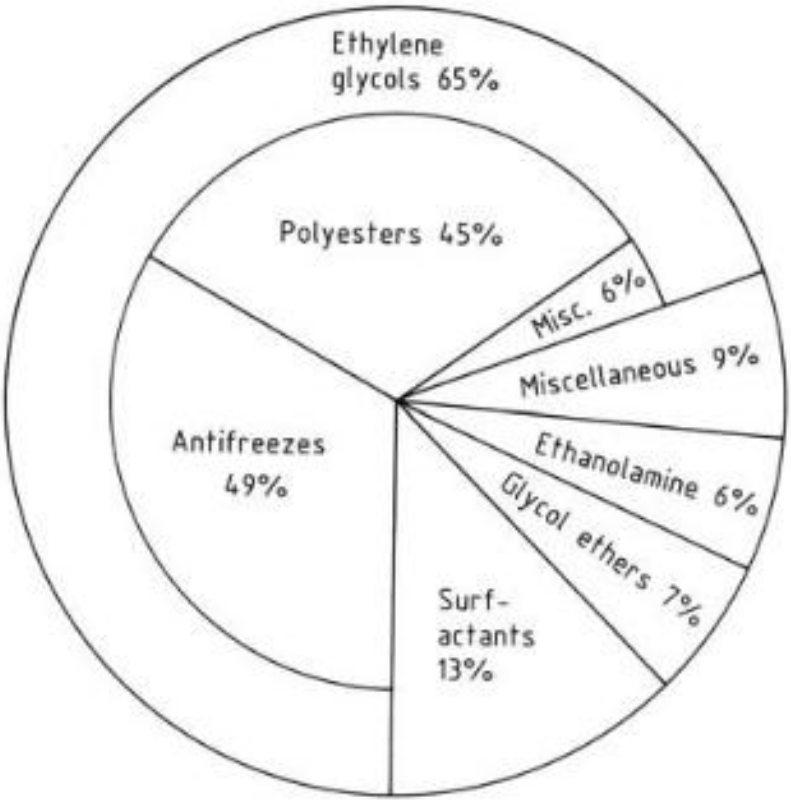


Figure 2.Uses of EO in chemistry[1]

I.4.Hazards and dangers of Ethylene-oxide:

Ethylene oxide is a highly reactive and flammable gas that can pose significant health and safety risks to humans and the environment[5]. Here are some of the potential dangers associated with ethylene oxide:

I.4.1.General danger classification:

H220—Extremely flammable gas

H280—Contains gas under pressure; may explode if heated

H315—Causes skin irritation

H319—Causes serious eye irritation

H331—Toxic if inhaled

H335—May cause respiratory irritation

H340—May cause genetic defects

H350—May cause cancer

H402—Harmful to aquatic life

H412—Harmful to aquatic life with long-lasting effects[2]

Figure 3.Ethylene-oxide danger stating label

I.4.2.Dangers to humans:

Carcinogenicity: Ethylene oxide has been classified as a known human carcinogen by several organizations, including the International Agency for Research on Cancer (IARC) and the US Environmental Protection Agency (EPA). Exposure to ethylene oxide has been linked to an increased risk of cancer, including leukemia, lymphoma, and breast cancer.

Acute toxicity: Ethylene oxide is highly toxic and can cause acute health effects such as respiratory irritation, headaches, dizziness, nausea, vomiting, and unconsciousness. Exposure to high concentrations can be lethal.

Chronic effects: Chronic exposure to ethylene oxide can cause long-term health effects such as neurotoxicity, reproductive toxicity, and genotoxicity.

Mutagenicity: Ethylene oxide is mutagenic due to its alkylating properties that causes dominant lethal mutations and chromosome aberrations in the DNA of workers exposed to it for an extended amount of time.[1]

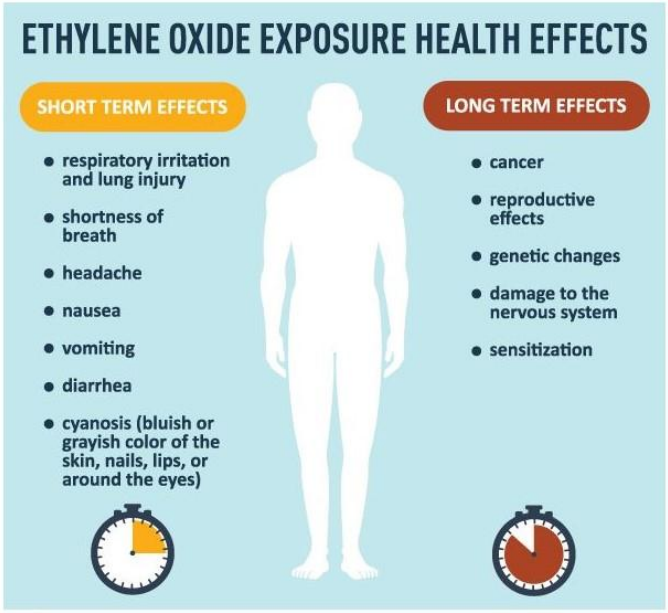


Figure 4.Effects of ethylene oxide exposure on human[6]

I.4.3.Dangers to environment:

Air pollution: ethylene-oxide is a volatile organic compound (VOC) that can contribute to air pollution when released into the atmosphere. It can react with other pollutants to form ground-level ozone, a major component of smog, which can cause respiratory problems and other health issues.

Water pollution: ethylene-oxide is water-soluble and can contaminate water sources if not properly disposed of. It can also degrade into other hazardous substances in water, such as ethylene glycol and ethylene chlorohydrin, which can be toxic to aquatic life and cause harm to ecosystems.

Soil contamination: ethylene-oxide can contaminate soil through spills or leaks during transportation or storage. It can also be absorbed by plants and accumulate in the food chain, potentially harming wildlife and humans.

Global warming: ethylene-oxide is a potent greenhouse gas that contributes to global warming. Its global warming potential is more than 1,000 times greater than carbon dioxide (CO2) over a 100-year time horizon

I.5.Properties of EO:

mp at 101.3 kPa	-112.5 C
bp at 101.3 kPa	10.8 C
Critical temperature	195.8 C
Critical pressure	7.2 MPa
Critical density	314 kg/m^3
Refractive index, n^7_D	1.3597
Explosive limits in air at 101.3 kPa lower upper	 2.6 vol % 100.0 vol %
Electrical conductivity	4x10^{-6} S/m
Dielectric constant at 1 C (liquid) at 15 C (vapor)	 13.9 1.01
Heat of combustion at 25 C, 101.3 kPa	 29.648 kJ/kg
Entropy of the vapor at 101.3 kPa 10.5 C 25.0 C	 5.439 kJ/kg.K 5.495 kJ/kg.K
Ignition temperature in air at 101.3 kPa	 429 C
Ignition energy in air at 101.3 kPa and 25 C	 0.087 mJ
Minimum ignition energy of the gas at 220 kPa and 100 C	 64 mJ
Decomposition temperature of the vapor at 101.3 kPa	 571 C
Heat of polymerization	2091 kJ/kg
Heat of fusion	117.86 kJ/kg
Heat of decomposition of the vapor	1901 kJ/kg
Coefficient of cubic expansion at 22 C at 55 C	 0.00161 0.00170
Heat of solution in water at 25 C	142.57 kJ/kg

Table.1.Properties of ethylene-oxide[1]

I.6.Conclusion:

In this chapter, we explore the fascinating compound known as ethylene oxide. Ethylene oxide is a cyclic ether, distinguished by its unique three-membered ring structure. Since its discovery in the early 1900s, ethylene oxide has become one of the most versatile chemical products, finding applications in various industries.

One of the key characteristics of ethylene oxide is its volatile nature, making it an essential component in the production of a wide range of chemicals. It serves as a building block for the synthesis of polymers, including polyethylene glycol, which is extensively used in industries such as cosmetics, pharmaceuticals, and personal care products. Ethylene oxide is also employed as a fumigant to control pests and insects in stored grains and agricultural products. The textile industry also relies on ethylene oxide for the production of certain fibers, such as polyester. Its ability to react with a variety of substances makes it a valuable intermediate in chemical synthesis. Furthermore, ethylene oxide plays a vital role in the medical field as a sterilizing agent for medical equipment and supplies, ensuring the safety and hygiene of healthcare practices.

While ethylene oxide offers numerous benefits in various industries, it is important to highlight its potential hazards. The compound is highly toxic to humans and has detrimental effects on the environment. Due to its toxicity, strict precautions and safety measures must be taken during handling and storage. Effective ventilation and protective equipment are essential to minimize the risks associated with ethylene oxide exposure.

In conclusion, ethylene oxide is a versatile and indispensable compound in modern industries. Its volatile nature and reactivity make it a valuable building block for the production of numerous chemicals and materials. However, the toxic nature of ethylene oxide demands responsible handling and adherence to safety protocols to protect both human health and the environment. Continued research and development in the safe and efficient use of ethylene oxide are essential to ensure its beneficial applications while minimizing associated risks.

Chapter II

The reactor

Chapter II:The reactor:

A Continuous Stirred-Tank Reactor (CSTR) is commonly used in the production of ethylene oxide (EO) through the direct oxidation of ethylene with oxygen or air. In this process, the reactants are continuously fed into a well-stirred tank reactor, where the reaction takes place at a constant temperature and pressure. The reactor is equipped with an agitator that ensures the reactants are well mixed and in contact with the catalyst[7].

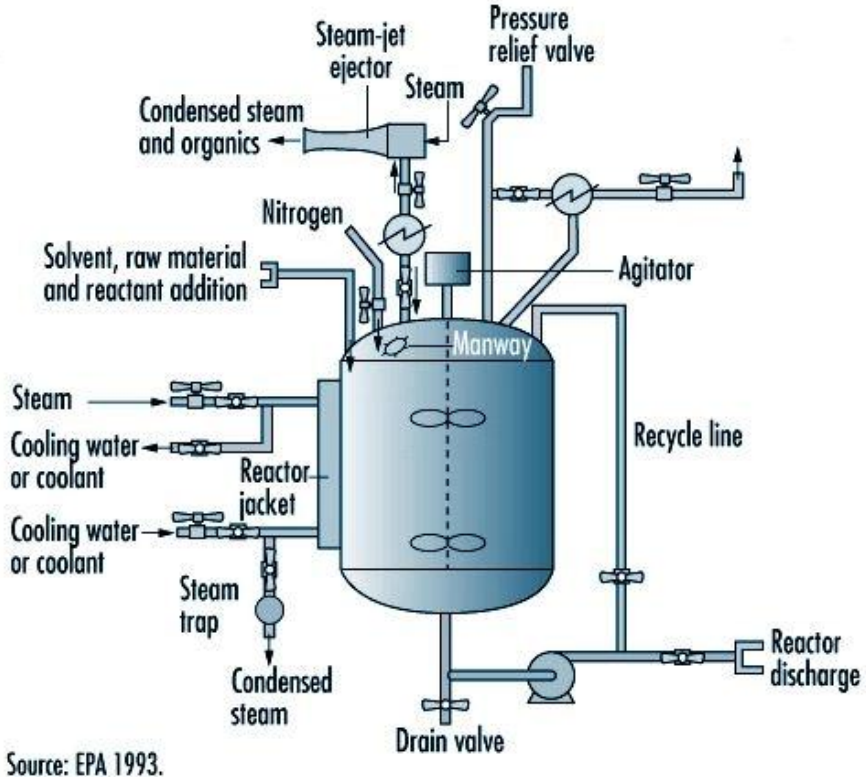


Figure 5.A diagram of a CSTR chemical reactor.

The CSTR is an efficient reactor design for the production of EO since it ensures a steady state operation, consistent product quality, and easy scale-up for commercial production. The reaction mixture is kept in a constant state of agitation to maximize mass transfer and heat transfer between the reactants and the catalyst surface, leading to a high yield of ethylene oxide.

In addition to CSTR, other reactor designs such as Plug Flow Reactor (PFR) and Fixed Bed Reactor (FBR) have also been used for EO production. However, CSTR remains the most commonly used reactor due to its high productivity and reliability.

II.1.Methods of production

There are two methods to produce EO which are:

II.1.1.The chlorohydrin:

The process involves the reaction of ethylene with hypochlorous acid (HOCl) to form ethylene chlorohydrin, which is then hydrolyzed to form EO and hydrochloric acid (HCl). The overall reaction can be represented as:

Reaction mechanism: The chlorohydrin process involves the reaction of ethylene with hypochlorous acid (HOCl) to form ethylene chlorohydrin (C2H5ClO). This reaction is typically carried out in the presence of a catalyst such as sulfuric acid or ferric chloride[8].

$C_2H_4 + HOCl \rightarrow C_2H_5ClO + HCl$

Hydrolysis: The ethylene chlorohydrin is then hydrolyzed with water to form EO and hydrochloric acid (HCl):

$C_2H5ClO + H_2O \rightarrow C_2H_4O + HCl$

One of the main disadvantages of the chlorohydrin process is the generation of large amounts of HCl, which must be handled and disposed of safely. In addition, the process is less efficient than the direct oxidation process, requiring more energy and producing more greenhouse gas emissions per unit of EO produced.

II.1.2.Direct oxidation:

The direct oxidation process for producing EO involves the reaction of ethylene with oxygen in the presence of a silver catalyst[9]. This process is also referred to as the "oxidation process" or "oxychlorination process." The reaction typically takes place at temperatures between 200-300°C and pressures of 1-2 atmospheres.

For direct oxidation two methods are used:

Air-based direct oxidation: The air-based direct oxidation method for producing EO involves the reaction of ethylene and oxygen in the presence of a silver catalyst at high temperatures and pressures. The reaction is exothermic and releases heat, which must be controlled to prevent overheating of the reactor. The reaction is typically carried out in a fixed-bed reactor, where the catalyst is packed into a fixed bed. The ethylene and oxygen are fed into the reactor and react over the catalyst, producing EO and heat.

The air-based direct oxidation method has several advantages over the chlorohydrin process, including higher yields, lower production costs, and lower environmental impact. The process does not produce any chlorinated byproducts and does not require the use of chlorine, which is a hazardous material. However, the air-based process does require the use of a large amount of energy and produces significant amounts of carbon dioxide.

Oxygen-based direct oxidation: The oxygen-base direct oxidation method is an alternative to the air-base direct oxidation method for the production of ethylene oxide (EO). In this method, pure oxygen is used instead of air, and the process takes place in a reactor containing a silver catalyst. The use of pure oxygen as the oxidizing agent increases the selectivity of the reaction towards EO, resulting in a higher yield of the desired product.

However, the use of pure oxygen in the process requires additional safety measures to prevent explosions, and the cost of producing and handling pure oxygen can be higher than that of using air. As a result, the choice of which method to use depends on a variety of factors, including the availability and cost of oxygen and the desired yield and purity of EO.

The direct oxidation process is the most common method for producing EO today, accounting for approximately 90% of global production. It is considered a more energy-efficient and environmentally-friendly process compared to the chlorohydrin process.

II.2.Reactor working principle:

In a continuous stirred-tank reactor (CSTR) for ethylene oxide production, a gas mixture of ethylene, oxygen, and an inert gas (such as nitrogen) is fed into the reactor along with a stream of recycled product gas. The mixture is then heated and pressurized to the operating conditions of the reactor.

The catalyst promotes the reaction between ethylene and oxygen to produce ethylene oxide. The reaction is exothermic, meaning it releases heat, so the reactor must be carefully cooled to maintain the desired temperature and prevent thermal runaway.

The main reactions happening in the reactor are:

$C_2H_4 + ½\ O_2 \rightarrow C_2H_4O$ (formation of ethylene oxide) (ΔH = -106,7 kJ/mol)

$C_2H_4 + 3\ O_2 \rightarrow 2\ CO_2 + 2\ H_2O$ (by products) (ΔH = -1323 kJ/mol)

As the reactants flow through the reactor, the conversion of ethylene to ethylene oxide gradually increases. The product gas, containing ethylene oxide, unreacted ethylene, oxygen, and inert gases, is withdrawn from the reactor and cooled to condense the ethylene oxide.

The product gas is then separated into different fractions using a series of distillation columns, with the highest purity ethylene oxide being the final product. Any unreacted ethylene and oxygen, as well as other by-products, are typically recycled back to the reactor for further processing. The performance equation for a Continuous Stirred Tank Reactor (CSTR) can be expressed as:

$$V \times \frac{dC}{dt} = Q(\mathrm{C_{in}} - \mathrm{C}) - \mathrm{V} \times \mathrm{r}$$

Where :

V is the volume of the reactor

C is the concentration of reactant in the reactor

t is time

Q is the flow rate of the reactant into the reactor

C_in is the concentration of the reactant in the feed stream

r is the reaction rate, which is a function of the concentration of the reactant and the activity of the catalyst

This equation describes the balance of mass in the reactor, taking into account the inflow and outflow of the reactant and the rate of the reaction occurring within the reactor. The objective of a CSTR is to maintain a steady state, where the concentration of reactant in the reactor remains constant over time.

