

MINISTRY OF HEALTH OF UKRAINE

**I. HORBACHEVSKY TERNOPIL NATIONAL MEDICAL UNIVERSITY OF
THE MINISTRY OF HEALTH OF UKRAINE**

APPROVE

Head of Department

Prof. Dmytro Vakulenko

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**STUDYING OF THE MODEL OF NON-IDEAL TUBULAR REACTOR FOR
PRODUCTION PROPYLENE GLYCOL**



Performed by

509 – Pharmacy

Ken – Woke Emmanuella

Academic supervisor:

Prof. Dmytro Vakuleno

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ABSTRACT

Propylene glycol is a versatile chemical substance that finds extensive application across multiple industrial domains. Its production requires a detailed understanding of reactor kinetics and architecture in order to be manufactured efficiently. This work simulates a non-ideal tubular reactor in an effort to clarify the intricacies involved in the manufacture of propylene glycol. The study explores the principles of tubular reactors, the kinetics and mechanisms of the synthesis of propylene glycol, and the modelling of reactor behaviour that is not ideal. Moreover, experimental analysis and validation are carried out to guarantee the created model's accuracy. The research also outlines future developments and optimisation techniques for the production of propylene glycol. The key to successful and long-lasting propylene glycol synthesis is a deep comprehension of non-ideal reactor behaviour.

Improving the manufacturing process's dependability, sustainability, and efficiency is the aim of the non-ideal tubular reactor model investigation. Comprehending the attributes of imperfect reactors, refining reactor blueprints, optimising operational circumstances, and guaranteeing precise modelling for pragmatic implementations are all part of this process. The report also looks at future developments in the manufacture of propylene glycol and sustainability issues.

INTRODUCTION

Tubular reactors are essential in chemical engineering because they offer a streamlined approach to a wide range of chemical processes. This section provides an overview of the basic principles of tubular reactors, with a focus on their practical use in industry [1].

There are various categories of tubular reactors.

Tubular reactors are highly adaptable systems utilised in several chemical processes, distinguished by their distinct properties [1].

1. Plug-Flow Reactor (PFR):

- Features: Uninterrupted movement of reactants with negligible radial mixing.
- Application: Well-suited for reactions requiring a precise and predetermined amount of time for completion.

2. Packed Bed Reactor:

- Features: Contains solid catalyst particles to increase surface reactions.
- Application: Frequently employed in catalytic processes, such as those found in petrochemical refining.

3. Fluidized Bed Reactor:

- Characteristics: Solid particles are suspended in a fluid, resulting in a state of fluidization.
- Application: Extensively used in processes that necessitate enhanced mass and heat transport, such as coal gasification.

Study of the movement and behaviour of fluids, as well as the patterns they create. An in-depth comprehension of the fluid dynamics of tubular reactors is crucial for maximising reaction efficiency. Important factors to take into account are [2]

1. Axial Dispersion:

- Definition: The phenomenon of concentration variation throughout the length of the reactor.

- Importance: Affects the distribution of the time that substances stay in a reactor and the overall performance of the reactor.

2. Radial Mixing:

- Definition: The process of fluid blending that occurs in the radial direction.
- Importance: Affects the consistency of reactant concentrations and temperature distributions.

3. Residence Time Distribution (RTD):

- Definition: The RTD refers to the probability distribution that represents the amount of time a particle remains in the reactor.
- Importance: Offers valuable information on the reactor's capacity to sustain consistent conditions.

Benefits of Tubular Reactor Design

Tubular reactors provide numerous advantages, such as the ability to be scaled up, precise determination of residence durations, and effective heat transfer. This section provides a comprehensive analysis of the advantages of tubular reactors, substantiated by empirical evidence showcasing their superior performance in comparison to alternative reactor types [1].

- **Enhanced Heat Transfer Efficiency:** The increased surface area in contact with the reactor walls enables more efficient heat exchange.
- **Precise Residence Time:** Accurate determination of residence times is essential for responses with specified temporal constraints.
- **Scalability:** Tubular reactors may be flexibly scaled up or down, making them adaptable to various production sizes.
- **Decreased Back Mixing:** Restricted radial mixing reduces the impact of back mixing, which is advantageous for reactions that have special demands.

The disadvantages of Tubular Reactor Design

Although tubular reactors have certain benefits, they also present difficulties. This section addresses potential hurdles, including hotspots, difficulties in temperature

management, and problems with catalyst dispersion. It also presents solutions to alleviate these issues.

- **Temperature Control Challenges:** Effectively managing temperature gradients can pose difficulties, perhaps resulting in the formation of hotspots.
- **Problems with the distribution of catalysts:** Achieving homogeneous dispersion of catalyst particles in packed bed reactors can be a difficulty.
- Fluidized bed reactors may experience issues with particle fouling and agglomeration, which can lead to potential complications.

Tubular reactors are used for reaction engineering.

This subsection establishes a link between the principles governing tubular reactors and the chemical reactions that take place inside them. This chapter offers fundamental knowledge that serves as a basis for future chapters. It delves into several facets of reaction engineering, such as the impact of reactant concentrations, temperature, and pressure on reaction kinetics.

Case Studies and Practical Applications

In order to exemplify abstract principles with practical implementations, this section incorporates case studies with tubular reactors. Studying successful implementations in various industries gives us a concrete grasp of how these reactors enable efficient chemical processes.

THE OBJECT OF RESEARCH AND METHODS OF STUDY

The aim of this study is to investigate the complexities and difficulties associated with the manufacturing of propylene glycol through the simulation of a non-ideal tubular reactor. The study explores the basic principles of tubular reactors, the kinetics and mechanisms involved in the synthesis of propylene glycol, and the modelling of non-ideal behaviour occurring in the reactor. I will utilise a secondary research methodology, extracting material from pre-existing publications and published academic and peer-reviewed studies in order to collect pertinent data.

The paper covers trends and sustainability, optimisation tactics, experimental investigation of propylene glycol production, and simulation results obtained from both the Plug Flow Reactor (PFR) and the Continuous Stirred-Tank Reactor (CSTR). Furthermore, it analyses the influence of other characteristics, such as tank arrangement, temperatures, and other relevant elements. In addition, the research offers a comprehensive overview of the mechanisms and kinetics involved in the manufacture of propylene glycol. It also includes a modelling of the behaviour of tube reactions.

Purpose of the Study

The objective of the study is to examine the modelling and simulation capabilities of a non-ideal tubular reactor in order to enhance the efficiency of the propylene glycol production process in the pharmaceutical business.

Research Objectives

The main goal is to examine literature sources that pertain to the models, methodologies, and environments utilised for simulating non-ideal tubular reactors in order to optimise the synthesis of propylene glycol in the field of pharmacy. Furthermore, the study seeks to do experimental modelling and determine the most favourable operational parameters for the manufacture of propylene glycol.

In order to achieve these goals, the following research tasks have been delineated:

- ✓ Perform an extensive examination of existing literature.
- ✓ Analyse the rate and processes involved in the synthesis of propylene glycol.
- ✓ Examine current methodologies for representing non-ideal behaviours in tubular reactors.
- ✓ Conduct empirical investigation, verification, and computer modelling of propylene glycol manufacturing.
- ✓ Execute optimisation strategies and investigate patterns in sustainable development.

Research Scope

The study centres on the environment utilised to simulate a non-ideal tubular reactor for the purpose of optimising propylene glycol synthesis processes in the field of pharmacy. The research focuses on developing a mathematical model to replicate the environment of a non-ideal tubular reactor for the purpose of optimising propylene glycol production in the field of pharmacy.

Research Methods

The study utilises bibliosemantic techniques to conduct literature search and review, mathematical modelling techniques to simulate non-ideal tubular reactor processes in order to optimise propylene glycol production, and analysis and generalisation of research findings.

Scientific and Practical Significance

The research involves a comprehensive examination of literature sources on models, methodologies, and environments used to simulate non-ideal tubular reactors in order to enhance the efficiency of propylene glycol synthesis in the field of pharmacy. The paper examines the rate and mechanisms of propylene glycol synthesis and discusses current methods for modelling deviations from optimal behaviour in tubular reactors. The study seeks to enhance the efficiency of the non-ideal tubular reactor for the synthesis of propylene glycol by experimental investigation, validation, and modelling. The research also concentrates on formulating optimisation strategies and investigating patterns in sustainable development.

CHAPTER 1

LITERATURE REVIEW

An examination of pertinent research papers in the topic of Propylene Glycol manufacturing.

The study titled "Recent advancements in catalytic conversion of glycerol into propylene glycol: A review" by Malaya R. N. et. al (2016) discusses the latest developments in the process of converting glycerol into propylene glycol using catalysts. The study asserts that the renewable nature of bio-glycerol makes it an attractive source for producing a wide range of chemicals. Selective hydrogenolysis of glycerol to create propylene glycol (PG) is a highly promising method for glycerol valorization. This process is particularly significant since it serves as a chemical intermediary in several applications. This article is a comprehensive review of advancements in catalytic conversion methods used to convert glycerol into propylene glycol. The subject matter includes progress in improving processes, the impact of preparation and activation methods on the effectiveness and longevity of catalysts, and the performance of various types of catalysts. In addition, this study examines the practicality of using bio-hydrogen and the difficulties involved in using crude glycerol for glycerol hydrogenolysis [3].

The upcoming paper for review is titled "Production of propylene glycol (1,2-propanediol) by the hydrogenolysis of glycerol in a fixed-bed downflow tubular reactor over a highly effective Cu–Zn bifunctional catalyst: effect of an acidic/basic support" and is authored by Dinesh Kumar Pandeya and Prakash Biswas [4]. This study involved the preparation and evaluation of different copper-zinc bimetallic catalysts supported on various oxides (V₂O₅, ZrO₂, TiO₂, CaO, and MgO) with acidic and basic properties. The catalysts were synthesised using a deposition-precipitation method. Their performance in the vapor-phase hydrogenolysis of glycerol to produce propylene glycol was assessed under specific conditions of 0.1 MPa and 220 °C. The catalysts were extensively characterised using various techniques such as BET, XRD, H₂-TPR, NH₃

and CO₂ TPD, N₂O adsorptive decomposition, TEM, XPS, FE-SEM, and TGA. Out of all the catalysts that were supported, the Cu–Zn/MgO catalyst exhibited the greatest selectivity for propylene glycol. The exceptional performance of the material can be due to its high dispersion of copper metal (about 5%), large surface area (approximately 23 m² g^{−1}), high basicity (0.25 mmol CO₂ g cat^{−1}), and the presence of partially reduced copper species (Cu₂O, CuO, and Cu⁰). The Cu-Zn/MgO catalyst achieved a glycerol conversion rate of roughly 98.5% with a selectivity of around 89% towards propylene glycol under the following reaction conditions: 220 °C, 0.72 MPa, and a weight hourly space velocity (WHSV) of 0.073 h^{−1}. This catalyst has the potential to maintain stability for a duration exceeding 84 hours [4].