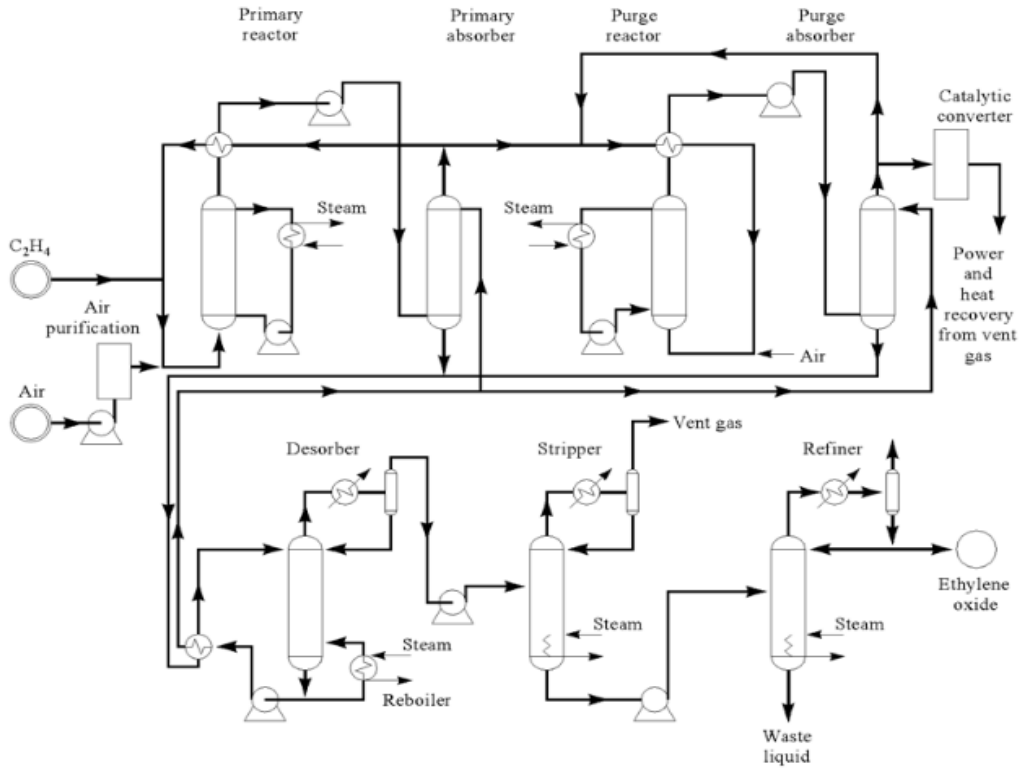


Figure 6.Direct oxidation of ethylene flow diagram

The process is continuously monitored and controlled to ensure the desired product purity and yield are maintained.

II.3.Catalyst:

A catalyst is a substance that speeds up a chemical reaction by providing an alternative pathway with a lower activation energy. It does not get consumed in the reaction and can be used over and over again. Catalysts work by providing a surface on which the reactant molecules can interact and react more easily, thus increasing the rate of the reaction. Catalysts can be used in a wide range of chemical reactions, from industrial processes to biological reactions within living organisms[10].

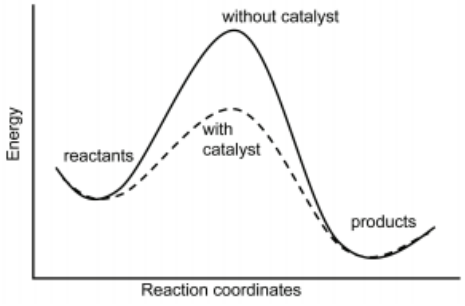


Figure 7.Graphe of the efficiency of using a catalyst

II.3.1.Types of catalysts:

There are two types of catalysts:

Homogeneous catalysts: homogeneous catalysts are catalysts that are present in the same phase (usually liquid) as the reactants. In homogeneous catalysis, the catalyst is uniformly distributed in the reaction mixture, enabling efficient contact with the reactants. Homogeneous catalysts typically have a high degree of selectivity and activity, allowing for precise control over the reaction conditions and products[11].

One of the main advantages of homogeneous catalysis is the ability to tune the activity and selectivity of the catalyst by modifying the structure and composition of the catalyst. However, homogeneous catalysts are often expensive, can be difficult to separate from the reaction mixture, and can pose environmental and safety risks.

Heterogeneous catalysts: Heterogeneous catalysts are a type of catalyst that exists in a different phase than the reactants. Heterogeneous catalysts are widely used in chemical processes due to their stability and easy separation from the reactants and products. They can be used in various forms such as powders, pellets, or supported on a substrate. The surface of the catalyst provides active sites for the reactants to adsorb and undergo chemical reactions, leading to the formation of products[12].

The reaction rate is typically described by the Langmuir-Hinshelwood model, which assumes that the reaction occurs in two steps:

(1) Adsorption of reactant molecules onto the catalyst surface.

(2) Reaction between the adsorbed molecules to form products.

The rate of reaction is then dependent on the adsorption rate, the reaction rate between the adsorbed molecules, and the desorption rate of the products. The rate expression for the LH model can be written as:

$$r = k \times \theta_A \times \theta_B$$

where

r is the reaction rate

k is the rate constant

θ_A is the fractional coverage of reactant A on the surface of the catalyst,

θ_B is the fractional coverage of reactant B on the surface of the catalyst.

The fractional coverage is related to the concentration of adsorbed molecules by the Langmuir isotherm:

$$\theta\_A = \frac{K\_A \times p\_A}{1 + K\_A \times p\_A}$$

$$\theta\_A = \frac{K\_B \times p\_B}{1 + K\_B \times p\_B}$$

where

K_A and K_B are the Langmuir adsorption constants for reactants A and B

p_A and p_B are the partial pressures of reactants A and B.

II.3.2.Description of the catalyst used in the process:

The silver-based catalyst used in the direct oxidation of ethylene to produce ethylene oxide has been extensively studied and optimized over the years. The catalytic activity and selectivity of the catalyst are highly dependent on a number of factors, including the size and morphology of the silver particles, the nature of the support material, and the reaction conditions[13].

One of the key factors affecting catalyst performance is the size and morphology of the silver particles. It has been found that smaller silver particles (typically 5-10 nm) are more active and selective than larger particles. This is because smaller particles have a higher surface area-to-volume ratio, which allows for more efficient use of the silver atoms in the catalyst. The morphology of the silver particles is also important, as particles with a high degree of crystallinity and low surface defect density have been found to be more active and selective.

Another important factor affecting catalyst performance is the nature of the support material. The support material serves to stabilize the silver particles and provide a high-surface-area substrate for the reaction to occur. Alumina and silica are commonly used as support materials, with alumina being the most widely used. The pore size and surface area of the support material can also affect catalyst performance, as these properties can influence the diffusion of reactants and products to and from the active sites on the silver particles.

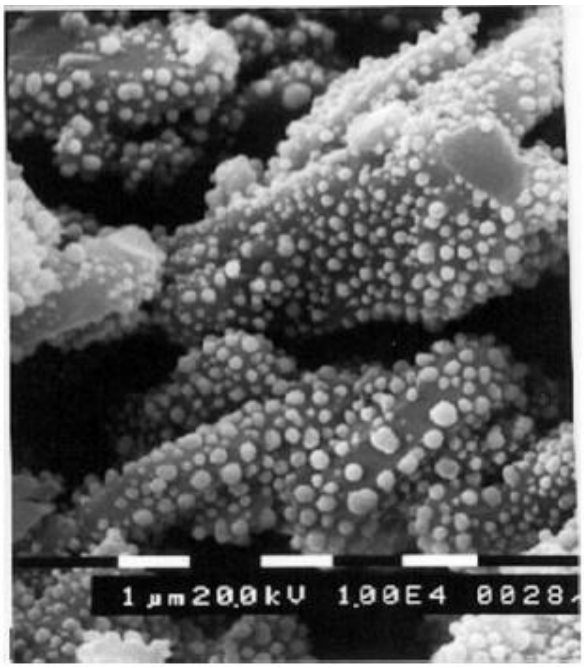


Figure 8.Microscopic view of silver catalyst[1]

Finally, the reaction conditions, including temperature, pressure, and feed composition, can have a significant impact on catalyst performance. The optimal conditions for maximum ethylene oxide production and minimum byproduct formation are typically around 200-300°C and 1-2 atm pressure. However, optimizing the reaction conditions is often a trade-off between maximizing ethylene oxide production and minimizing byproduct formation, as different reaction conditions can lead to different product distributions.

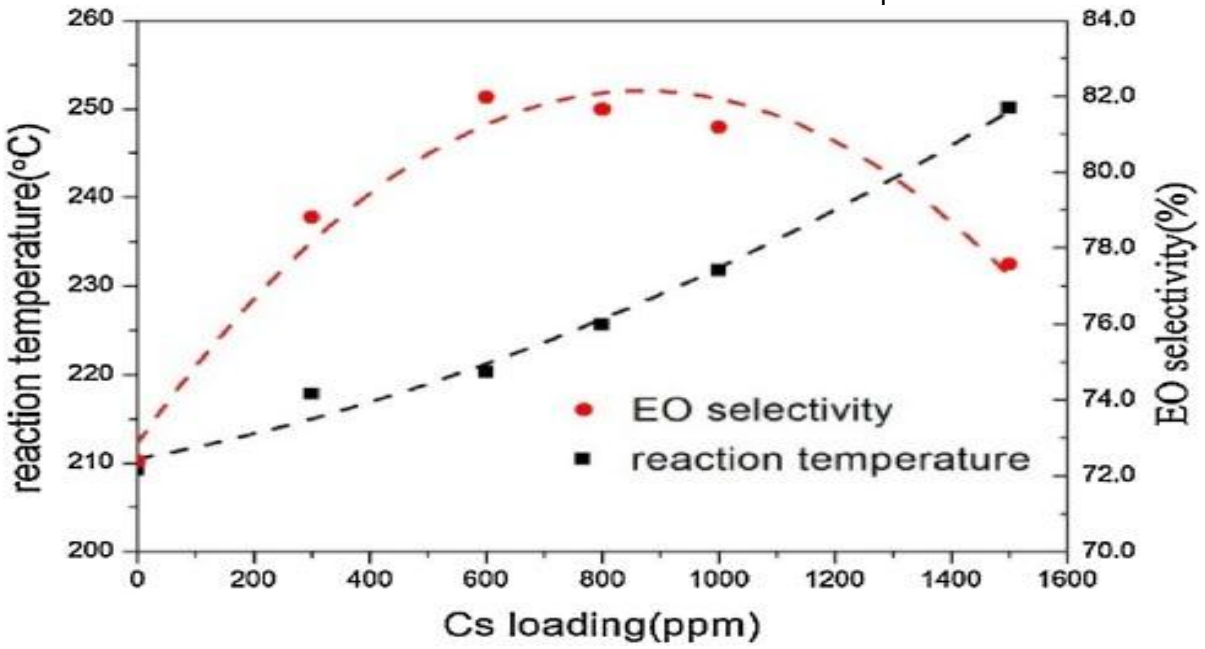


Figure 9.The coloration between the temperature degree and the selectivity of the catalyst[13]

II.4.Mathematical modeling:

The control system employed in the EO plant discussed in this model consists of a Yokogawa DCS Centum XL. This control system is integrated with an mM PC, enabling the transmission of setpoints to the DCS for operational control. To ensure the safe handling of emergencies, the plant is equipped with two PLCs: Honeywell IPC 620-35 and Alan Bradley PLC 3/10. The Honeywell PLC is equipped with dual CPUs, enabling the implementation and monitoring of two separate copies of the plant trip logic, thereby enhancing redundancy and system reliability.

II.4.1.Kinetics:

In ethylene oxide production, the two competing reactions that occur are the desired oxidation of ethylene to ethylene oxide and the undesired oxidation of ethylene oxide to carbon dioxide and water. These reactions can be represented as follows:

Desired reaction: $C_2H_4 + 1/2O_2 \rightarrow C_2H_4O$ (II.1)

Undesired reaction: $C_2H_4O + 1/2O_2 \rightarrow CO_2 + H_2O$ (II.2)

The challenge in ethylene oxide production is to maximize the yield of the desired reaction while minimizing the extent of the undesired reaction. This is typically achieved through the use of carefully designed reactors and catalysts, as well as process conditions that favor the desired reaction.

The kinetics of the reaction in ethylene oxide production is complex and is influenced by various factors, including the catalyst type, temperature, pressure, and reactant concentrations. The reaction kinetics can be described by mathematical models that relate the rate of the reaction to these factors.

The reaction is typically modeled using a Langmuir-Hinshelwood mechanism, which assumes that the reaction occurs in two steps: adsorption of the reactants on the catalyst surface, followed by a surface reaction that produces the desired product. The rate of the reaction is then given by the following equation:

$$ri = \frac{k_r^i \times P_E \times P_O^{ni}}{1 + k_E^i \times P_E + k_C^i \times P_C + k_H^i \times P_H + k_{EO}^i \times P_{EO}} \quad \text{(II.3)}$$

The selectivity expression is a way to quantify the efficiency of a chemical reaction in producing a desired product. In the context of EO production, selectivity refers to the percentage of ethylene that is converted to EO, as opposed to other byproducts such as carbon dioxide or carbon monoxide.

The selectivity expression can be written as:

Selectivity(S) = moles of C_2H_4O produced / moles of C_2H_4 consumed (II.4)

If xl and *x2* are, respectively, the number of moles of *EO* and *CO2* produced, then:

$$S = \frac{x1}{x1+\frac{x2}{2}} \quad \text{(II.5)}$$

If *x1i* and x2i are the mole fractions of *EO* and *CO2* , respectively, at the inlet and *x1o* ,*x2o* the corresponding values at the outlet, it can be shown that xl and *x2* are given by:

$$S = \frac{x1o-x1i}{1+\frac{x1o}{2}} \quad \text{(II.6)}$$

$$x2 = x2o - x2i - \frac{x2o \times x1}{2} \quad \text{(II.7)}$$

The EO plant described in this model is equipped with a Yokogawa DCS Centum XL for control purposes. It is connected to an mM PC, which facilitates the provision of setpoints to the DCS. In case of emergencies, two PLCs, namely the Honeywell IPC 620-35 and Alan Bradley PLC 3/10, are responsible for initiating plant trips. The Honeywell PLC comprises two CPUs, each implementing and monitoring a copy of the plant trip logic. Consequently, the EO plant possesses three parallel protection mechanisms to handle emergencies, including runaways.

II.4.2.Model development:

$$\frac{\partial[\overline{C2H4}]}{\partial t} = -\frac{v}{\epsilon} * \frac{\partial[\overline{C2H4}]}{\partial x} - r1 - r2 \quad \text{(II.8)}$$

$$\frac{\partial[\overline{O2}]}{\partial t} = -\frac{v}{\varepsilon} * \frac{\partial[\overline{O2}]}{\partial x} - 0.5r1 - 3r2 \quad \text{(II.9)}$$

$$\frac{\partial[\overline{C2H4O}]}{\partial t} = -\frac{v}{\varepsilon} * \frac{\partial[\overline{C2H4O}]}{\partial x} - r1 \quad \text{(II.10)}$$

$$\frac{\partial[\overline{CO2}]}{\partial t} = -\frac{v}{\varepsilon} * \frac{\partial[\overline{CO2}]}{\partial x} - 2 * r2 \quad \text{(II.11)}$$

$$\rho C_P * \frac{\partial \overline{T}}{\partial t} = -\frac{v}{\varepsilon} * \rho C_P * \frac{\partial \overline{T}}{\partial x} - \frac{4U}{dt} * \left(\overline{\overline{T}} - T_c\right) + \overline{UA}(\overline{T} - \overline{T}_s) \quad \text{(II.12)}$$

We assume that each particle is uniformly heated, and there is no significant resistance to the diffusion of gases within the solid particles. Therefore, only the energy balance equations need to be considered for the solid phase.

$$\rho C_P * \frac{\partial \overline{T_s}}{\partial t} = r1(-\Delta H_1) + r2(-\Delta H_2) + \overline{UA}(\overline{T} - \overline{T}_s) \quad \text{(II.13)}$$

The initial conditions at t = 0 are:

$$[\overline{C2H4}] = C_1^0 \quad \text{(II.14)}$$

$$[\overline{O2}] = C_2^0 \quad \text{(II.15)}$$

$$[\overline{C2H4O}] = C_3^0 \quad \text{(II.16)}$$

$$[\overline{CO2}] = C_4^0 \quad \text{(II.17)}$$

$$\overline{T} = T_r \quad \text{(II.18)}$$

$$\overline{T}_s = T_r \quad \text{(II.19)}$$

The symbol T_r represents room temperature. The boundary conditions for the system are defined as follows: at x = 0, the concentration conditions are equal to the initial conditions. The temperature of the incoming gas is gradually increased to reach the final value. This behavior is represented in the model as follows: at x = 0:

$$\overline{T} = T^0 \quad \text{(II.20)}$$

With the help of the following dimensionless variables

$$\tau = \frac{tv}{\varepsilon L} \quad \text{(II.21)}$$

$$\xi = \frac{x}{L} \quad \text{(II.22)}$$

$$[C2H4] = \frac{[\overline{C2H4}]}{C_1^0} \quad \text{(II.23)}$$

$$[O2] = \frac{[\overline{O2}]}{C_1^0} \quad \text{(II.24)}$$

$$[C2H4] = \frac{[\overline{C2H4O}]}{C_1^0} \quad \text{(II.25)}$$

$$[CO2] = \frac{[\overline{CO2}]}{C_1^0} \quad \text{(II.26)}$$

$$T = \frac{\overline{T} - T_r}{10T_r} \quad \text{(II.27)}$$

$$T_s = \frac{\overline{T_s} - T_r}{10T_r} \quad \text{(II.28)}$$

$$Da1 = \frac{\varepsilon L}{v C_1^0} r1 \quad \text{(II.29)}$$

$$Da2 = \frac{\varepsilon L}{v C_1^0} r2 \quad \text{(II.30)}$$

$$H_{num1} = \frac{\varepsilon L r1(-\Delta H1)}{10 v \rho_s C_{ps} T_r} \quad \text{(II.31)}$$

$$H_{num2} = \frac{\varepsilon L r2(-\Delta H2)}{10 v \rho_s C_{ps} T_r} \quad \text{(II.32)}$$

$$Bi = \frac{\varepsilon L U}{v \rho C_p dt} \quad \text{(II.33)}$$

$$Bi_s = \frac{\varepsilon L \overline{UA}}{v \rho_s C_{ps}} \quad \text{(II.34)}$$

$$\beta = \frac{T_c}{10 T_r} - 0.1 \quad \text{(II.35)}$$

$$\gamma = \frac{\rho_s C_{ps}}{\rho C_p} \quad \text{(II.36)}$$

$$\frac{\partial [C2H4]}{\partial \tau} = -\frac{\partial [C2H4]}{\partial \xi} - Da1 - Da2 \quad \text{(II.37)}$$

$$\frac{\partial [O2]}{\partial \tau} = -\frac{\partial [O2]}{\partial \xi} - 0.5Da1 - 3Da2 \quad \text{(II.38)}$$

$$\frac{\partial [C2H4O]}{\partial \tau} = -\frac{\partial [C2H4O]}{\partial \xi} + Da1 \quad \text{(II.39)}$$

$$\frac{\partial [CO2]}{\partial \tau} = -\frac{\partial [CO2]}{\partial \xi} + 2Da2 \quad \text{(II.40)}$$

$$\frac{\partial T}{\partial \tau} = -\frac{\partial T}{\partial \xi} + 4Bi(\beta - T) + Bi_s \gamma (T_s - T) \quad \text{(II.41)}$$

$$\frac{\partial T_s}{\partial \tau} = H_{num1} + H_{num2} + Bi_s (T - T_s) \quad \text{(II.42)}$$

The model described above does not consider the axial dispersion term due to certain challenges associated with obtaining the appropriate boundary conditions. Initially, an attempt was made to set the derivatives of the variables at the reactor's end to zero. However, as explained by Schiesser (1996), this condition would imply that a moving front must exit the system with zero slope, which is not physically realistic. This anomaly arises because the Péclet number is

extremely large, on the order of 10^6. Consequently, the model simplifies by excluding the axial dispersion terms, eliminating the need for the second boundary condition. To avoid numerical difficulties arising from the jump between the initial condition given by Eq. 18 and the boundary condition described by Eq. 20, it is necessary to replace Eq. 20 with:

$$\overline{T} = T_r + (T^0 - T_r)(1 - e^{-0.1r}) \quad \text{(II.43)}$$

II.4.3.Module proving;

Below are the parameter values utilized in this model, which have been determined using standard correlations. These parameter values are assumed to remain constant throughout the analysis. The value of UA is obtained by dividing the heat of reaction by the anticipated temperature difference between the average solid temperature and the gases, which is assumed to be approximately 5°C.