The paper by Memon et al. (2022) examines the heat and mass transfer in a Multicomponent tubular reactor with a cooling jacket during the thermal decomposition of propylene oxide in water. The process is an irreversible, first-order reaction that releases heat, resulting in the formation of propylene glycol with an enthalpy of -84,666 J/mol. The reaction rate is governed by the Arrhenius equation, where the activation energy is adjusted between 75,000 and 80,000 J/mol, but the frequency factor remains constant. In order to maintain smooth flow, it is necessary to keep the Reynolds number between the range of 100 to 1000 [5].

The study of heat and mass transfer involves solving three interconnected partial differential equations that govern the transfer of mass, momentum, and energy. These equations are solved using the chemistry interface in COMSOL Multiphysics 5.4. The quantity of propylene oxide is initially varied between 2 to 3%, and the thermal conductivity of the mixture is evaluated within the range of 0.599 to 0.799. The study by Memon et al. (2022) found that when the Reynolds number grows, the compound's deactivation rate falls.

At a lower activation energy and Reynolds number of 100, the breakdown of propylene oxide achieves an approximate 99.8% conversion, leading to the highest possible total enthalpy change in the tubular reactor. Upon examining the correlation between Sherwood numbers and Nusselt numbers, it was inferred that there is an inverse

relationship between convective heat transfer and convective mass transfer at high Reynolds numbers [5].

The paper titled "Catalytic conversion of glycerol to propylene glycol: synthesis and technology assessment" by Chiu, Chuang-Wei focuses on developing a method that can be used for large-scale production of propylene glycol from glycerol. The objective is to achieve high conversions and yields in the process (Chiu, 2018). The fundamental comprehension of glycerol technology produced in this study provides the foundation for future research on extracting more commodity chemicals from natural sources.

Acetol was created successfully by dehydrating glycerol, which acted as a temporary intermediary. This indicates that excellent selectivity in producing propylene glycol can be attained in two phases. By employing reactive distillation technology, the equilibrium was effectively manipulated in favour of the intended direction, leading to increased yields. This catalytic process provides an alternate method for producing propylene glycol by utilising renewable resources. A study by Chiu (2018) has shown that it is possible to transform glycerol into propylene glycol using a copper-chromite catalyst using low-pressure vapor-phase catalytic processing. This technique underwent rigorous testing in a continuous process to address problems related to scalability and its suitability for large-scale production. Using a vapor-phase reaction method, glycerol can be transformed into propylene glycol effectively in a single reactor.

A validated proposal for a two-step reaction process has been put forward to produce propylene glycol from glycerol, utilising an acetol intermediate. A large-scale process is theoretically feasible [6].

Another study titled "An Experimental Study of the Pyrolysis and Oxidation of Ethylene Glycol and Propylene Glycol in a Jet-Stirred Reactor" was conducted by Suphaporn Arunthanayothin, Olivier Herbinet, and Frédérique Battin-Leclerc [7]. This study empirically investigates the pyrolysis and oxidation mechanisms of ethylene glycol (EG) and propylene glycol (PG), which act as representative substitutes for pyrolysis oils derived from biomass. These oils possess similar structures to sugars. This study involves the preliminary examination of these high-boiling dioxygenated

compounds (with boiling points around 470 K for EG and 461 K for PG) using a fused silica jet-stirred reactor. The tests consist of subjecting a combination of 1% fuel and helium to pyrolysis and oxidation processes within a temperature range of 600–1200 K. Studies using ethylene glycol involve oxidation using three distinct equivalency ratios ($\phi = 0.5, 1.0, \text{ and } 2.0$), whereas studies with propylene glycol are conducted only under stoichiometric conditions [7]. The residence time is set at a constant value of 2 seconds, and the pressure is about equal to atmospheric pressure (107 kPa). The experimental findings clearly show noticeable differences in the reactivity of both fuels. Comparing simulations using a thorough kinetic model with a comparative analysis reveals significant differences, highlighting the need for additional improvement in diol chemistry within these models. The rate-of-production and sensitivity analyses identify important pathways that require further investigation to gain a more thorough understanding of glycol combustion chemistry. These pathways include the simultaneous decomposition reactions of the fuel and the potential replacement of its analogue, aldehyde, with ethenol [7].

The research titled "Simultaneous production of lactic acid and propylene glycol from glycerol using solid catalysts without external hydrogen" by Lu Liu and X. Philip Ye [8] demonstrates exploring the conversion of glycerol, a by-product of biodiesel production, into value-added chemicals is essential for the sustainability of the biodiesel business. A catalytic pathway has been developed to convert glycerol into racemic lactic acid by utilising a stable foundation and a copper-based catalyst. This approach revealed a new pathway in which hydrogen is produced during the conversion of glycerol to lactic acid. This hydrogen may be used on-site to make propylene glycol with the help of a copper-based catalyst [8]. The synergistic effects of a base catalyst (such as CaO, MgO, or SrO) and a copper-based dehydrogenation catalyst (including Cu, CuO, Cu₂O, or Cu₂Cr₂O₅) were examined in experimental experiments. Multiple combinations of catalysts and reaction conditions were investigated in order to attain controllable yields of lactic acid and propylene glycol. The combined employment of CuO and CaO was prioritised due to their cost-effectiveness and simplicity of recyclability. Under

optimised reaction conditions, the production of lactic acid reached a yield of 52 mol%, along with a yield of 31 mol% of propylene glycol [8].

The paper titled "Simulation Study of Propylene Glycol Formation from Propylene Oxide and Water: Effect of Reactor Type, Reactant Ratio, Temperature, and Reactor Configuration" by Eko Ariyanto et al., (2024) investigates the influence of reactor type, configuration, temperature, and reactant ratio on the production of propylene glycol from propylene oxide and water. The study utilises HYSYS simulation software. The reactor types investigated encompass Continuous Stirred Tank Reactors (CSTR) and Plug Flow Reactors (PFR). The investigation examines the impact of varying the mole ratio of propylene oxide to water on the reactant ratio. Modifying the reaction temperature from 24 to 40 °C investigates the impact of temperature. The simulation findings from HYSYS indicate that the Plug Flow Reactor (PFR) shows higher conversion rates when compared to the Continuous Stirred Tank Reactor (CSTR). Furthermore, the successive continuous stirred-tank reactor (CSTR) configuration results in a greater conversion rate compared to the parallel CSTR architecture, as stated by Ariyanto et al. in 2024. Raising the reaction temperature from 24 to 40 °C improves the conversion of propylene oxide to propylene glycol. The maximum conversion is achieved when the reactant ratio is 1:1, namely between propylene oxide and water. These findings provide valuable information on how to improve the efficiency and cost-effectiveness of propylene glycol processes. The study proposes that the use of PFR configuration, sequential CSTR design, higher reactor temperatures, and ideal reactant ratios can greatly enhance the efficiency of propylene glycol synthesis [10].

CHAPTER 2

KINETICS AND MECHANISM OF PROPYLENE GLYCOL PRODUCTION, MODELLING NON-IDEAL BEHAVIOUR IN TUBULAR

KINETICS AND MECHANISM OF PROPYLENE GLYCOL PRODUCTION

The production of propylene glycol entails an intricate sequence of chemical processes, given its significant utility in several industries [10]. In order to enhance the efficiency of the synthesis process, it is essential to have a comprehensive grasp of the kinetics and mechanisms that govern its production. This chapter explores the complex chemistry involved in the manufacture of propylene glycol, including the reactions, rate laws, procedures, and techniques for determining kinetic parameters [10].

Chemical reactions involved in the synthesis of propylene glycol

The creation of propylene glycol necessitates a range of chemical reactions that are contingent upon the initial substances used and the selected technique of manufacturing. The following main reactions are involved in the production of propylene glycol [11]:

Derived from propylene oxide:

✚ Hydrolysis Reaction: Propylene oxide ($\text{CH}_3\text{CHCH}_2\text{O}$) reacts with water (H_2O) and a catalyst (such as an acid or base) to undergo hydrolysis and form propylene glycol:

The reaction between $\text{CH}_3\text{CHCH}_2\text{O} + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{CHOHCH}_2\text{OH}$.

✚ The ring opening reaction can be achieved by opening propylene oxide, and then adding water to produce propylene glycol.

The reaction of $\text{CH}_3\text{CHCH}_2\text{O} + \text{H}_2\text{O}$ yields $\text{CH}_3\text{CHOHCH}_2\text{OH}$.

From Glycerol:

1. Hydrogenolysis is a chemical reaction in which glycerol ($\text{C}_3\text{H}_8\text{O}_3$) is converted into propylene glycol using high-pressure hydrogen and a catalyst such

as copper chromite. The chemical equation represents the reaction between $C_3H_8O_3 + H_2$, resulting in the formation of $CH_3CHOHCH_2OH$.

2. Dehydration and Hydrogenation: Glycerol can be subjected to dehydration, a process in which water is removed, and then hydrogenation, a process in which hydrogen is added, resulting in the production of propylene glycol: The chemical formula $C_3H_8O_3$ can be converted to CH_2OHCH_2OH and further to $CH_3CHOHCH_2OH$.

3. Etherification is a chemical process where glycerol reacts with alcohols to produce propylene glycol ethers. These reactions are the main processes involved in the production of propylene glycol. Optimal yield and selectivity of propylene glycol can be achieved by adjusting variables such as temperature, pressure, and catalysts, depending on the production technique. In addition, commercial synthesis methods may include side reactions or additional purification processes in order to attain the necessary level of purity and quality of propylene glycol [11].

Rate laws and reaction mechanisms

Rate Determining Step: It is essential to identify the rate-determining step in the reaction pathway. Usually, the rate-determining phase is characterised by the slowest elementary reaction, which ultimately determines the total rate of the synthesis process.

Rate Equation: The rate equation establishes the correlation between the reaction rate (r) and the concentrations of reactants. An example of a hypothetical rate equation can be written as: $r = k[A]^m[B]^n$ where k represents the rate constant, $[A]$ and $[B]$ denote the concentrations of reactants, and m and n indicate the reaction orders with respect to each reactant.

Reaction Mechanisms

1. **Fundamental Stages:** It is crucial to comprehend the sequence of fundamental stages that constitute the entire reaction mechanism. Every step corresponds to a straightforward and well defined reaction that involves a distinct number of molecules.
2. **Intermediates and Transition States:** Reaction mechanisms frequently involve intermediates, which are temporary species created during the reaction, and transition states, which are high-energy states that molecules must traverse during the reaction. These factors are essential in defining the routes and kinetics of reactions.
3. The identification of the rate-determining step within the reaction mechanism is essential for determining the overall rate law. The rate of the reaction is determined by the slowest step.
4. **Catalysts and Reaction Mechanism:** Catalytic species can be involved in the reaction mechanism, modifying the pathway and reducing the activation energy, therefore impacting the reaction rate [11].