It should be noted that the choice of UA leads to the model reaching steady state in approximately 10 minutes. If a larger UA value is selected, the steady state will be reached sooner with a smaller temperature difference. Conversely, reducing UA will delay the attainment of steady state. Therefore, accurately tuning the model requires understanding the time required for the reactor to reach steady state. Unfortunately, dynamic information of this nature is unavailable from the plant. Additionally, due to the hazardous nature of the EO reactor startup, a proprietary and meticulous procedure is employed. Considering the startup scenario assumed in this report, a value of 10 minutes appears reasonable to engineers and operators experienced with the plant.

V	1.0	m/s
ε	0.6	
ρ	12.0	kg/m^3
C_p	1000	Joules/Kg/K
U(liq)	330	Joules/s/m^2/K
U(vap)	190	Joules/s/m^2/K
D_t	0.0389	m
L	12.8	m
ρ_s	890	kg/m^3
C_{ps}	1000	Joules/Kg/K
$\overline{UA}$	100000	Joules/s/m^3/K
$(-\Delta H_1)$	103246	Joules/gmole of C_2H_4
$(-\Delta H_2)$	1321716	Joules/gmole of C_2H_4

Table 2.Parameters of the reactor

Gases	Input	output	
		sim	plant
C_2H_4	31.36	28.55	28.84
O2	6.30	3.19	4.26
C_2H_4O	0.03	2.45	2.45
CO2	2.35	3.14	3.14

Table 3.Results of the simulation

II.5.Conclusion:

In this chapter, our focus is on the production method of ethylene oxide, a crucial compound in the ethylene-based chemical industry. Traditionally, ethylene oxide was produced using the chlorohydrin method. However, in our study, we explore the direct oxidation of ethylene in a Continuous Stirred Tank Reactor (CSTR) as an alternative production method.

The CSTR design offers several advantages for this application. It allows for efficient mixing of the reactants and maintains continuous contact between the reactants and the catalyst. This ensures optimal reaction conditions and enhances the conversion of ethylene to ethylene oxide. The CSTR's ability to maintain a homogeneous reaction mixture throughout the process enhances the reaction kinetics and improves the overall efficiency of ethylene oxide production.

Choosing the appropriate catalyst is crucial for achieving high selectivity towards ethylene oxide. In our study, we utilize a silver-based catalyst, known for its exceptional selectivity in the ethylene oxidation reaction. Silver catalysts are widely used in industry due to their high activity, stability, and availability. By employing a silver catalyst in our CSTR, we aim to maximize the production of ethylene oxide while minimizing unwanted byproducts.

The direct oxidation of ethylene in a CSTR with a silver-based catalyst offers numerous benefits. It provides a more streamlined and efficient production process compared to the chlorohydrin method. Additionally, the utilization of a readily available and selective catalyst ensures a higher yield of ethylene oxide.

By exploring this production method in our study, we aim to optimize the production process of ethylene oxide, enhance its selectivity, and improve overall efficiency. This research contributes to the advancement of ethylene oxide production techniques, opening avenues for further optimization and innovation in the industry.

Chapter III

Sliding mode control approach

Chapter III:Sliding mode control approach:

In the past few decades, significant advancements have been made in the field of linear control systems, leading to the resolution of many problems in this area. However, with the advent of modern technology and the demand for more sophisticated control laws to meet stringent design specifications, the importance of nonlinear control systems has become increasingly evident[14].

Real-world systems inherently exhibit nonlinear behavior, especially when considered over a wide operating range. Although many systems can be approximated as linear around certain operating points under specific assumptions, their true nature is nonlinear.

In recent years, researchers from various fields such as process control, biomedical engineering, robotics, and aircraft and spacecraft control have shown a keen interest in the design and analysis of nonlinear control strategies. This is driven by the fact that many practical problems involve dealing with nonlinearities, including improving upon existing linear control systems, analyzing challenging nonlinear behaviors, addressing model uncertainties, and seeking design simplicity[14].

The future of nonlinear control systems appears promising as there are still many aspects of nonlinear theory that need to be developed to meet the design requirements of numerous nonlinear systems. Nonlinear control theory finds applications in various domains, including cyber-physical systems, communication, energy, healthcare, big data research, robotic systems, small unmanned aerial vehicles (UAVs), and AC electrical motors.

Looking back at the history of nonlinear control theory, its origins can be traced back to the 18th century when the first nonlinear governor was designed to control steam engines. The development of nonlinear control theory can be divided into three distinct eras, each contributing theories and concepts that have advanced the field.

The first era, spanning from the 1880s to the 1950s, saw the emergence of influential works such as Poincare's concepts of limit cycles and the phase plane method, Lyapunov's stability analysis of dynamical systems, Van der Pol's study of limit cycles in oscillator dynamics, Bode's frequency response and bode plotting, Krylov and Bogoliubov's describing function method, Nyquist's feedback theory, Lur'e's work on absolute stability, and Hamel and Tsypkin's accurate

evaluation of limit cycles in relay systems in the time and frequency domain. This era also witnessed the development of sliding mode control (SMC) by Emelyanov. The second era, from 1960 to 1989, marked the beginning of modern nonlinear control, further advancing the field with new concepts and methodologies[15].

III.1.Nonlinear control:

Nonlinear control techniques have emerged as significant contributors to modern control theory, primarily due to their ability to effectively handle the inherent nonlinearity present in many practical engineering systems and ensure stability across a broad operating range. In the subsequent section, we will explore recent advancements and research directions in three prominent nonlinear control strategies: sliding mode control, back-stepping control, and feedback linearization control.

These approaches offer valuable insights and methodologies for addressing the challenges posed by nonlinear systems and achieving desirable control performance.

III.1.1.Back-stepping control:

BSC is considered as the most popular technique, especially for controlling high order systems. The applications of BSC have widely involved several practical systems. One notable drawback of traditional BSC is the issue of "explosion of terms," resulting from repeated differentiation of virtual inputs. This leads to increased complexity of the controller, particularly for higher-order systems, which presents challenges in practical implementation. To address this problem, Dynamic Surface Control (DSC) based on fractional-order filters has been proposed as a solution. Additionally, the use of disturbance observers has been suggested as another remedy.

Furthermore, the strict feedback form requirement for designing BSC for nonlinear systems poses another limitation. To overcome this drawback, various solutions have been presented in the literature, such as model-free backstepping normal form and block backstepping approaches.

It should be noted that an exact mathematical model of the system is typically required for designing the controller when using the backstepping technique, which represents a third potential limitation[15].

Overall, these advancements and alternative approaches aim to overcome the challenges associated with BSC and enhance its practical applicability in controlling nonlinear systems.

III.1.2.Feedback linearization control:

Feedback linearization control is a widely used approach for controlling nonlinear systems. It offers the advantage of canceling out the nonlinear terms in a system, enabling the use of linear control techniques to design the control law. The applications of Feedback Linearization Control (FLC) span across various domains, including Maglev trains, microgrids, and converters.

However, a significant drawback of FLC is the removal of useful nonlinear terms from the system dynamics. This can limit the control capabilities and the ability to fully exploit the nonlinear behavior of the system. Another challenge associated with FLC is its limited robustness in the presence of uncertainties. Uncertain factors can degrade the control performance and introduce undesirable effects.

To address these issues, the use of disturbance observers has been proposed as a means to alleviate the impact of uncertainties. Disturbance observers can estimate and compensate for the effect of disturbances and uncertainties, enhancing the robustness and performance of the control system when combined with FLC[15].

By incorporating disturbance observers, the limitations of FLC can be mitigated, allowing for improved control performance and increased robustness in the presence of uncertainties. This combination of techniques offers a promising avenue for effectively controlling nonlinear systems.

III.1.3.Sliding mode control:

In the formulation of control problems, discrepancies between the actual plant and the mathematical model used for controller design often arise[15]. These discrepancies can be attributed to various factors such as unmodeled dynamics, parameter variations, or the simplification of complex plant behavior in the model. It is crucial for engineers to ensure that the resulting controller can achieve the desired performance levels in practice, despite these plant/model mismatches. This need has spurred the development of robust control methods that aim to address this challenge. One prominent approach in robust controller design is the sliding mode control methodology[16].

Chapter III Sliding mode control approach

Sliding mode control (SMC) has gained significant popularity as a control technology over the past 60 years. It is particularly well-suited for complex nonlinear dynamic systems due to its simplicity and robustness against uncertainties and disturbances. Its foundation lies in the principles of Lyapunov theory, which guarantees asymptotic stability. In the 1990s, a novel variant of SMC known as terminal sliding mode control (TSMC) was introduced. TSMC has been extensively studied and applied, offering robust control with tunable finite-time convergence, fast response, high precision, and strong robustness. In recent years, there has been a growing interest in this specific control technology[17].

The subsequent section will delve into further details of this control strategy, exploring its principles, methodologies, and applications.

III.2.General Development of Sliding Mode Control:

Sliding mode control (SMC) is a specialized form of nonlinear control that has emerged as a powerful and robust strategy for dealing with incompletely modeled or nonlinear systems since its inception in the 1950s. SMC distinguishes itself by employing a discontinuous control action that switches between two distinct system structures, creating a unique type of system motion known as the sliding mode, which exists within a specified manifold. This characteristic of motion within the manifold offers robustness against parameter variations and complete rejection of external disturbances. The analysis and design of SMC have been extensively explored in the literature, covering both theoretical foundations and practical implementation considerations[18].

While sliding mode control (SMC) provides a robust and straightforward approach for synthesizing controllers in linear and nonlinear processes, its application to chemical processes poses certain challenges. Firstly, developing a comprehensive model for chemical processes is often challenging due to the complexity of the process itself and limited knowledge of certain process parameters. Secondly, most process models relating the controlled and manipulated variables tend to be higher-order, adding complexity to the resulting sliding mode controller. In general, the traditional procedures of SMC yield complex controllers with multiple parameters, making the tuning process difficult. Consequently, the conventional approaches of SMC encounter limitations when applied to chemical processes[19].

III.3.Variable structure system:

The concept of sliding mode control (SMC) originates from the variable structure system (VSS) framework, where the system's structure undergoes changes during the evolution of its dynamics. In VSS, the system's structure is switched or altered in a way that ensures the closed-loop system's asymptotic stability. However, in SMC, the system trajectory is constrained to remain on a predetermined manifold through the application of a discontinuous control signal. In this case, the vector fields on either side of the sliding manifold act towards the manifold, guiding and maintaining the trajectory along it. This phenomenon, where the system dynamics switch between two structures while enforcing sliding mode, is referred to as sliding mode.

SMC is considered a special category within the VSS framework, as it involves switching along a predetermined manifold, leading to a discontinuous system behavior on that manifold. While it is not necessary for sliding mode to be enforced in the system from the initial instant, it must initiate within a finite time for the system to be considered in sliding mode. In a controlled dynamical system, the control law is often designed to bring about sliding mode, giving rise to what is known as sliding mode control. This control strategy is responsible for achieving and maintaining the sliding mode behavior within the system[20].

III.4.Sliding surface:

The sliding surface in sliding mode control is a mathematical construct or a hyperplane that separates different operating regions of a system. It is designed such that the system dynamics drive the states of the system to the sliding surface and subsequently maintain them on that surface. The sliding surface acts as a reference trajectory or a desired state for the system.

The specific form of the sliding surface depends on the control objective and the characteristics of the system being controlled. It is typically defined as a function of the system states, and its equation determines the conditions that must be satisfied for the system to enter and remain in the sliding mode.

The choice of the sliding surface is crucial as it directly influences the behavior and performance of the sliding mode control system. The design of the sliding surface often involves considering stability criteria, desired performance objectives, and system-specific requirements. It can be a linear or nonlinear function of the system states, depending on the complexity of the system dynamics and the control objectives.

In summary, the sliding surface in sliding mode control defines the desired state or trajectory that the system should track, and it plays a vital role in achieving robust and precise control performance.

III.5.Fundamental Theory of SMC:

The fundamental concept of sliding mode control (SMC) is to establish a surface along which the system can smoothly slide towards its desired final value. This surface defines the objective of SMC. As the system's state crosses the sliding surface, the structure of the controller is intentionally modified based on a predetermined control law[19].

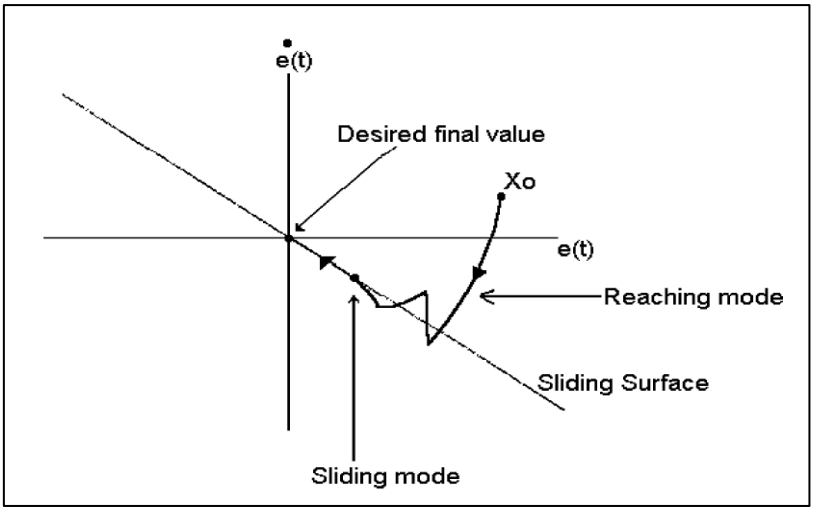


Figure 10.Graphical interpretation of SMC[21].

Let us consider the following nonlinear system:

$$\dot{x} = f(x,t) + g(x,t)u(t) \quad \text{(III.1)}$$

Where $x \in R^n$ is the state variable vector, $u(t) \in R^m$ is the control input, $f(.,.)$ and $g(.,.)$ are continuous functions in x, u and t vector fields.

The sliding mode controller is designed as:

$$u(t) = [u_1(t)u_2(t) \dots u_m(t)]^T \quad \text{(III.2)}$$

$$u_i(t) = \begin{cases} u_i^+(t), & if\ s_i(x) > 0, \\ u_i^-(t), & if\ s_i(x) < 0, \end{cases} \quad i = 1,2,3,\dots,m \quad \text{(III.3)}$$

Where $u_i^+(t) \neq u_i^-(t)$, and $s(x) \in R^m$ called sliding manifold is the switching vector function $s(x) = [s_1(x)s_2(x) \dots s_m(x)]^T$.

It undergoes discontinuities on the surface $s(x) = 0$.

It is important to note that the design of the sliding mode control law (III.3) is aimed at achieving two objectives: reaching the sliding surface (s(x) = 0) and subsequently maintaining motion on the sliding surface. To fulfill these objectives, the control law u(t) needs to satisfy the "reachability condition," which ensures that the system reaches and remains on the sliding surface.

III.5.1.Reaching phase:

The condition for the system (III.1) to satisfy the reachability condition can be expressed as follows:

$$s(x)\dot{s}(x) < 0 \quad \text{(III.4)}$$

This condition (III.4) ensures that the system trajectory always moves towards the sliding surface. A more stringent reachability condition, known as the 'η-condition,' is defined as:

$$s(x)\dot{s}(x) \leq -\eta|s(x,t)| \quad \text{(III.5)}$$

Here, η is a positive scalar. The condition (III.5) guarantees that the sliding surface is reached within a finite time period, even in the presence of uncertainty. The system state trajectories that satisfy either condition (III.4) or (III.5) are referred to as the reaching phases[18].

III.5.2.SMC Design Methods:

In the literature, various design methods for sliding mode control (SMC) have been proposed, typically involving two steps:

Step 1: Designing a sliding manifold s(x) that ensures desired performance in the sliding mode, such as stability, disturbance rejection, and tracking.

Step 2: Designing a discontinuous feedback control u(t) that guides the system states to reach the sliding manifold within a finite time, thus achieving and maintaining the desired performance.

To simplify the implementation, the sliding variable $s_i(x)$, where $s_i(x) = 1,2,3,\dots,m$, is chosen as a linear combination of the state variables, represented as:

$$s_i(x) = \sum_{j=1}^{m} \alpha_j x_j(t) \quad \text{(III.6)}$$

Here, α_j denotes the sliding coefficients, and $x_j(t)$belongs to the state vector x(t). The primary objective of the sliding mode controller is to drive the system state trajectories onto the specified sliding surface within a finite time and maintain them there for all subsequent time. In the following section, we will discuss typical strategies employed in sliding mode control[18].

III.5.3.Equivalent-Control-Based Design:

For the system (III.1), assuming that the term $\frac{\partial s}{\partial x} g(x,t)$ is non-singular, and the control law $u(t)$ is designed as follows:

$$u(t) = u_{eq}(t) + u_N(t) \tag{III.7}$$

Where $u_{eq}(t)$ represents a continuous component and $u_N(t)$ represents a discontinuous component.

The equivalent control $u_{eq}(t)$ is derived from the so-called equivalent control method, i.e., in the case when $s(x) = \dot{s}(x) = 0$. Thus, $u_{eq}(t)$ is calculated as:

$$u_{eq}(t) = -\left(\frac{\partial s}{\partial x} g(x,t)\right)^{-1} \frac{\partial s}{\partial x} f(x,t) \tag{III.8}$$

Substituting the above equivalent control (III.8) into the original system (III.1), it follows that the motion of sliding mode is determined by:

$$\dot{x}(t) = \left[I_n - g\left(\frac{\partial s}{\partial x} g(x,t)\right)^{-1} \frac{\partial s}{\partial x}\right] f(x,t) \tag{III.9}$$

Where (III.9) is considered as the equation of the sliding mode in the manifold $s(x) = 0$. The high frequency switching action $u_N(t)$ can be designed as:

$$u_N(t) = -\beta\left(\frac{\partial s}{\partial x} g(x,t)\right)^{-1} sign(s(x)), \beta > 0 \tag{III.10}$$

Such that the derivative of the Lyapunov function $V = \frac{1}{2} s^T(x) s(x)$ is negative, that is:

$$\dot{V} = s^T(x)\dot{s}(x) = s^T(x)\frac{\partial s}{\partial x} g(x,t) u_N(t) < -\beta \|s(x)\| \tag{III.11}$$

The physical meaning of the equivalent control can be interpreted as the low-frequency component of the discontinuous control law $u(t)$, because the high frequency $u_N(t)$ can be filtered out by a low pass filter of the system.

$$\tau\dot{z} + z = u(t), \tau \ll 1 \tag{III.12}$$

Which means $z \simeq u_{eq}$.

III.5.4.Reaching Law Approach:

The reaching law specifies the dynamics of a switching function, which can be described by the following differential equation:

$$\dot{s}(x) = -\gamma sign\big(s(x)\big) - Kg(s(x)) \quad \text{(III.13)}$$

Where:

$$\gamma = diag[\varepsilon_1 \varepsilon_2, \dots, \varepsilon_m], \qquad \varepsilon_i > 0$$

$$K = diag[k_1 k_2, \dots, k_m], \qquad k_i > 0$$

$$sign\big(s(x)\big) = \begin{bmatrix} sign(s_1(x)) \\ sign(s_1(x)) \\ : \\ : \\ sign(s_m(x)) \end{bmatrix}, g\big(s(x)\big) = \begin{bmatrix} g_1(s_1(x)) \\ g_2(s_2(x)) \\ : \\ : \\ g_2(s_m(x)) \end{bmatrix}$$

$$g_i(0) = 0, s_i(x) g_i\big(s_i(x)\big) > 0, i = 1,2,3, \dots, m$$

Equation (III.13) is a general form of reaching law, and some special cases are:

1-The constant rate reaching law:

$$\dot{s}(x) = -\gamma sign(s(x))$$

2-The constant plus proportional rate reaching law:

$$\dot{s}(x) = -\gamma sign\big(s(x)\big) - Ks(t)$$

3-The power rate reaching law:

$$\dot{s}(x) = -\varepsilon_i |s_i(x)|^{\alpha} sign\big(s_i(x)\big), \quad 0 < \alpha < 1$$

The reaching law approach not only guarantees the reaching condition but also specifies the dynamics of the motion during the reaching phase[18].

III.5.5.Chattering Problem:

In practical scenarios, an ideal sliding mode is not achievable because it would require control actions to switch at an infinitely high frequency. Due to various switching imperfections, such as time delays and small-time constants in the actuators, the discontinuous

nature of the feedback control leads to a specific dynamic behavior near the sliding surface. This phenomenon is commonly known as chattering.

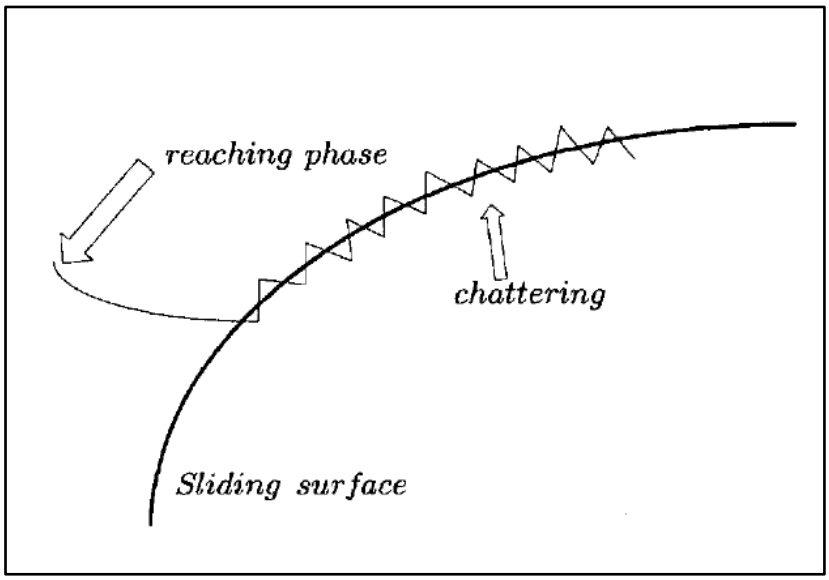


Figure 11.The chattering phenomenon[22].

This phenomenon is considered a drawback because even if it is filtered at the output of the process, it can still excite high-frequency modes that are modeled. This ultimately deteriorates the system's performance and can even result in instability. Moreover, chattering contributes to increased wear of moving mechanical components and higher heat losses in electrical power circuits. Consequently, numerous approaches have been suggested in the literature to mitigate or attenuate the effects of chattering[21].

III.5.6.Main approaches to alleviate or limit the chattering problems:

III.5.6.A.Boundary layer approach:

To address this issue, a common approach is to introduce a boundary layer in the vicinity of the sliding surface. The aim is to replace the discontinuous control action with a continuous one when the system operates within this boundary layer. To achieve this, the discontinuous component of the controller can be modified or adapted.

$u_N(t) = -K_s \text{sign}(s(x))$

is often replaced by the saturation control:

$u_N(t) \approx -K_s \frac{s(x)}{\|s(x)\|+\delta}$

for some, preferably small, $\delta > 0$.

The boundary layer approach has been utilized extensively to the practical applications. However, this method has some disadvantages such as:

- While introducing a boundary layer can eliminate chattering, it often results in a finite steady-state error in the system.

- The thickness of the boundary layer is subject to a trade-off relationship between the control performance of sliding mode control and the mitigation of chattering.

- It's important to note that within the boundary layer, the system's robustness and accuracy characteristics are no longer guaranteed[18].

II.5.6.B.Reaching law approach:

One approach to reducing chattering is to decrease the magnitude of the discontinuous control, which directly affects the amplitude of chattering. However, this technique has an impact on the robustness of the controller and can degrade the transient response of the system. Therefore, there exists a trade-off between reducing chattering and maintaining system performance. A compromised approach is to decrease the amplitude of the discontinuous control, denoted as $u_N(t)$, when the system state trajectories are close to the sliding surface (to reduce chattering), and to increase the amplitude when the system states are far from the sliding surface. This approach aims to strike a balance between chattering reduction and maintaining desirable system performance[18].

III.5.6.C.Dynamic SMC approach:

The core concept behind the dynamic sliding mode control (SMC) approach is to incorporate an integrator or a strictly proper low-pass filter between the SMC and the plant being controlled. This concept is visually depicted in the following diagram:

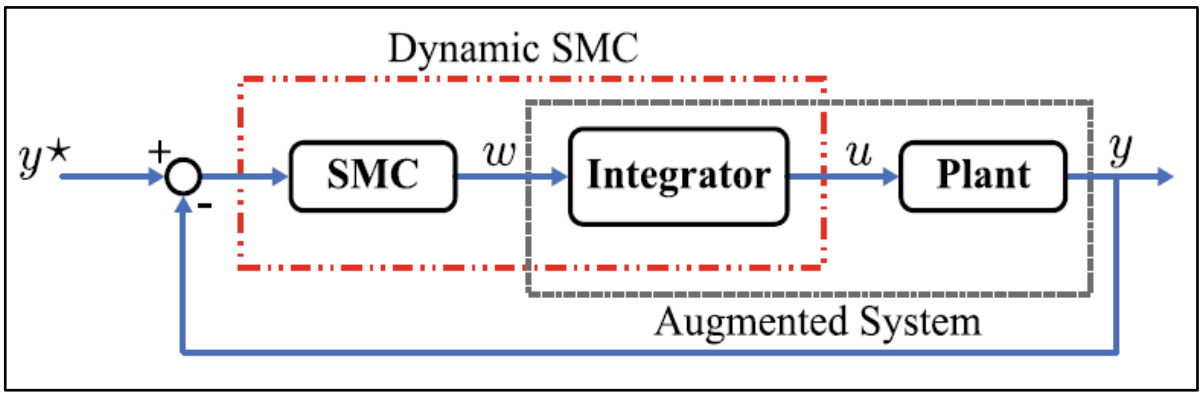


Figure 12 The concept of a dynamic SMC approach[21]

Chapter III Sliding mode control approach

In the dynamic sliding mode control approach, the time derivative of the control input, ω, is considered as the new control input for the augmented system. By incorporating a low-pass integrator, the high-frequency chattering in ω is effectively filtered out. As a result, the control input to the actual plant, u, becomes continuous, providing a potential means to reduce chattering. This method can effectively eliminate chattering and achieve zero steady-state error. However, it is important to acknowledge that the system order is increased by one, and as a trade-off, the transient responses of the system may be compromised[18].

III.6.Application areas of Sliding Mode Control:

The Sliding Mode control technique has made significant advancements across various control domains. In hydraulic or pneumatic control, on/off valves are commonly used, which have two stable states: fully open or fully closed. These valves allow for switching frequencies of 0 Hz.

In applications such as electric drives for machine tools or robotic systems, precise control of rotation speed or position is required. Sliding Mode control offers undeniable advantages in terms of high-performance dynamic behavior and the ability to enforce limits on certain quantities, such as current and rotation speed[23].

It is worth mentioning that in certain fields like chemical processes and metallurgy, on/off controllers are commonly employed.

III.7.Advantages of Sliding Mode Control:

This control technique exhibits the following characteristics[23]:

- The system response demonstrates robustness and insensitivity to variations in certain parameters, load disturbances, and disturbances.

- It only necessitates knowledge of an upper bound for V, simplifying the control process.

- The selection of the switching surface offers significant flexibility and independence.

- The control action is made smoother by the inclusion of an equivalent control term, which can be eliminated by increasing V.

III.8.Higher Order Sliding Mode Control:

Higher Order Sliding Mode Control (HOSMC) is a powerful approach for mitigating chattering. It involves applying the discontinuous control signal to higher-order time derivatives

of the sliding variable. This design enables not only the convergence of the sliding variable itself to the origin but also the convergence of its higher-order time derivatives. By not directly affecting the system input with the discontinuous control, chattering is inherently reduced. In the upcoming section, we will delve into the problem formulation of HOSMC and review some widely recognized algorithms for Second Order Sliding Mode Control[24].

Problem Formulation:

Let us consider an uncertain nonlinear system:

$$\begin{cases} \dot{x}(t) = f(x,t) + g(x,t)u, \\ y(t) = s(x,t), \end{cases} \quad \text{(III.14)}$$

where $x \in R^n$ is the state vector and $u \in R$ is the control input. The sliding variable s is a measured smooth output-feedback function and $f(x,t)$ and $g(x,t)$ are uncertain smooth functions. Let us recall the definition of relative degree of a system:

The relative degree, denoted as $\boldsymbol{r}$, of System (III.14) is defined as the smallest order of time derivatives of the output y(t) in which the control input u explicitly appears. It is assumed that the relative degree $\boldsymbol{r}$ is globally well defined, uniform, and time invariant for System (III.14). Additionally, it is assumed that the associated zero dynamics of the system are asymptotically stable.

This implies that there exist appropriate functions $\tilde{\varphi}(x,t)$ and $\tilde{\gamma}(x,t)$ such that the following conditions are satisfied:

$$y^{(r)} = \tilde{\varphi}(x(t),t) + \tilde{\gamma}(x(t),t)u(t) \quad \text{(III.15)}$$

The functions $\tilde{\gamma}(x(t),t)$ and $\tilde{\varphi}(x(t),t)$ are assumed to be bounded by positive constants γ_m , γ_M and $\bar{\varphi}$, such that:

$$0 < \gamma_m \leq \tilde{\gamma}(x(t),t) \leq \gamma_M, \quad |\tilde{\varphi}(x(t),t)| \leq \bar{\varphi} \quad \text{(III.16)}$$

Defining: $s^{(i)} = \frac{d^i}{dt^i} y$; the higher order sliding manifold of degree $\boldsymbol{r}$ is defined as:

$$S^{(r)} = \left\{ x \in R^n | s^{(0)} = s^{(1)} = \cdots = s^{(r-1)} = 0 \right\} \quad \text{(III.17)}$$

Then Higher Order Sliding Mode is defined as:

There exists an ideal Higher Order Sliding Mode regime of r^{th} order if there exists a finite time T_s such that all solutions of System (III.15) are in $S^{(r)}$ for all $t > T_s$.

More precisely, let us introduce $z = [z_1 z_2 \dots z_r]^T \coloneqq \left[s\ \dot{s} \dots s^{(r-1)}\right]^T$. Then (III.17) is equivalent to $z = 0$. Since the only available information on $\tilde{\varphi}(x(t), t)$ and $\tilde{\gamma}(x(t), t)$ are the bounds (III.16), it is natural to consider a more general control system instead of System, such as:

$$\dot{z} = z_{i+1}, \quad i = 1,2, \dots r-1 \tag{III.18}$$

$$z_r = \varphi(t) + \gamma(t)u$$

Where the new functions φ and γ are arbitrary measurable functions that verify the condition:

$$\text{(H1)} \quad \varphi(t) \in I_\varphi \coloneqq [-\bar{\varphi}, \bar{\varphi}], \quad \gamma(t) \in I_\gamma \coloneqq [-\gamma_m, \gamma_M] \tag{III.19}$$

Where $\bar{\varphi}, \gamma_m, \gamma_M$ are positive constants. In consequence, we are in fact dealing with the differential inclusion:

$$z_1^{(r)} \in I_\varphi + u\, I_\gamma \tag{III.20}$$

The objective of designing HOSM controllers for System (III.14), with respect to s, is to achieve the stabilization of System (III.20) at the origin, ideally within a finite time. Since these controllers are implemented as discontinuous feedback laws u = U(z), it is necessary to interpret the solutions of (III.20) in the Filippov sense, which is defined as follows:

At the points of discontinuity in (III.20), the right-hand vector set is expanded to include the convex hull of the set of velocity vectors obtained by approaching z from all directions in the r-dimensional space, while avoiding sets of zero measure.

A control algorithm is considered to establish a real sliding mode of order r with respect to s when, for any local set of initial conditions and for any finite time interval $[t_1, t_2]$, there exist constants $\Delta_1, \Delta_2, \dots, \Delta_r$ such that, for all $t_1 > t_2$, the following inequalities are satisfied:

$$|s| \le \Delta_1\ |\dot{s}| \le \Delta_2\ \dots \left|s^{(r-1)}\right| \le \Delta_r \tag{III.21}$$

III.8.1.Examples of Second Order Sliding Mode Controllers:

After the introduction to Higher Order Sliding Mode (HOSM), let's explore a few well-known algorithms for Second Order Sliding Mode (SOSM), namely the super-twisting, twisting, and sub-optimal algorithms. In SOSM, the objective is for the sliding variable s and its first time derivative ˙s to converge to zero within a finite time[24].

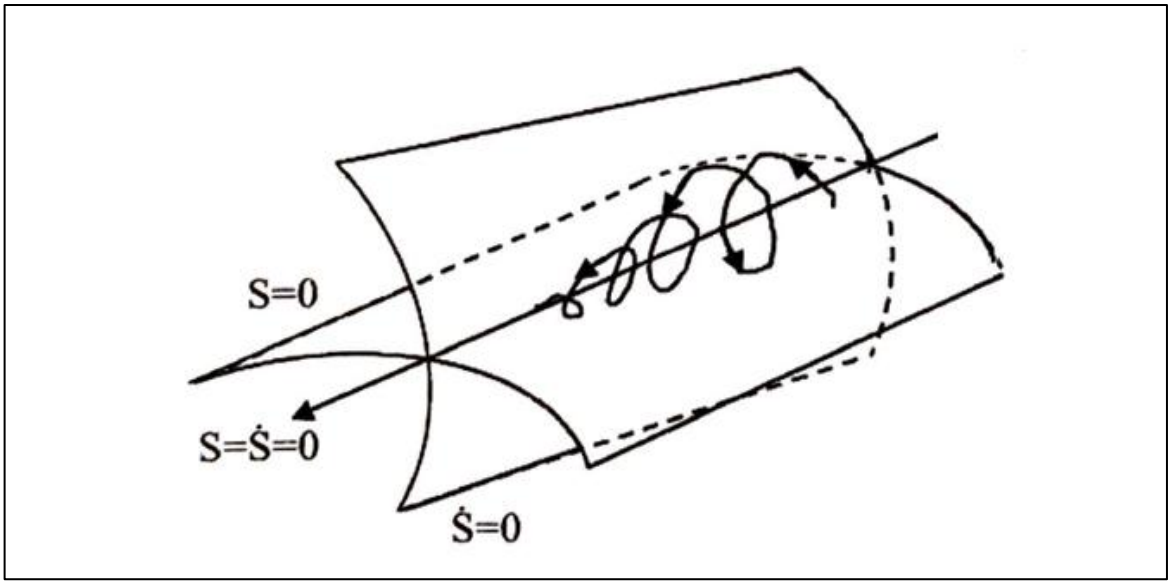


Figure 13. Second order sliding mode trajectory[24].