Experimental Determination of Rate Laws

1. The initial rate approach entails measuring the first rates of a reaction while manipulating the initial concentrations of the reactants. Through the examination of how alterations in the amounts of reactants impact the rate, one can infer the reaction order in relation to each reactant.
2. **Integrated Rate Laws:** Integrated rate laws elucidate the alterations in the concentrations of reactants as time progresses. Plotting the concentration against time on a graph allows one to ascertain the reaction sequence and the rate constant.
3. The isolation method is a technique used to determine the rate law for a specific stage in a complex reaction. It includes purposely manipulating the circumstances, such as concentration and temperature, which only affect that

particular phase. This allows for the isolation and study of that step in order to determine its rate law [11].

Temperature Dependence Studies

1. The Arrhenius equation is a mathematical expression that relates the rate constant (k) of a reaction to the temperature (T):

$k = A * e^{(-E_a/RT)}$. The variables in the equation are defined as follows: A represents the pre-exponential factor, E_a represents the activation energy, R represents the gas constant, and T represents the temperature. The activation energy can be calculated by analysing the slope of the Arrhenius plot, which is obtained by measuring the rate constants at various temperatures.

2. The Eyring equation offers a more comprehensive comprehension of the activation energy by taking into account the principles of the transition state theory. It establishes a connection between the rate constant and several factors such as temperature, activation energy, and the enthalpy and entropy of activation.

3. Reaction Calorimetry:

✓ Differential Scanning Calorimetry (DSC) is a technique used to detect the heat flow related to chemical reactions in relation to temperature. Through the examination of alterations in heat flow, one can ascertain the activation energy and reaction kinetics.

✓ Isothermal Microcalorimetry is a method used to detect the heat changes that occur during a chemical reaction at a consistent temperature. This technique provides valuable data on the reaction kinetics and the amount of heat released over a period of time.

4. Computational Methods: Theoretical calculations in computational chemistry employ methods such as quantum mechanics/molecular mechanics (QM/MM) simulations, density functional theory (DFT), or molecular dynamics

(MD) to accurately predict reaction paths, transition states, and kinetic parameters [11].

MODELLING NON – IDEAL BEHAVIOUR

Non-ideal behaviour in propylene glycol production refers to deviations from ideal circumstances, including changes in reactant concentrations, temperature differences, pressure fluctuations, or inefficiencies in the reactor [12]. This chapter explores the complexities of non-ideal behaviour and emphasises the significance of accurate modelling to enhance manufacturing processes.

TYPES OF NON-IDEAL BEHAVIOUR

- **Non-Ideal Behaviour in Fluid Dynamics and Mixing:** This topic focuses on the various types of non-ideal behaviour that can occur in fluid flow patterns, such as axial dispersion and radial mixing. It also examines how these behaviours can affect the distribution of reactants and the amount of time they spend in the system [12]
- **The limitations of heat and mass transmission are investigated in this study.** This includes analysing heat gradients, restrictions in mass movement, and how these factors impact reaction speeds and selectivity [12].
- **Chemical Equilibrium and Reactions:** Examines departures from ideal chemical equilibrium and the presence of secondary reactions that impact the amount and purity of the final product.

Modelling techniques for non-ideal behaviour

- **Mathematical Models:** Explores mathematical representations employed to illustrate non-ideal behaviour, encompassing models for axial dispersion, mixing, heat transport, and mass transfer in reactors.
- **Computational Fluid Dynamics (CFD)** is a field that focuses on utilising simulations to visually and analytically examine fluid flow patterns, temperature distributions, and concentration gradients within a reactor.

- **Empirical and Semi-Empirical Models:** This section explores the use of empirical methods that utilise experimental data to account for non-idealities, as well as semi-empirical correlations to forecast reactor performance [13]

Verification and adjustment

- Experimental validation emphasises the need of using experimental data to confirm and improve the developed models, guaranteeing their accuracy and dependability.
- **Parameter Estimation and Calibration:** This section explores methods for determining and adjusting model parameters using experimental data in order to improve the accuracy of model predictions.

Utilisation in Reactor Design and Optimisation

- **Reactor Design Modifications:** This section explores how non-ideal modelling can provide valuable insights for making changes to reactor design in order to enhance performance and efficiency [13]
- **Optimisation Strategies:** This section examines methods for improving operating conditions, including flow rates, temperature profiles, and catalyst distributions, using models that account for non-ideal behaviour

Factors contributing to non-ideal behaviours in chemical reactions

i. Mixing and Reactor Design

- **Incomplete Mixing:** Insufficiently uniform mixing of reactants inside the reactor can result in concentration gradients, which can have an impact on reaction rates and the production of products.
- **Reactor Geometry:** Irregularities or intricate shapes within the reactor might lead to non-optimal flow patterns, which can result in ineffective mixing and distribution of residence time [13].

ii. Constraints on the transfer of mass and heat

- Mass transfer limitations can occur when the diffusion rates of reactants or products are slow in the bulk fluid or across different phases. This can particularly affect reactions in heterogeneous systems [13].
- Heat transfer problems can arise in a reactor when there is an uneven distribution of temperature or inadequate heat transfer. These issues can lead to temperature gradients that can impact the rates of reaction and the selectivity of the process [13].