III.8.1.A.Super-twisting Algorithm:

Super-twisting is a continuous SOSM controller for systems of relative degree 1. It requires the boundedness of the time derivative of perturbation, i.e. for the system $\dot{z}_1 = \varphi(t) + \gamma(t)u$, the condition $|\dot{\varphi}| \leq \bar{\phi}$ needs to be satisfied. Let us introduce $\varphi = z_2$, then the control objective becomes the stabilization of the following differential inclusion:

$$\dot{z}_1 \in z_2 + [\gamma_m, \gamma_M]u \tag{III.22}$$

$$z_2 \in [-\bar{\phi}, \bar{\phi}]$$

Super-twisting algorithm is expressed as follows:

$$u = -K_p|z_1|^{\frac{1}{2}}sign(z_1) - \int_0^t K_i sign(z_1)dt \tag{III.23}$$

Where K_p and K_i are positive constants:

$$K_p = k_p\sqrt{L}, \quad K_i = k_i L$$

$$L = \frac{\phi}{\gamma_m}, k_i > 1, k_p > \sqrt{-2k_i + 2\sqrt{k_i^2 + 2k_i + 2}} \tag{III.24}$$

It should be noted that the structure of Super-twisting algorithm could be considered as a nonlinear finite time version of the PI Controller[24].

III.8.1.B.Twisting Algorithm :

The Twisting algorithm is a discontinuous Second Order Sliding Mode (SOSM) controller commonly employed for systems with a relative degree of 2. Its amplitude switches between two values based on the quadrant in which the system state resides. Let's consider the following differential inclusion derived from the equation:

$$\begin{cases} \dot{z}_1 = z_2 \\ \dot{z}_2 \in [-\bar{\phi}, \bar{\phi}] + [\gamma_m, \gamma_M]u \end{cases} \tag{III.25}$$

The twisting controller is given as:

$$u = \begin{cases} -K_m sign(z_1) & if \ z_1 z_2 < 0, \\ -K_M sign(z_1) & if \ z_1 z_2 \geq 0, \end{cases} \tag{III.26}$$

Where K_m and K_M are some positive constants. Twisting algorithm can be written in another compact form:

$$u = -l_1 sign(z_1) - l_2 sign(z_2) \tag{III.27}$$

Where l_1 and l_2 satisfy:

$$\gamma_m(l_1 + l_2) - \bar{\varphi} > \gamma_M (l_1 - l_2) + \bar{\varphi},$$

$$\gamma_m(l_1 - l_2) > \bar{\varphi} \tag{III.28}$$

This algorithm can be considered as a nonlinear robust version of the classical PD controller[24].

III.8.1.C.Sub-optimal Algorithm:

The Sub-optimal algorithm is a discontinuous Second Order Sliding Mode (SOSM) controller typically employed for systems with a relative degree of 2. Consequently, its formulation is similar to that of the twisting algorithm. The sub-optimal controller is defined as:

$$u = \lambda(t) u_M sign\left(z_1 - \frac{z_1(t_M)}{2}\right)$$

$$\lambda(t) = \begin{cases} 1 & if\ z_1(t) \geq z_1(t_M), \\ \lambda^* & if\ z_1(t) \geq z_1(t_M), \end{cases} \quad \text{(III.29)}$$

Where t_M is the last moment at which $z_2 = 0$. In order to ensure finite time convergence, the gains λ^* and u_M should fulfill the following condition:

$$\lambda^* \in (0,1] \cap \left(0, \frac{3\gamma_m}{\gamma_M}\right)$$

$$u_m > max\left(\frac{\bar{\varphi}}{\lambda^* \gamma_m}, \frac{4\bar{\varphi}}{3\gamma_m \lambda^* \gamma_M}\right) \quad \text{(III.30)}$$

Like twisting, this algorithm can also be considered as a nonlinear robust version of the classical PD controller[24].

III.8.2.Advantages of Higher Order Sliding Mode:

The utilization of this control technique is motivated by its numerous advantages, which can be summarized as follows[25]:

- The control setting and the convergence time do not depend on each other, allowing for independent determination of these factors.

- The trajectory generation facilitates convergence in finite time from the initial moment, providing robust behavior of the control law throughout the system's response.

- Reduction or elimination of chattering phenomenon and asymptotic precision improvement.

- Applicability of the control in sliding modes of any order, higher or equal to the system's relative degree.

- Ease of parameter tuning, contributing to the simplicity of setting the control parameters.

III.9.conclusion:

In this chapter, our focus has been on nonlinear control approaches, structure variables systems theory, and sliding modes. The utilization of sliding mode control has been extensively studied in the operation of nonlinear systems, where the presence of uncertainties in parameters and variables does not compromise its robustness. One of the notable advantages of sliding mode control is its flexibility in choosing different shapes for the sliding surface, allowing for adaptable control strategies. Additionally, the use of multiple sliding surfaces concurrently opens up possibilities for advanced control schemes.

Moreover, we have delved into the realm of higher-order sliding mode control, particularly emphasizing the well-established second-order sliding mode. This approach ensures that the system's convergence to desired states occurs within a finite time frame, making it particularly suitable for systems with a relative degree higher than one. By incorporating higher-order sliding modes, we aim to enhance the accuracy of asymptotic behavior and mitigate the occurrence of chattering phenomena, which can adversely affect system performance.

In light of the advantages offered by sliding mode control, we have sought to apply this technique to our case study: the continuous stirred tank reactor (CSTR). The primary objective is to design a control law that ensures the reactor's robust operation in the face of parameter variations and external disturbances. This control law will be further developed and explored in the subsequent chapter, where we will delve into the implementation details and evaluate its effectiveness.

Overall, this chapter has laid the groundwork for understanding the principles and benefits of sliding mode control, particularly in the context of nonlinear systems. The exploration of higher-order sliding mode control and its potential advantages has provided insights into more advanced control strategies. These insights will guide us in the application of sliding mode control to the specific challenges posed by the continuous stirred tank reactor, as we strive to develop a robust and efficient control solution.

Chapter IV

Simulation and results

Chapter IV: Simulation and results

In this chapter we will be simulating and optimizing the production of the ethylene oxide in a Continuous Stirred Tank Reactor using a sliding mode controller in MATLAB Simulink to regulate the process. The primary objective of this chapter is to investigate the effectiveness of a sliding mode controller in maintaining the desired production rate and optimizing the robustness of the system and optimizing it to be more cost effective.

In our work we will be using the non-linear SMC to maximize the profit from the process by elevating the ethylene production rate by manipulating the feed rate and concentration of ethylene and the reactor cooling mantel temperature to obtain the optimal the best production rate with the lowest cost possible.

IV.1.Process description:

The process starts with the feed of ethylene (C_2H_4) and an oxygen-containing gas, such as air or pure oxygen, into the CSTR. These reactants are mixed and introduced into the reactor, which is a large vessel equipped with agitation mechanisms to ensure thorough mixing and uniform reaction. Inside the CSTR, the ethylene and oxygen undergo a controlled chemical reaction, facilitated by a catalyst, to produce ethylene oxide. The reaction is exothermic, meaning it releases heat energy during the process. To maintain a suitable reaction temperature cooling jacket is employed to remove excess heat generated.

The reaction kinetics play a crucial role in determining the production rate and product quality. The concentration of reactants, temperature, and pressure influence the reaction rate and selectivity. Therefore, we employ the SMC to ensure that the reactor is running in the most optimal state to drive the system states onto a sliding surface in a finite time and maintain them there. By continuously adjusting the control inputs based on the sliding surface and system dynamics, the sliding mode controller can effectively regulate the ethylene oxide production process. Through the simulation in MATLAB Simulink, the behavior of the CSTR system, including reactant concentrations, temperature profiles, and production rate, can be observed and analyzed under various operating conditions.

Chapter IV Simulation and results

Overall, the simulation of ethylene oxide production in a CSTR with a sliding mode controller provides valuable insights into the control and optimization of this chemical process. It allows for the exploration of control strategies to enhance production efficiency, product quality, and operational stability while considering the challenges associated with nonlinear dynamics, uncertain parameters, and disturbances.

IV.2.Reaction parameters:

In this specific process there are 3 reactions that occur simultaneously. These 3 reactions are:

C_2H_4 + 0.5*O2 -> C_2H_4O

C_2H_4 + 3*O2 -> 2*CO2 + 2*H2O

C_2H_4O + 2.5*O2 -> 2*CO2 + 2*H2O

The first one is the one we need while the other 2 are undesirable as they diminish the ethylene oxide production by turning it into other unwanted by-products.

In this module there are the following 3 inputs:

* C_2H_4 concentration in the feed

*Reactor cooling jacket temperature

* C_2H_4 feed rate

And these 4 states:

*Gas density in the reactor

* C_2H_4 concentration in the reactor

* C_2H_4O concentration in the reactor

*Temperature in the reactor

All these variables were taken from the book computers and chemical engineering Vol 92 and for the purpose of our study all the parameters are dimensionless and of the same order[26].

IV.3.Ojective of simulation:

The main objective of the control system is to optimize the production rate of ethylene oxide (C_2H_4O) and optimizing the consumption rate of the ethylene (C_2H_4), which directly affects the profitability of the process. This optimization is achieved by maximizing the C_2H_4O production rate at any steady-state operating point while considering the availability of C_2H_4 in the feed stream as it is the most expensive reactant in this project.

The C_2H_4O production rate is calculated as the product of the concentration of C_2H_4O in the reactor (represented by variable x3) and the total volumetric flow rate exiting the reactor (given by the ratio u3/u1 multiplied by x4).

The operating point of the system is determined by three inputs. The first input, u1, represents the C_2H_4 concentration in the feed, and it can be manipulated by the SMC controller. The second input, u2, corresponds to the cooling jacket temperature, which is maintained at a stable level. The third input, u3, represents the C_2H_4 feed rate and indicates the amount of ethylene available from an upstream process. Increasing the feed rate enhances the achievable C_2H_4O production rate. In this context, both u2 and u3 are considered as measured disturbances that affect the system.

Overall, the control system aims to maximize the production rate of ethylene oxide by adjusting the C_2H_4 concentration in the feed (u1) while considering the stability of the cooling jacket temperature (u2) and the available ethylene feed rate (u3). The optimization of these parameters ensures efficient and profitable operation of the ethylene oxide production process.

IV.4.Sliding mode controller design:

IV.4.1.Sliding surface:

The sliding surface equation in sliding mode control is a mathematical expression that defines the desired state trajectory for the system. It represents the condition that the system states should satisfy in order to achieve sliding mode behavior. The specific form of the sliding surface equation can vary depending on the system dynamics and the control objectives.

In the context of the ethylene oxide production process, the sliding surface equation can be formulated based on the desired control objective. Since the primary goal is to maximize the C_2H_4O production rate, the sliding surface equation could be designed to ensure that the concentration of C_2H_4O in the reactor (x3) and the total volumetric flow rate exiting the reactor (u3/u1 * x4) are appropriately balanced.

A possible sliding surface equation for this scenario could be:

$$s = x3 - (\frac{u3}{u1}) \times x4$$

Here, s represents the sliding surface, x3 is the concentration of C_2H_4O in the reactor, u3/u1 is the ratio of the C_2H_4 feed rate to the C_2H_4 concentration in the feed, and x4 is the total volumetric flow rate exiting the reactor. The sliding mode controller aims to drive the system states onto this sliding surface and maintain them there to achieve the desired control objective of maximizing the C_2H_4O production rate.

IV.4.2.The reactor:

We describe the reactor with the following script:

```
function dxdt = reactor(x,u)
%% Parameters
gam1 = -8.13;
gam2 = -7.12;
gam3 = -11.07;
A1 = 92.80;
A2 = 12.66;
A3 = 2412.71;
B1 = 7.32;
B2 = 10.39;
B3 = 2170.57;
B4 = 7.02;
%% Kinetic rate expressions
r1 = exp(gam1/x(4))*(x(2)*x(4))^0.5;
r2 = exp(gam2/x(4))*(x(2)*x(4))^0.25;
r3 = exp(gam3/x(4))*(x(3)*x(4))^0.5;
%% ODEs from mass and energy balances
V = u(3)/u(1);
dxdt = zeros(4,1);
dxdt(1) = V*(1 - x(1)*x(4));
dxdt(2) = V*(u(1) - x(2)*x(4)) - A1*r1 - A2*r2;
dxdt(3) = -V*x(3)*x(4) + A1*r1 - A3*r3;
```

```
dxdt(4) = (V*(1 - x(4)) + B1*r1 + B2*r2 + B3*r3 - B4*(x(4) -
u(2)))/x(1);
```

IV.4.3.Controller:

To design the SMC controller we use the following script:

```
function [u1, err] = fcn(x,dx,u2, u3,errp,ref)
%% Parameters
gam1 = -8.13;
gam2 = -7.12;
gam3 = -11.07;
A1 = 92.80;
A2 = 12.66;
A3 = 2412.71;
B1 = 7.32;
B2 = 10.39;
B3 = 2170.57;
B4 = 7.02;
coef1=0.1;
coef2=1.6;
err=x(2)-ref;
s=(coef1*err)+errp;
%% Kinetic rate expressions
r1 = exp(gam1/x(4))*(x(2)*x(4))^0.5;
r2 = exp(gam2/x(4))*(x(2)*x(4))^0.25;
r3 = exp(gam3/x(4))*(x(3)*x(4))^0.5;
%% ODEs from mass and energy balances
u1=   (u3/(x(4)*(-(A1*r1)-(A2*r2)+u3)))*(-x(2)+(-coef2*sign(s)-
coef1*errp));
V = u3/u1;
dxdt = zeros(4,1);
dxdt(1) = V*(1 - x(1)*x(4));
dxdt(2) = V*(u1 - x(2)*x(4)) - A1*r1 - A2*r2;
dxdt(3) = -V*x(3)*x(4) + A1*r1 - A3*r3;
```

```
dxdt(4) = (V*(1 - x(4)) + B1*r1 + B2*r2 + B3*r3 - B4*(x(4) -
u2))/x(1);
y = u3/u1*x(3*x(4);
```

IV.4.4.Initial parameters:

The cooling jacket temperature: Tc = 1.1

C2H4 availability: C2H4A = 0.175

The plant initially operates at u0 = 0.5

To find the states at the steady state we use (fsolve):

x0=real(fsolve (@(x) reactor(x,[u0;Tc;C2H4A]),rand(1,4),optimopt))

for the optimal the ethylene oxide production rate we sweep through the range of the ethylene concentration in the feed using (fsolve) as follows:

```
uRange = 0.1:0.1:3;
EORate = zeros(length(uRange),1);
optimopt = optimoptions('fsolve','Display','none');
for ct = 1:length(uRange)
   xRange = real(fsolve(@(x) reactor(x,[uRange(ct);Tc;C2H4A]),rand(1,4),optimopt));
   EORate(ct) = C2H4A/uRange(ct)*xRange(3)*xRange(4);
end
```

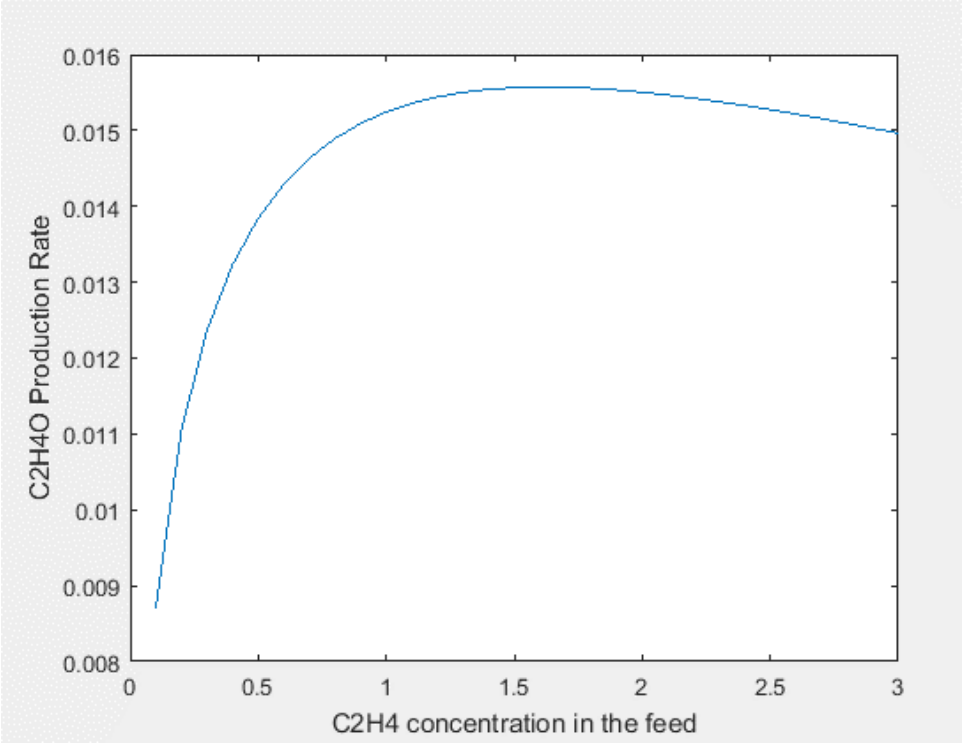


Figure 15. The relation between the ethylene concentration and the production rate of EO

IV.5.Simulink design:

Using the models from the previous chapter we get the following Simulink design :

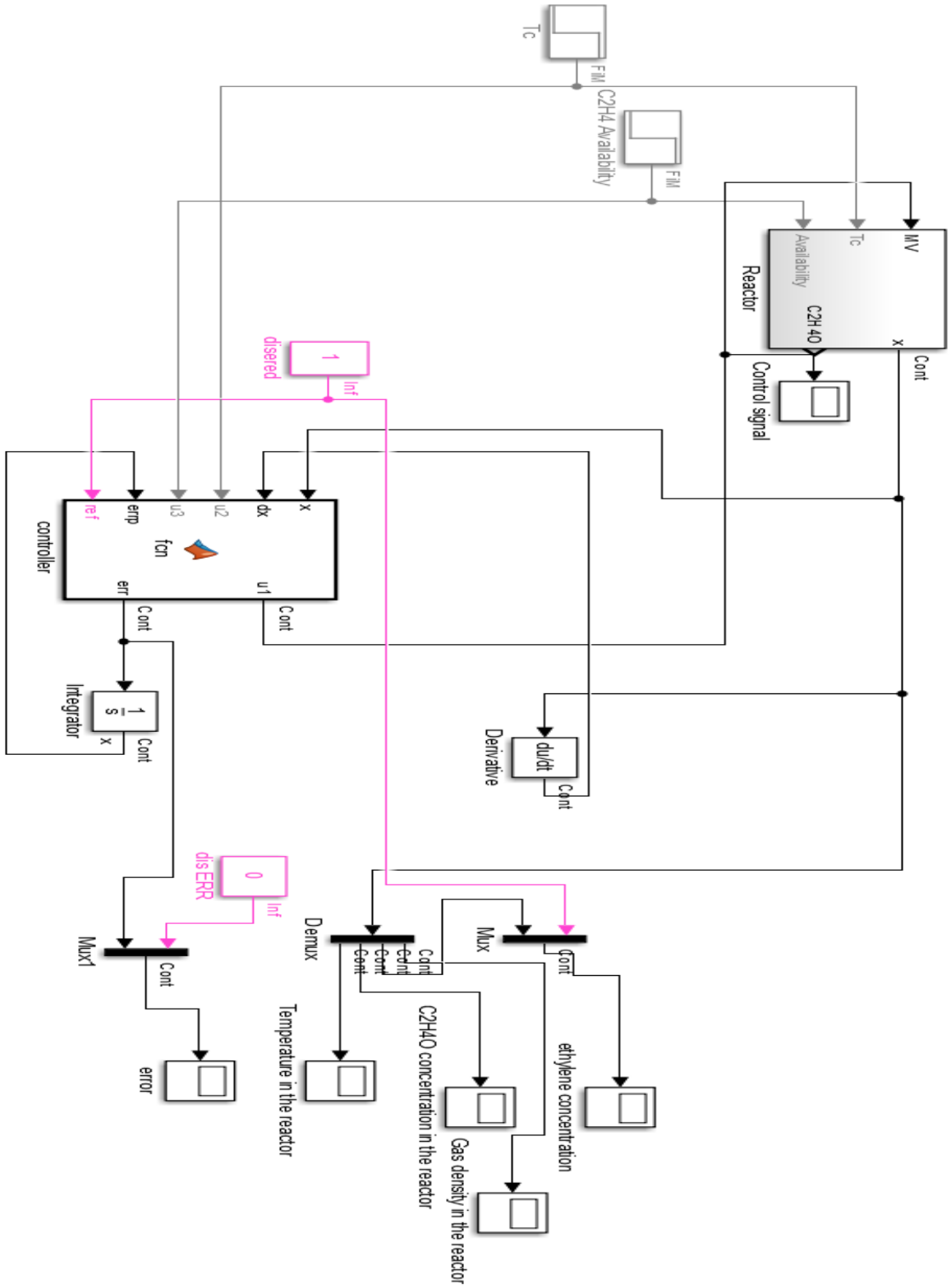


Figure 16. Process simulink

The 2 inputs in this simulation are the ethylene availability and the cooling mantel temperature, where at the start the C_2H_4 availability is 1.5 then is increased to 2.5 at 200s , the temperature starts at 1.1 then it is increased to 1.15 at 100s . These parameters are fed into both the reactor and the SMC controller after setting the simulation time to 300 we get the following results.

IV.6.Simulation results and analysis;

IV.6.1.The Ethylene oxide produced;

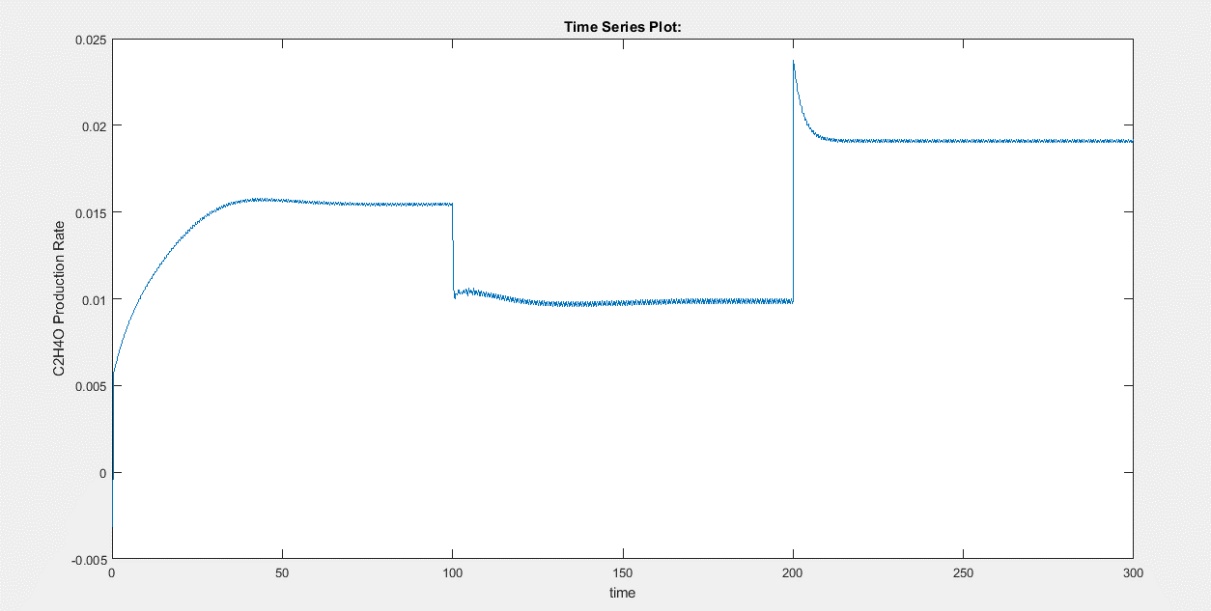


Figure 17. EO production rate evolution

Figure 16 illustrates the evolution of Ethylene oxide production throughout the simulation. Initially, the temperature of the cooling jacket is set to 1.1 and is maintained at this value for the first 100 seconds. At the 100-second mark, the temperature is increased to 1.15 due to the exothermic nature of the reaction. This change in temperature leads to a decrease in the optimal C_2H_4O production rate from 0.0156 to 0.0135.

Simultaneously, the availability of C_2H_4 is set to 0.175 and remains constant for the first 200 seconds. At the 200-second mark, the availability of C_2H_4 is increased to 0.25. This increase in C_2H_4 availability results in an increase in the optimal C_2H_4 O production rate from 0.0135 to 0.0195.

During the initial 100 seconds, the Sliding Mode Controller (SMC) gradually adjusts the C_2H_4 O plant to the true optimal condition while adhering to the constraints of the cooling jacket temperature and C_2H_4 availability.

In the subsequent 100 seconds, the cooling jacket temperature increases from 1.1 to 1.15. SMC controller smoothly adjusts the plant to the new optimal condition of 0.0135, as expected.

Moving forward, in the next 100 seconds, the availability of C_2H_4 increases from 0.175 to 0.25. Once again, the SMC controller efficiently guides the plant to the new optimal steady state of 0.0195.

Overall, Figure 16 provides insights into how the control algorithms respond to changes in the cooling jacket temperature and **C_2H_4** availability. The SMC controller demonstrate their ability to optimize the C_2H_4O production process, achieving the desired production rates while maintaining stability and adhering to the specified constraints. The simulation results validate the effectiveness of these control strategies in ensuring optimal operation of the continuous stirred tank reactor for ethylene oxide production.

IV.6.2.The gas density in the reactor:

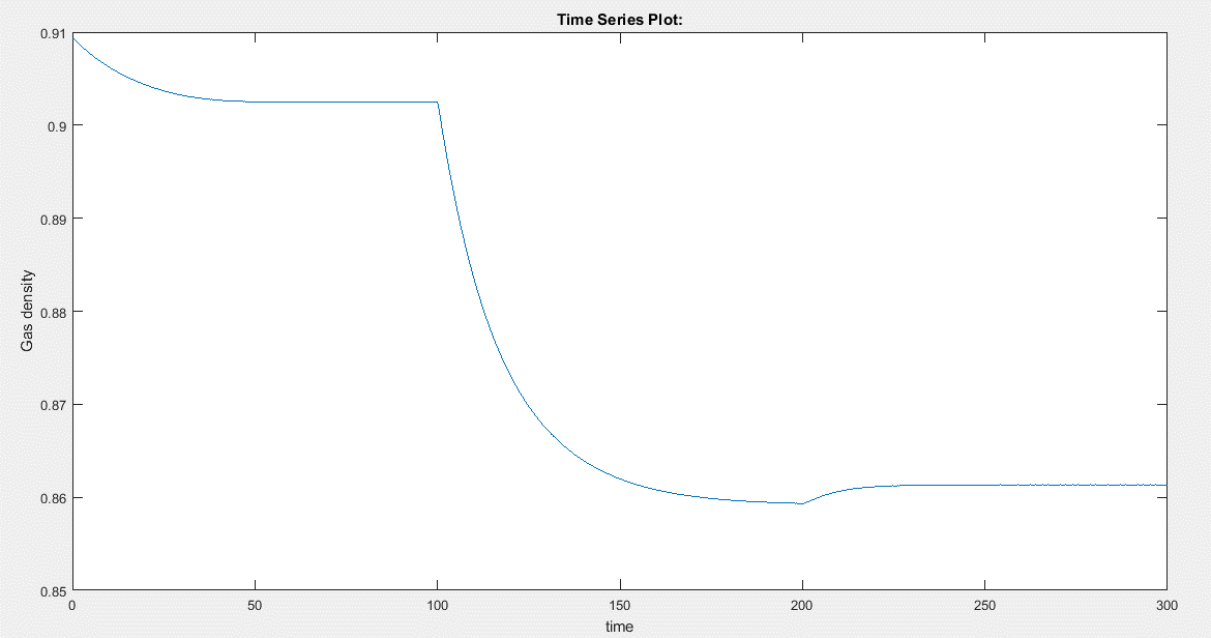


Figure 18 .The gas density in the reactor

In Figure 17, the gas density in the reactor is depicted throughout the simulation. Initially, the gas density is at its highest value, around 0.9. However, at around 100 seconds, as the temperature increases, the gas density decreases to approximately 0.88.

This observation can be attributed to the relationship between gas density and temperature. As the temperature rises, the gas molecules become more energetic and spread out, resulting in a decrease in gas density. The increase in temperature in the cooling jacket causes the gas molecules in the reactor to expand and occupy a larger volume, leading to a decrease in gas density.

At 200 seconds, even with the increase in ethylene availability, the gas density does not improve significantly. This behavior is primarily influenced by the temperature of the cooling jacket.

The cooling jacket temperature plays a crucial role in regulating the overall temperature of the reactor and affects the gas density.

It is important to note that gas density is a crucial parameter to monitor and control in the production of ethylene oxide. Optimal gas density ensures efficient reaction rates and product formation. The fluctuations in gas density observed in Figure 17 highlight the impact of temperature on the system and the need for careful temperature control to maintain the desired gas density.

To optimize the gas density, it is essential to carefully manage the cooling jacket temperature and ensure it remains within the desired range. By controlling the cooling jacket temperature effectively, it is possible to stabilize the gas density and improve the overall efficiency of the ethylene oxide production process.

IV.6.3.The EO concentration in the reactor:

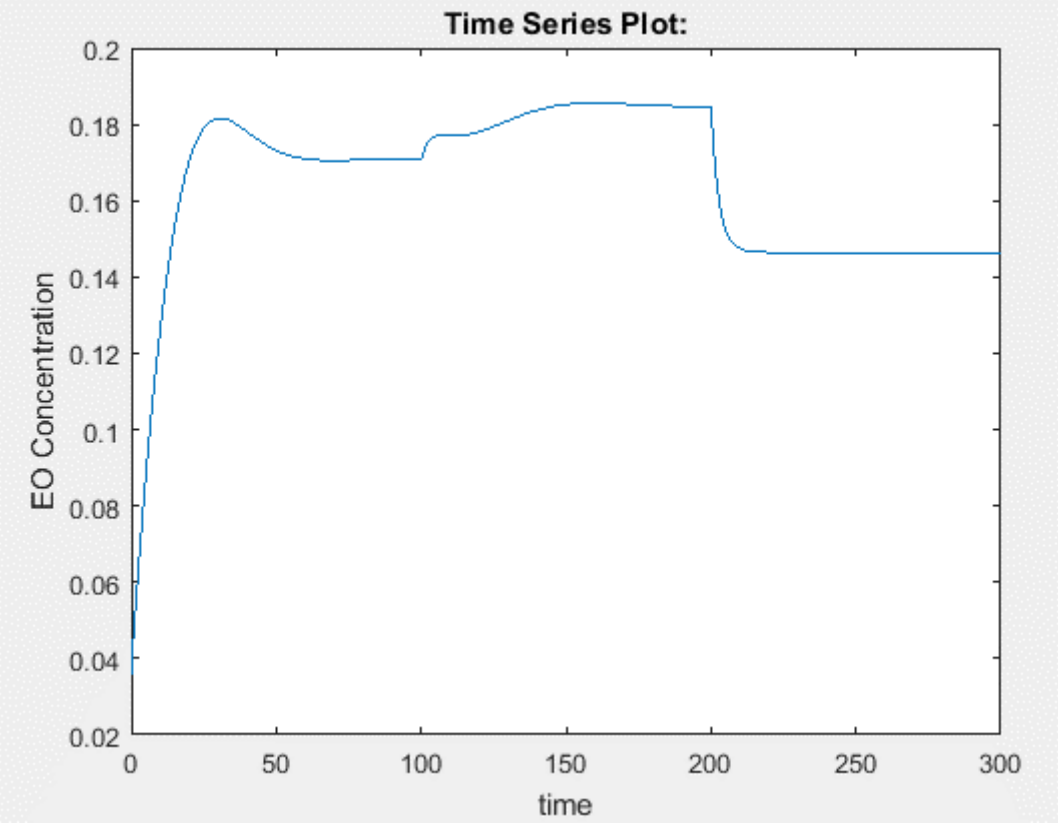


Figure 19.The evolution of the EO concentration in the reactor over the simulation time

Figure 18 provides insights into the evolution of the ethylene oxide (EO) concentration in the reactor throughout the simulation. At the start of the simulation, the EO concentration quickly reaches 0.17 within approximately 20 seconds and stabilizes at this value for the first 100

seconds. This initial stability indicates that the controller is able to maintain the desired EO concentration in the presence of the given initial conditions.

After the 100-second mark, there is a noticeable change in the cooling mantle temperature, which results in an increase in the EO concentration to 0.18. This change in temperature has an impact on the reaction kinetics and leads to a higher EO concentration. However, at the 200-second mark, as the availability of ethylene (C_2H_4) increases, the EO concentration decreases to 0.15. This change in availability affects the reaction rate and subsequently influences the EO concentration.

Throughout these variations in the cooling mantle temperature and ethylene availability, the controller demonstrates its ability to effectively regulate the EO concentration. It responds to the changing conditions by adjusting the control inputs to maintain the desired concentration levels. The successful control of the EO concentration is crucial for ensuring the desired product quality and meeting the production requirements.

Figure 18 provides a visual representation of the controller's performance in maintaining the EO concentration within the desired range despite changes in the process conditions. This control capability ensures the stability and reliability of the ethylene oxide production process in the continuous stirred tank reactor.

IV.6.4.The reactor temperature;

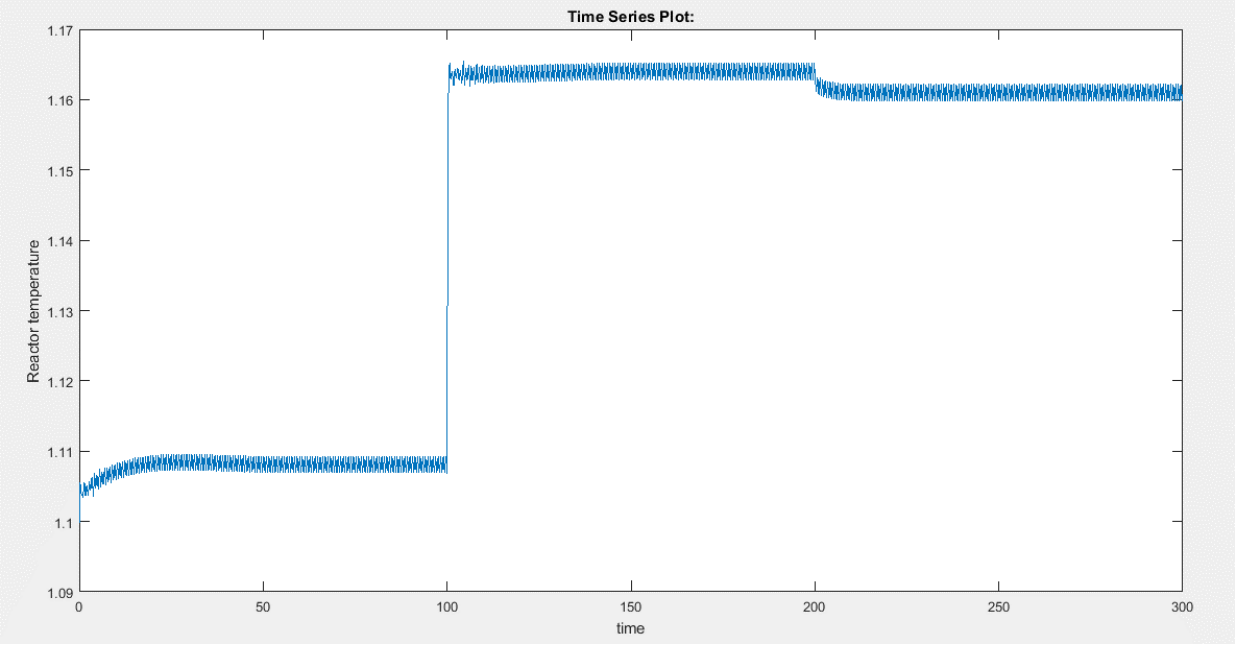


Figure 20.The temperature of the reactor

Initially set at 1.1, the temperature gradually increased to 1.16 at t=100s. This rise in temperature was attributed to the exothermic nature of the reaction occurring inside the reactor.