iii. Chemical Equilibrium and Side processes

- Incomplete Conversion: Reversible processes may fail to reach equilibrium because of inadequate residence time or unfavourable thermodynamics.
- Side reactions refer to undesirable chemical events that occur alongside the main reaction pathway. These side reactions can have a negative impact on the yield or purity of the desired product [13].

iv. Catalyst Presence

- Deactivation or Inefficiency: The presence of catalysts might result in lower catalytic activity or selectivity due to catalyst deactivation, poor distribution, or incorrect utilisation.

v. Irregular Reaction Kinetics

- Non-Ideal Kinetics: Non-ideal behaviour in reaction kinetics can occur due to deviations from conventional kinetic behaviour, such as non-elementary reactions or unexpected dependence on reactant concentrations.

vi. Transport Phenomena and Fluid Dynamics

- Axial Dispersion: The non-uniform fluid velocity distribution across the reactor's cross-section can lead to axial dispersion, which can impact the uniformity of reactant concentration.
- Radial mixing refers to the process of distributing reactants evenly around the radius of a reactor. When radial mixing is poor, it can result in an uneven distribution of reactants, which can cause the reactor to behave in a non-ideal manner [13].

vii.Operational settings

- Temperature and Pressure Variations: Any changes or deviations from the ideal temperature and pressure settings can have an effect on the speed of reactions and the balance between reactants and products.
- Insufficient flow rates or inadequate residence time might hinder the completion of reactions, hence impacting the yields of products [13].

Emphasises the application of mathematical modelling.

The mathematical modelling of non-ideal tubular reactors involves the formulation of equations that describe the behaviour of the reactor when it is not operating under ideal conditions. Below is an outline that specifically highlights the emphasis on mathematical modelling of non-ideal tubular reactors [2].

1) Equations governing transport phenomena:

- The mass balance equations are derived by taking into account axial dispersion and radial mixing, and considering the fluctuations in reactant concentrations along the length and radius of the reactor.
- The energy balance equations are formulated by taking into account the heat transfer processes and temperature changes in order to represent the thermal behaviour of the reactor [2].

2) Fluid Dynamics and Reactor Behaviour

- Axial Dispersion Model (ADM): The axial dispersion model is introduced to explain the uneven distribution of reactants along the length of the reactor. This involves the use of partial differential equations (PDEs).
- The Radial Dispersion Model (RDM) is a model that takes into account the effects of radial mixing. It specifically addresses the issue of non-uniform concentration distribution across the cross-section of the reactor.

3) Study of the rate at which chemical reactions occur and the state of balance between reactants and products in a chemical system

- Chemical reaction rate equations involve incorporating rate laws and reaction mechanisms into transport equations to accurately represent the kinetics of chemical reactions happening in a reactor [2].
- Chemical equilibrium models involve analysing equilibrium reactions and accounting for any deviations from ideal chemical equilibrium conditions, if they exist, by employing suitable equilibrium models.

4) Mathematical Expressions for Non-Idealities [14]

- Empirical Correlations: Using empirical correlations or experimental data to include non-idealities, such as dispersion coefficients or mixing factors, in the mathematical models.
- Numerical approaches: Utilization of numerical techniques (such as finite difference, finite element, or finite volume approaches) to solve the intricate set of differential equations that describe the behaviour of the reactor.

5) Model Validation and Parameter Estimation [14]

- Experimental Validation: It is crucial to validate mathematical models using experimental data in order to assure the accuracy and reliability of modelling non-ideal reactor behaviour

CHAPTER 3

EXPERIMENTAL ANALYSIS, VALIDATION AND SIMULATION

To comprehend and maximise the efficiency of tubular reactors, experimental verification and analysis are of utmost importance. This chapter delves into the methodologies, approaches, and significance of experimental research in defining and verifying the behaviour of tubular reactors in practical settings.

Various methodologies are used to investigate and quantify deviations from ideal conditions in order to characterise non-ideal reactor behaviour. Methods for describing less-than-ideal reactor behaviour are summarised here [5].

Experimental Methods

- **Concentration Profiling:** By analysing concentration profiles along the length and cross-section of the reactor with experimental data, we can gain insights into mixing and dispersion.
- **Temperature Measurements:** By keeping an eye on changes in temperature, we can find thermal gradients that impact reaction rates and equilibrium [5].

Residence Time Distribution (RTD) Analysis

- The purpose of a tracer study is to learn about the mixing efficiency and patterns of fluid flow by injecting tracers and then analysing their distribution to get the RTD.

Reaction Kinetics Studies

- **Reaction Rate Analysis** involves studying the pace at which a reaction occurs under various situations in order to get insights into its kinetics and detect any deviations from expected behaviour.
- **Catalyst Performance Evaluation:** The process of evaluating the effectiveness and efficiency of a catalyst by measuring its activity and selectivity, with the goal of identifying any shortcomings or loss of effectiveness [5].

Computational Fluid Dynamics (CFD)

- **Numerical Simulations:** Utilising computational fluid dynamics (CFD) simulations to visually represent the patterns of fluid flow, distributions of

temperature, and gradients of concentration within the reactor, facilitating comprehension of non-ideal conditions.

Heat and Mass Transfer Analysis

- **Measurement of Heat Transfer Coefficient:** Assessing heat transfer coefficients to analyse thermal behaviour and possible deviations in heat transport [8].
- **Mass transfer studies** involve the analysis of mass transfer rates in order to discover any constraints or variations that may affect the efficiency of a reaction.