The exothermic reaction released heat energy, which resulted in an increase in the overall temperature of the system. As the reaction progressed, the heat generated accumulated, causing the temperature to rise steadily. This phenomenon is commonly observed in exothermic reactions, where the heat produced exceeds the heat dissipated or removed from the system.

As the reaction progressed, the heat generated accumulated, causing the temperature to rise steadily. This phenomenon is commonly observed in exothermic reactions, where the heat produced exceeds the heat dissipated or removed from the system.

The increase in the cooling mantle temperature played a significant role in regulating the reactor temperature. By adjusting the cooling jacket temperature, the excess heat generated by the reaction could be effectively managed and removed from the system. The cooling jacket acted as a heat sink, absorbing the excess heat and maintaining the desired temperature range.

The control of the cooling mantle temperature is crucial for maintaining the stability and efficiency of the reactor. Proper temperature regulation ensures that the reaction proceeds optimally, preventing any undesirable side reactions or deviations from the desired product specifications.

The observed temperature increase at t=100s highlights the dynamic nature of the reactor system and the importance of proactive temperature control strategies. By continuously monitoring and adjusting the cooling mantle temperature, the system can maintain optimal operating conditions and enhance the production of ethylene oxide.

IV.6.4.The ethylene concentration and the error:

As both the ethylene concentration in the feed and error are tied with the controller parameters they require fine tuning of different of the controller mostly the coefficients of the u1 equation

$$u1 = u3/(x(4) \times (-(A1 \times r1) - (A2 \times r2) + u3)) \times (-x(2) + (-coef2 \times sign(s) - coef1 \times errp))$$

As the production of the EO is already optimized we now focus on optimizing the consumption the ethylene as it is the most expensive reactant it needs to be optimized, the optimization of the ethylene and the elimination of the error is done by manipulating the coefficients 1 and 2, we used the trial and error method to pin point the most optimal values for these parameters

Case 1:

Coef1 > 2 while Coef2 > 2 or Coef2 < 0.5

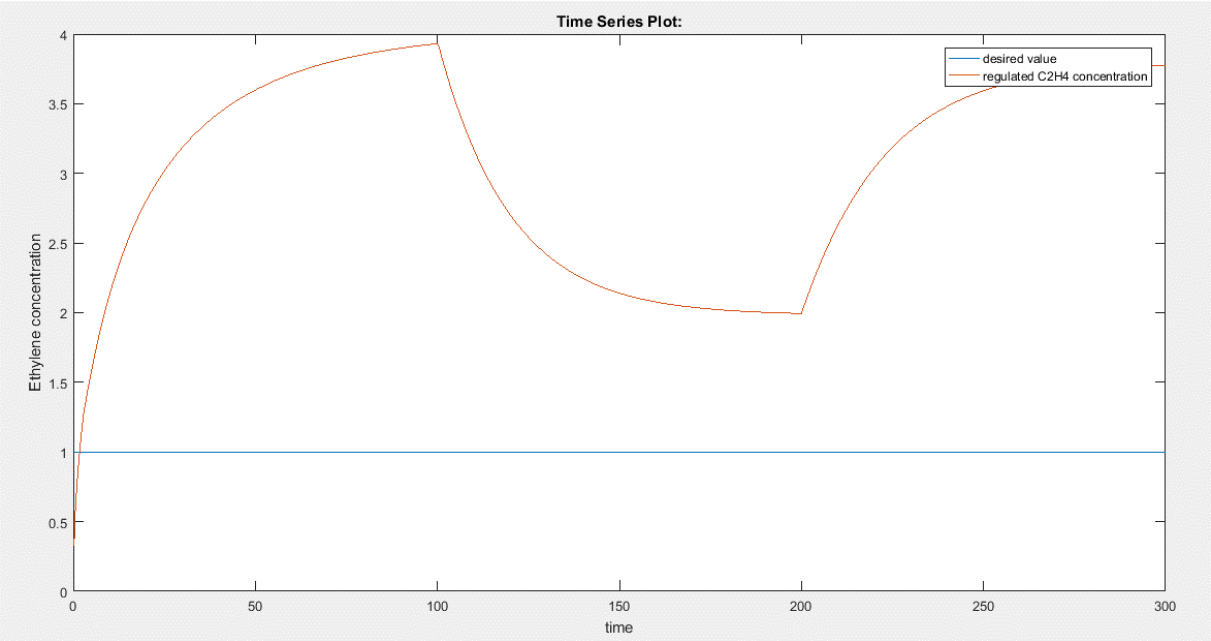


Figure 21.The evolution of the ethylene concentration in case 1

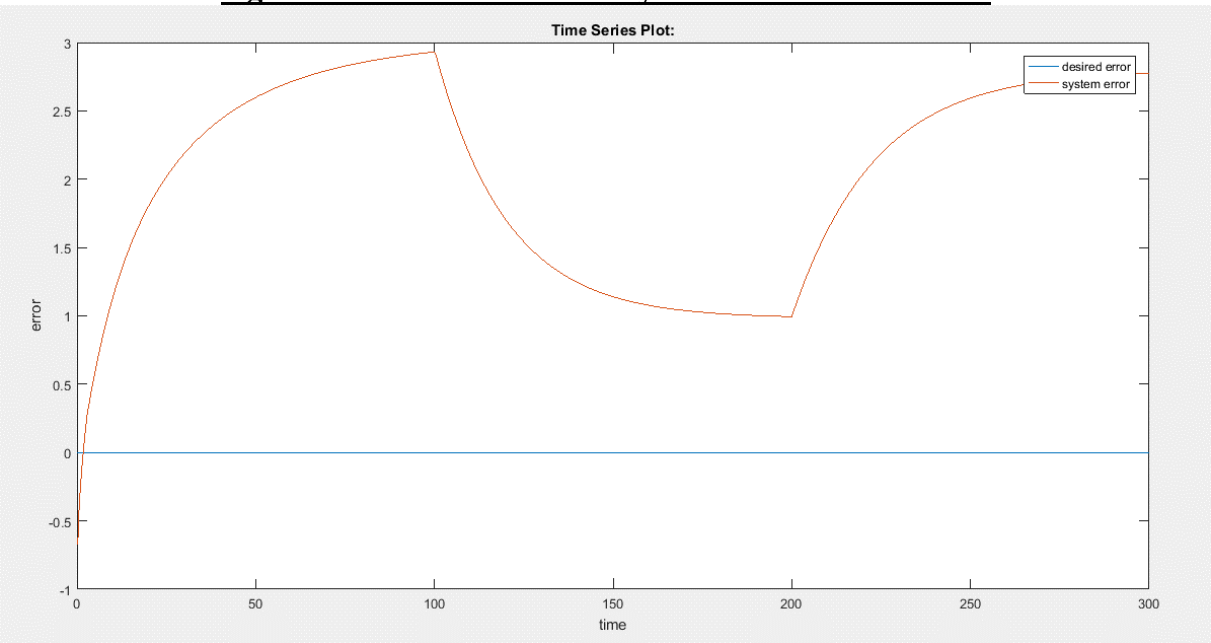


Figure 22.The system error in case 1

In case one, it is observed that the ethylene concentration, and the error jump abruptly above their respective desired values of Ce=1 and ERR_des=0. This behavior indicates that the controller coefficients used in this scenario lead the system to an unstable state.

The sudden jump in the ethylene concentration and error beyond the desired values suggests that the controller's response is excessively aggressive or sensitive. It fails to maintain the system within the desired operating range and instead pushes it towards instability.

To rectify this issue, it is necessary to reevaluate and adjust the controller coefficients to ensure stability. By carefully tuning the controller parameters, it becomes possible to achieve a more robust and stable control of the ethylene concentration, preventing such sudden jumps and maintaining the system within the desired operating conditions.

Therefore, it is crucial to carefully analyze the controller design and fine-tune the coefficients to strike a balance between performance and stability, ensuring that the system operates within safe and desired boundaries.

Case 2:

Coef1<1.4 and 0.5<Coef2<1.2

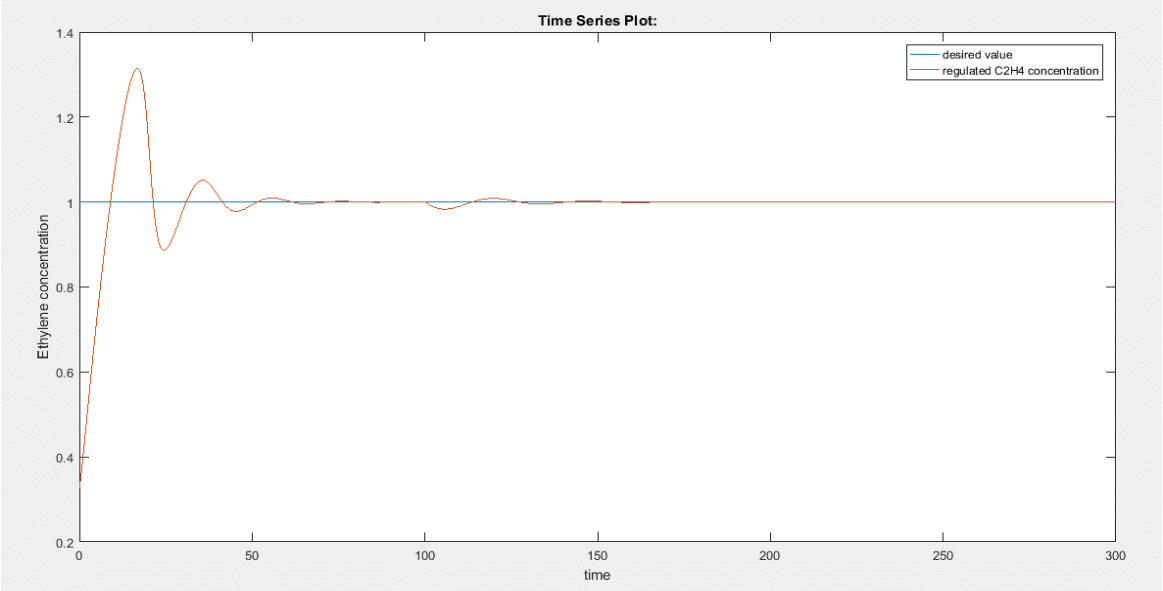


Figure 23.The evolution of the ethylene concentration in case 2

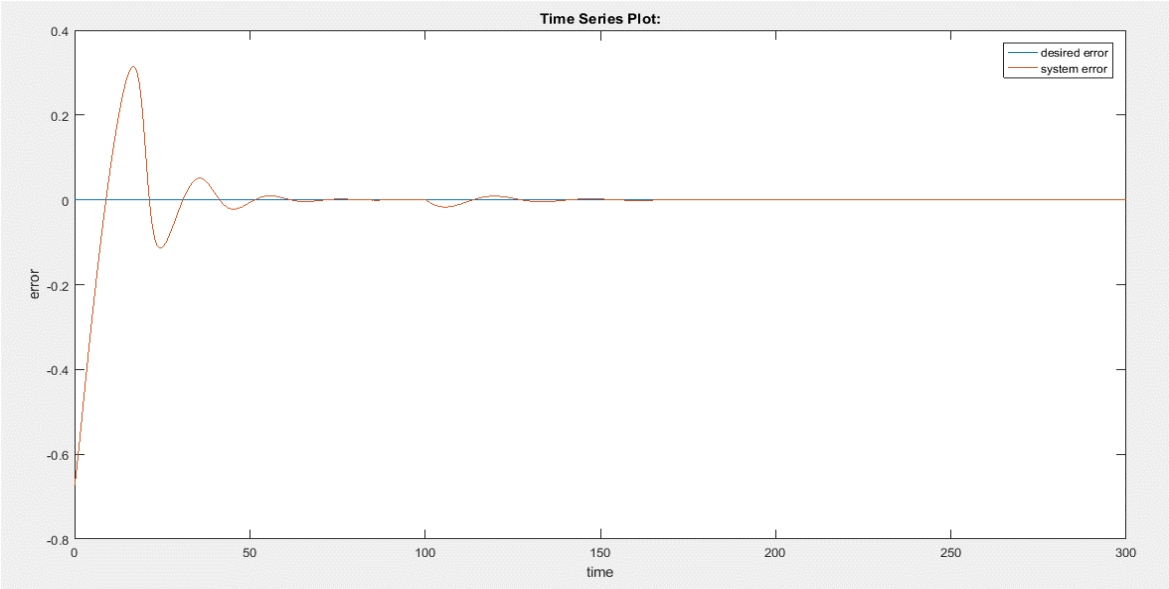


Figure 24.The system error in case 2

In case 2, the controller demonstrates improved performance compared to case 1. The controller successfully guides both the Ethylene concentration and the error towards the desired optimal points of 100% for the ethylene concentration and 0% for the error. However, during the process, slight oscillations are observed before the system stabilizes at the optimal values.

These oscillations indicate that the controller is initially working at values slightly above 100% for the ethylene concentration and below 0% for the error. While these values are not physically possible, they are a result of the controller's adjustment process as it strives to reach the optimal setpoints. The oscillations occur due to the controller's attempt to fine-tune the system and eliminate any deviations from the desired values

To further improve the controller's performance and eliminate the oscillations, fine-tuning of the controller's coefficients may be necessary. By adjusting the controller's parameters, it is possible to strike a balance between stability and response speed, ensuring smooth and precise control without overshooting the optimal values.

Overall, case 2 demonstrates the capability of the sliding mode controller to guide the system towards the optimal operating point, albeit with slight oscillations. The controller's effectiveness in bringing the system back to the desired range highlights its robustness and ability to regulate the process variables effectively.

Case 3:

Coef1>0.1 and Coef2>1.6

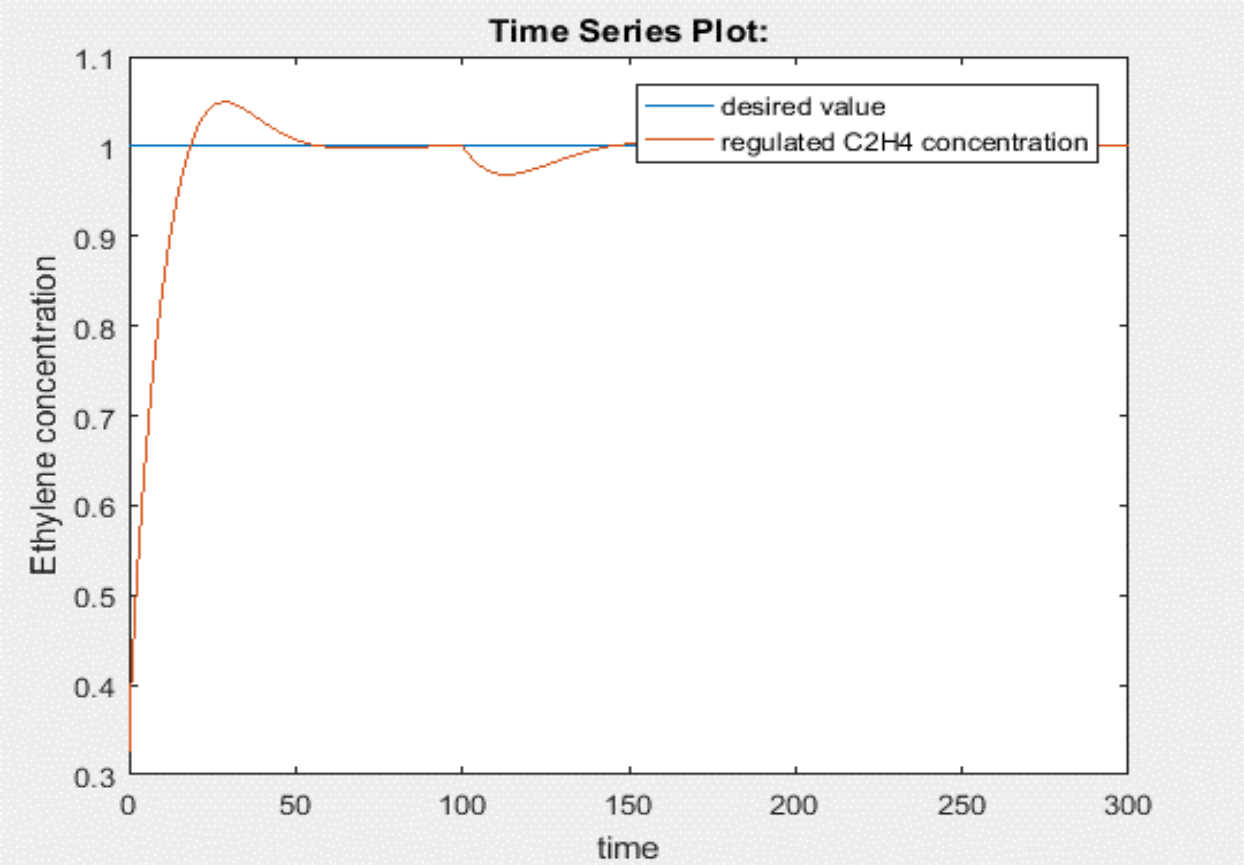


Figure 25.The evolution of the ethylene concentration in case 3

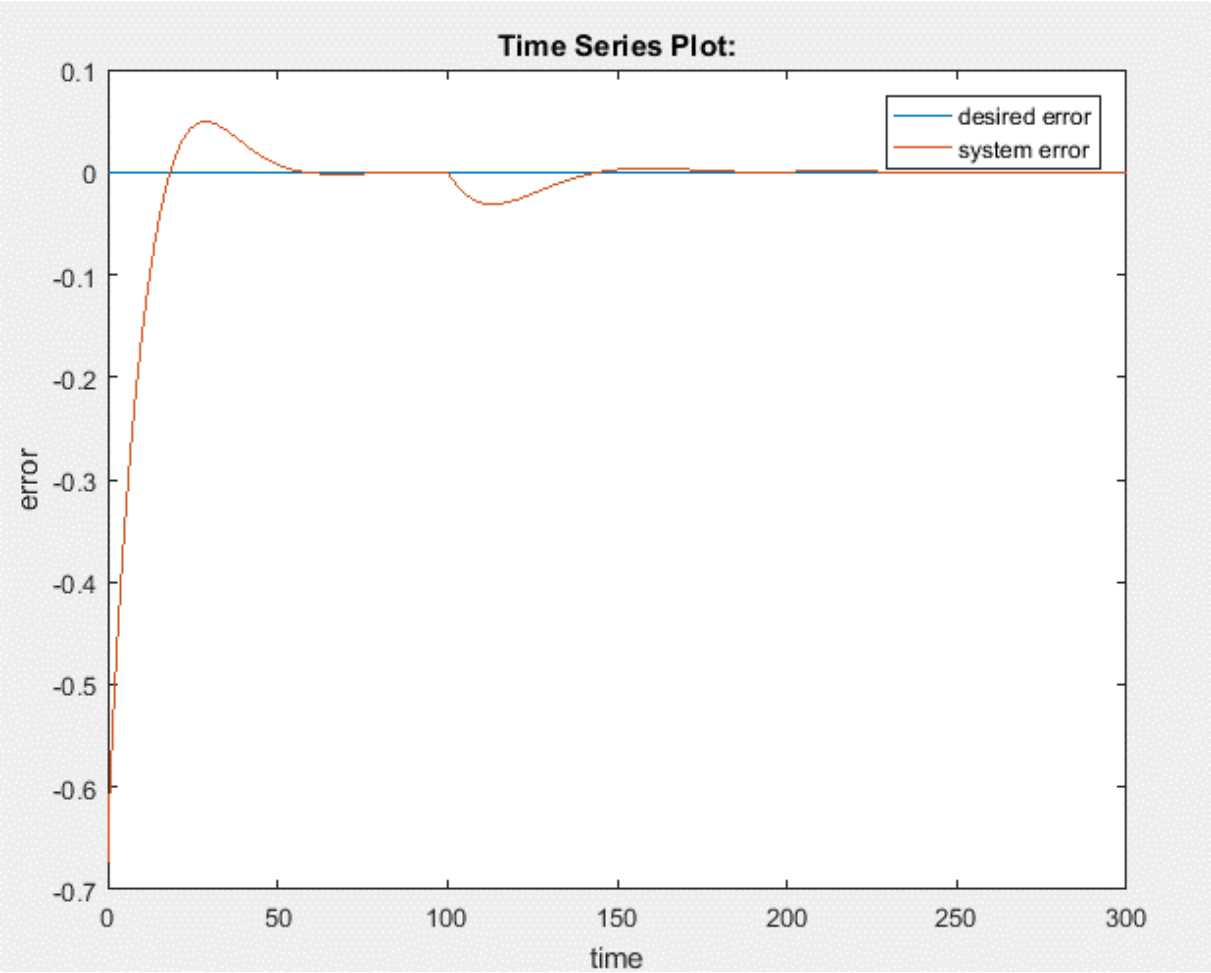


Figure 26.The system error in case 3

In case 3, significant improvements are observed compared to the previous cases. The controller successfully reduces the oscillations, and both the Ethylene concentration and the error reach the desired values in a relatively shorter time. However, it is worth noting that the ethylene concentration still exceeds the 100% mark, which is not acceptable as it exceeds the physical limits of the system.

Despite the faster convergence and reduced oscillations, the controller coefficients still require further optimization to ensure that the system operates within the allowable range. The current settings may result in an overshoot, causing the ethylene concentration to temporarily exceed the desired maximum value. Fine-tuning the coefficients can help strike a balance between stability and response speed, ensuring that the system remains within the acceptable operating limits.

By refining the controller's parameters, it is possible to achieve a more precise and controlled response, eliminating any deviations beyond the acceptable limits. The optimization process

aims to find the optimal combination of coefficients that guarantees stable and accurate control without exceeding the predefined constraints.

The case 3 results indicate that although the controller has made significant improvements in terms of convergence and oscillation reduction, further adjustments are needed to fine-tune the system's response. By optimizing the coefficients, the controller can achieve the desired performance, maintaining stability while operating within the defined bounds.

In summary, case 3 demonstrates the effectiveness of the sliding mode controller in reducing oscillations and improving convergence speed. However, the ethylene concentration briefly exceeding the acceptable limit highlights the need for continued optimization of the controller's coefficients to ensure precise control and adherence to the system's operational constraints.

Case 4:

Coef1=0.1 and Coef2=1.6

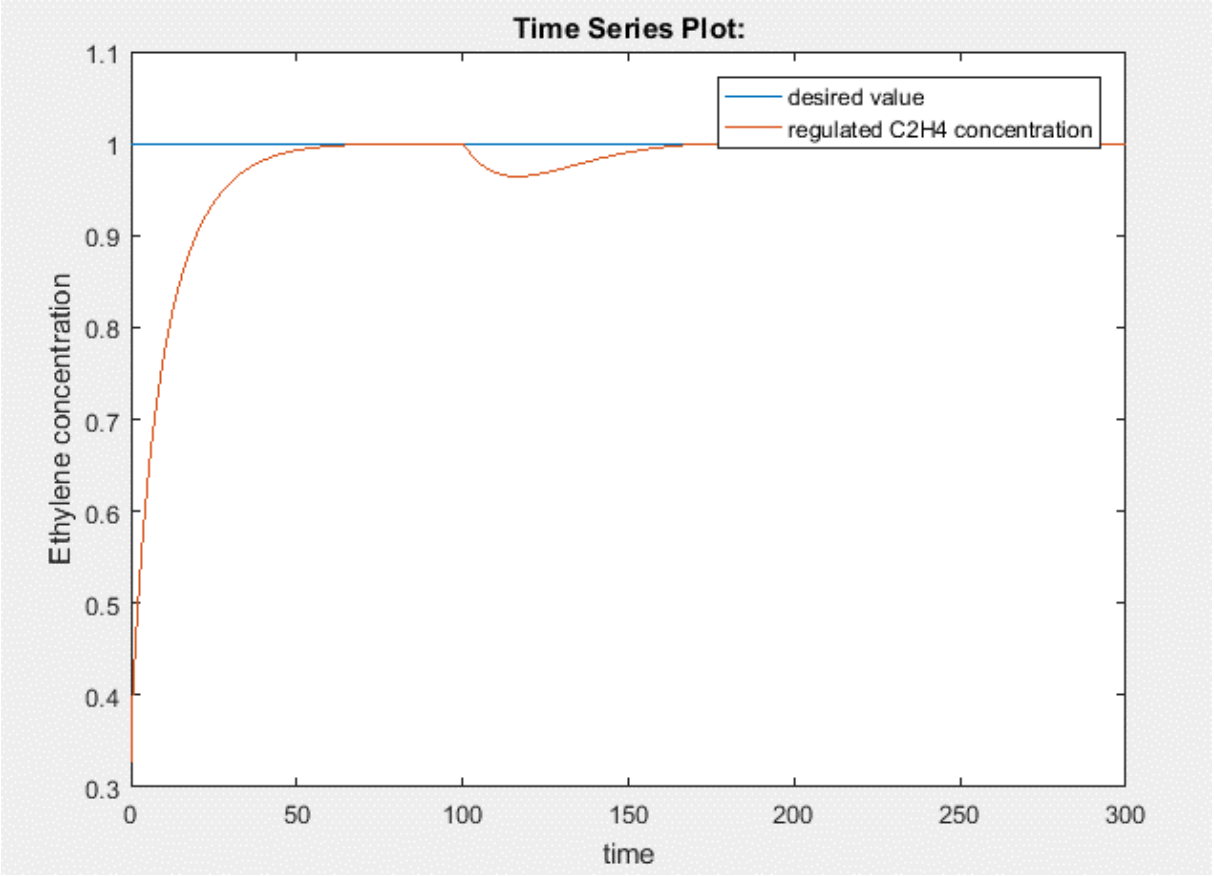


Figure 27.The evolution of the ethylene concentration in case 4

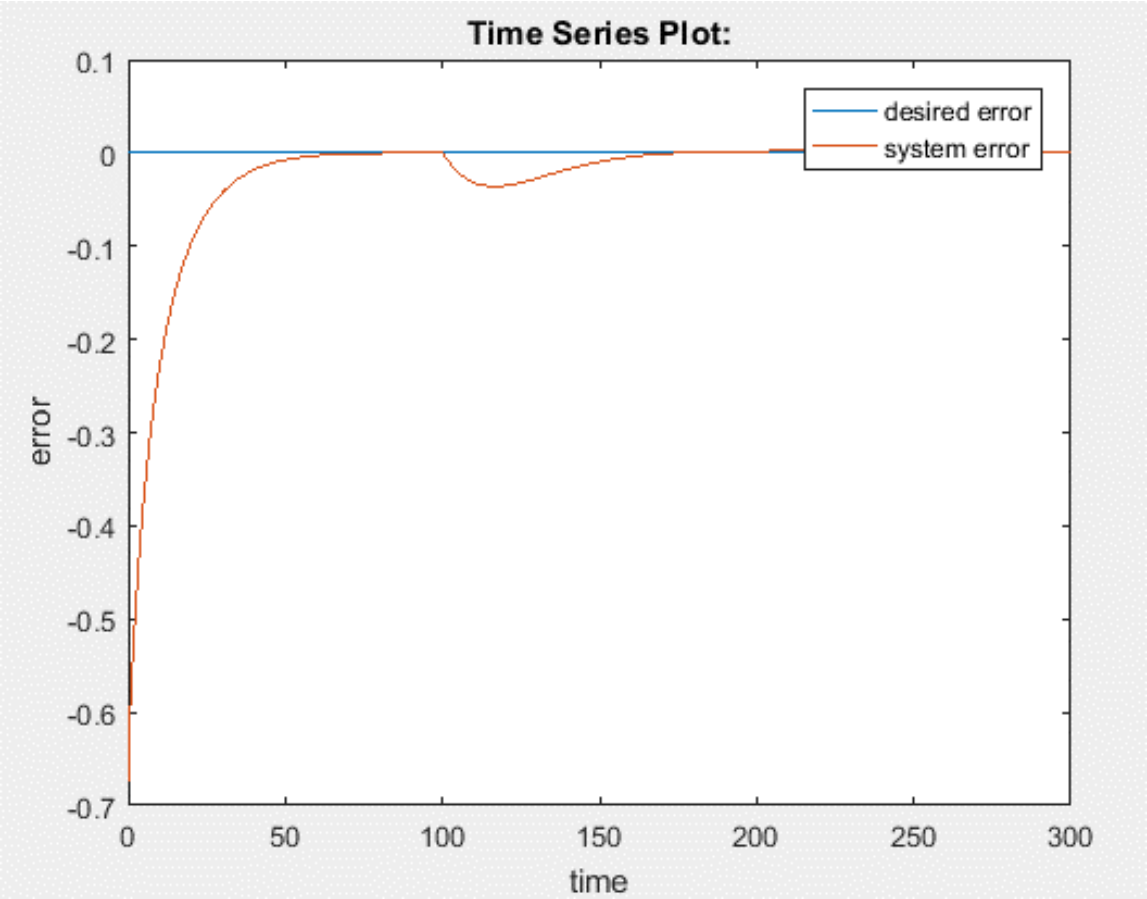


Figure 28.The system error in case 4

In case 4, significant improvements are observed in the controller's performance compared to the previous cases. The controller successfully guides both the ethylene concentration and the error to their optimal values without any oscillations. However, achieving this precise control comes at the expense of response speed.

The slower response speed in case 4 indicates that the controller prioritizes stability and accuracy over rapid adjustments. It ensures that the ethylene concentration remains within the acceptable limit of 100% without exceeding it. This trade-off between response speed and stability is acceptable in this context, as the primary objective is to reach the most optimal point while adhering to the system's limitations.

By sacrificing some speed in the control action, the controller eliminates any overshoot or oscillations that might occur, providing a smooth and stable operation. This not only ensures the system's safety but also allows for more precise control of the ethylene concentration.

The results in case 4 demonstrate the effectiveness of the sliding mode controller in achieving the desired target without surpassing the system limit. While the response speed may be slower

compared to other cases, the trade-off is justifiable in the context of maintaining the system's integrity and operating within the defined constraints.

Overall, the controller's ability to reach the optimal values without exceeding the system limit is a significant achievement. It showcases the controller's capability to provide robust and stable control while ensuring the ethylene concentration remains within the permissible range. The trade-off between response speed and stability in case 4 demonstrates the controller's ability to prioritize system safety and precision, making it a suitable choice for controlling the production of ethylene oxide in a CSTR.

The result:

After analyzing the results of the four cases, it is evident that the choice of coefficients plays a crucial role in the performance of the sliding mode controller for optimizing the production of ethylene oxide in the CSTR. Based on the observed behavior and system response, it can be concluded that the most optimal coefficients for this particular system are 0.1 for coefficient 1 and 1.6 for coefficient 2.

The selection of these coefficients allows the controller to effectively regulate the ethylene concentration and minimize the error, while maintaining stability and adhering to the system constraints. The optimized coefficients strike a balance between fast response and stability, leading to accurate control without compromising the system's integrity.

By setting coefficient 1 to 0.1, the controller exhibits a moderate control action, allowing for a controlled and gradual adjustment of the system variables. This helps in preventing overshoots and reducing oscillations, leading to smoother and more stable operation.

On the other hand, coefficient 2 is set to 1.6, which introduces a higher control gain to ensure a more robust response. This value allows the controller to swiftly correct any deviations from the desired setpoint, facilitating faster convergence towards the optimal values.

The choice of these coefficients reflects a compromise between response speed and stability. The optimized coefficients enable the controller to effectively handle disturbances, maintain precise control, and ensure the ethylene concentration remains within the acceptable range.

However, it is important to note that the selection of optimal coefficients may vary depending on the specific characteristics of the system, including the dynamics and desired performance

criteria. Further experimentation and tuning may be required to fine-tune the controller's parameters for different operating conditions and system requirements.

In conclusion, the selection of coefficients 0.1 for coefficient 1 and 1.6 for coefficient 2 yields a well-balanced sliding mode controller for optimizing the production of ethylene oxide in the CSTR. These coefficients enable the controller to achieve stable and accurate control while minimizing oscillations and ensuring the system operates within the desired range.

IV.7.Conclusion:

In conclusion, this chapter focused on the simulation of ethylene oxide (EO) production in a continuous stirred tank reactor (CSTR) using a sliding mode controller in MATLAB Simulink. The controller was designed to regulate optimize the production of

Through the simulation, we observed the dynamic behavior of the system under different conditions. We examined the effects of changing the cooling jacket temperature and the C_2H_4 availability on the optimal EO production rate. The sliding mode controller demonstrated its ability to adapt to these changes and maintain the EO production at the desired levels.

The results showed that the controller effectively regulated the process variables and ensured the stability and optimal performance of the system. It successfully adjusted the process conditions to reach the desired EO concentration and minimize oscillations. However, there were trade-offs to consider, such as the response speed and stability, which required further tuning of the controller coefficients.

Overall, the simulation provided valuable insights into the control of EO production in a CSTR using sliding mode control. It highlighted the importance of accurate control of process variables to achieve optimal production rates and maintain product quality.

Conclusion

Conclusion:

In conclusion, the study focused on optimizing the production of ethylene oxide in a Continuous Stirred Tank Reactor (CSTR) using a sliding mode controller simulated in MATLAB Simulink. The following key conclusions can be drawn from the study:

* Sliding mode control (SMC) is an effective control strategy for optimizing the production of ethylene oxide in a CSTR. It provides robustness against uncertainties and disturbances, ensuring stability and improved performance of the system.

* The sliding mode controller successfully regulated key process variables such as cooling jacket temperature and C_2H_4 availability, allowing the system to reach and maintain optimal conditions for ethylene oxide production.

* The simulation results demonstrated the ability of the sliding mode controller to smoothly adjust the plant to new optimal conditions when there were changes in cooling jacket temperature and C_2H_4 availability. This ensured consistent and efficient production of ethylene oxide.

* The optimization of ethylene oxide production in the CSTR resulted in improved selectivity and minimized consumption of ethylene, leading to cost savings and increased process efficiency.

* The study highlighted the importance of parameter tuning in the sliding mode controller to strike a balance between stability and system response speed. Further refinement of controller coefficients can enhance performance and optimize the trade-off between stability and response time.

* The simulation provided valuable insights into the behavior of the system and demonstrated the effectiveness of the sliding mode control approach in optimizing ethylene oxide production. This knowledge can be utilized for real-world implementation and process optimization in industrial settings.

Overall, the study demonstrated the potential of in implementing sliding mode control in the chemical production field. The findings contribute to the existing body of knowledge in the field of process optimization and control, offering valuable insights for researchers, engineers, and practitioners in the chemical industry.

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