Modelling Approaches

- **Mathematical Models:** Developing mathematical models that incorporate axial dispersion, radial mixing, and reaction kinetics to accurately explain and forecast the behaviour of non-ideal reactors [8]
- **Empirical correlations** are utilised to establish a relationship between experimental data and model parameters, hence improving the accuracy of non-ideal models.

Sensitivity Analysis

- **Parameter Sensitivity Studies:** Conducting sensitivity analyses to identify critical parameters influencing reactor performance and assessing their impact.

Comparison with Ideal Models

- **Benchmarking Against Ideal Models:** Contrasting the behaviour of non-ideal reactors with idealised models in order to measure and comprehend the degree of deviations.

Through the utilisation of these methods, scientists and technicians can thoroughly analyse the behaviour of reactors that do not meet ideal conditions. This allows for well-informed choices about optimisation, enhancements in design, and effective operation in chemical procedures.

DATA COLLECTION AND VALIDATION

Data collection and validation play a crucial role in maintaining the accuracy of models, which is essential for constructing dependable and efficient mathematical representations of intricate systems. Below is a concise overview that emphasises the crucial elements, as presented [8]:

Data Collection

1. Foundation of Understanding:
 - Data collection is the initial and essential process of gathering information about the actual behaviour of a system in the real world. This process provides factual observations that theoretical models strive to represent accurately.
2. Parameter Estimation:
 - Accurate data collection is crucial for estimating parameters, enabling researchers to identify model parameters that correspond to observable system dynamics.
3. Model Calibration:
 - Collected data enables the adjustment of models, bringing theoretical predictions in line with experimental observations and enhancing the model's ability to make accurate predictions.

Validation for Model Accuracy

1. Comparison with Real-world Behavior:
 - Validation is the process of comparing the predictions made by a model with the data that has been obtained. The goal is to make sure that the mathematical representation of the system appropriately reflects its real-world behaviour [14].
2. Identifying Discrepancies:
 - Validation is a process that detects differences between model predictions and experimental outcomes, indicating areas where the model may need to be improved or modified.

3. Enhancing Predictive Power:
 - Iterative data validation enhances the predictive capability of the model, rendering it a more resilient instrument for comprehending and forecasting system behaviour across diverse circumstances.
4. Guiding Model Development:
 - Validation drives the refinement of more advanced models, leading to modifications or enhancements that can better represent the intricacies of the system.
5. Optimization and Decision-making:
 - Precise models, verified using real-world data, establish a strong basis for optimisation endeavours and well-informed decision-making in diverse applications.

Ensuring Model Reliability

1. Reducing Uncertainty:
 - Thorough data validation minimises uncertainties related to theoretical models, enhancing trust in the model's capacity to accurately depict the system.
2. Facilitating Trust in Results:
 - Model validation instills confidence in the outcomes produced by the model, rendering it a dependable instrument for researchers, engineers, and decision-makers.

Industry Applications

- Validated models are essential in industrial contexts for developing efficient processes, optimising operations, and making educated decisions that affect productivity and resource utilisation.

THE ROLE OF EXPERIMENTAL VALIDATION IN PRACTICAL APPLICATION

Experimental validation plays a crucial role in practical applications by confirming that theoretical models adequately depict real-world systems (Wang and Yuan, 2016).

Below is an analysis of the importance of experimental validation in many practical scenarios:

1. Process Optimization

- Identification of Optimal Conditions:
 - Experimental validation enables the determination of the most effective operating conditions, allowing enterprises to optimise processes for improved efficiency and productivity.
- Fine-tuning Parameters:
 - Validating theoretical models by experimental allows for the adjustment of model parameters, ensuring that simulations closely match observed behaviours in real processes.

2. Product Development

- Quality Assurance:
 - Experimental validation in product development ensures the dependability of theoretical predictions, assisting in quality assurance by confirming that the product satisfies predetermined requirements.
- Material Selection:
 - Validating material qualities and behaviours through tests is essential in areas like materials science and engineering, since it helps determine the appropriate materials for certain applications.

3. Environmental Impact Assessments

- Accurate Predictions for Regulatory Compliance:
 - Experimental validation is crucial in environmental research to provide accurate predictions of contaminant dispersion, which helps in meeting regulatory criteria and reducing environmental damage.

4. Pharmaceuticals and Medicine

- Drug Development and Efficacy:

- Experimental validation is essential in pharmaceutical research to evaluate the effectiveness, harmfulness, and safety of drugs. It offers crucial insights into the potential practical consequences of novel therapies.
- Biomedical Devices:
 - Experimental validation is crucial for biomedical devices since it assures that the equipment functions in accordance with its intended purposes, hence enhancing the dependability and safety of medical innovations.

5. Energy Systems

- Efficiency Improvements:
 - Experimental validation plays a crucial role in the advancement and refinement of energy systems, leading to enhanced efficiency in areas like the production and storage of renewable energy.
- Safety Protocols:
 - Validating theoretical models in the design of energy infrastructure guarantees compliance with safety norms and laws, reducing potential risks linked to system breakdowns.

6. Aerospace and Automotive Engineering

- Vehicle Performance:
 - Experimental validation is of utmost importance in aerospace and automotive engineering since it allows for the assessment of vehicle performance. It ensures that theoretical models are able to effectively predict elements like as aerodynamics, fuel efficiency, and structural integrity.
- Safety Standards:
 - Validating theoretical models is crucial for ensuring compliance with safety requirements, since it offers actual evidence that confirms the dependability and safety of aviation and vehicle systems.

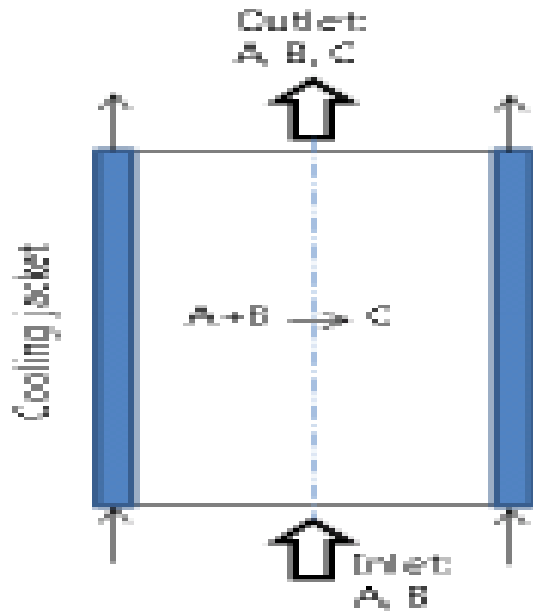
7. Climate Modelling

- Predicting Climate Changes:
 - Experimental validation in climate modelling enhances the accuracy of long-term climate forecasts and informs decision-making in climate-related policies.

SIMULATIONS

The Embedded Model

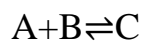
The Embedded Model (Liu & Ye, 2015) describes a systematic process that involves the exothermic chemical interaction between propylene oxide and water, resulting in the production of propylene glycol. This chemical reaction takes place inside a cylindrical reactor that is equipped with a cooling jacket to prevent any explosions from occurring.



Above is a sketch of the reactor geometry.

The reaction takes place in the liquid phase and in the presence of a solvent. The density of the reactor solution is presumed to remain generally constant, even when there are changes in composition and temperature. Based on these assumptions, it is possible to establish a comprehensive velocity profile along the radius of the reactor.

MODEL DEFINITION:



The reaction (Deng W., 2019) entails the reversible transformation of species A, B, and C in their liquid state. A symbolises propylene oxide, B symbolises water, and C symbolises propylene glycol. The reaction kinetics are expected to follow a first-order rate law with respect to the concentration of A, under the assumption that the

concentration of water is in excess and remains constant. Furthermore, if we assume that propylene oxide and propylene glycol have the same transport properties and are both present in a water solution with low concentration, we can estimate the concentration of propylene glycol (referred to as species C) based on the concentration of propylene oxide (referred to as species A) and the stoichiometry of the reaction.

The model equations elucidate the fundamental concepts of conserving both material and energy inside the system. The variables of interest in the reactor are the concentration (c) and temperature (T). There is also a variable called the temperature within the cooling jacket (T_j), which is placed along the length of the reactor where the cooling jacket is positioned.

The reactor's material and energy conservation equations are formulated based on two distinct variables: the radial direction (r) and the axial direction (z). The above equations form a coupled system of two partial differential equations (PDEs) that are defined along the r and z axes.

The equation governing material conservation within the reactor is as follows:

$$D_{\text{eff}} \frac{1}{r} \frac{\partial c_A}{\partial r} + D_{\text{eff}} \frac{\partial^2 c_A}{\partial r^2} + D_{\text{eff}} \frac{\partial^2 c_A}{\partial z^2} - 2U \left(1 - \left(\frac{r}{R}\right)^2\right) \frac{\partial c_A}{\partial z} + r_A = 0$$

where D_{eff} denotes the effective diffusion coefficient, c_A the concentration of species A, U the average flow velocity, R the radius of the reactor, and r_A the reaction rate.

The reactor's energy conservation equation is as follows:

$$k \frac{1}{r} \frac{\partial T}{\partial r} + k \frac{\partial^2 T}{\partial r^2} + k \frac{\partial^2 T}{\partial z^2} - 2U \left(1 - \left(\frac{r}{R}\right)^2\right) \rho C_P \frac{\partial T}{\partial z} - r_A (-\Delta H_{Rx}) = 0$$

where k denotes the thermal conductivity, T temperature, ρ density, C_P the heat capacity, and ΔH_{Rx} the heat of reaction.

The temperature of the cooling jacket is presumed to vary exclusively in the axial direction, specifically over the length of the reactor. Therefore, the energy equation for the cooling jacket is formulated using the z-coordinate.

$$\frac{\partial T_j}{\partial z} = \frac{2\pi R U_k (T - T_j)}{m_J C_{PJ}}$$

where m_J denotes the mass flow rate of the coolant, C_{PJ} its heat capacity, and U_k the heat transfer coefficient between the reactor and the cooling jacket.

The boundary conditions define the specific values of concentration and temperature at the inlet of the reactor. On the other hand, at the outlet, the flow of material and energy moving away is mostly affected by advection and is described appropriately. The heat flux on the reactor wall is directly proportional to the difference in temperature between the reactor and the cooling jacket.

$$-\frac{\partial T}{\partial r}(R, z) = \frac{U_k}{k}(T - T_j)$$

The simulation results are remarkably fascinating. With the default input settings, the conversion profiles along radial cut lines demonstrate both the lowest and highest values, as depicted in Figure 3 below. One of the difficulties faced by students in Fogler's book is to clarify and understand these profiles.

Here, we can clarify that the profile is determined by the combination of the exothermic reaction, the advective term, and the cooling impact from the jacket. The conversion rate is reduced in the middle of the reactor due to the significant decrease in flow velocity. This is because the reactants penetrate deeply into the reactor before experiencing reaction, as indicated by label 1 in Figure 3 [3].

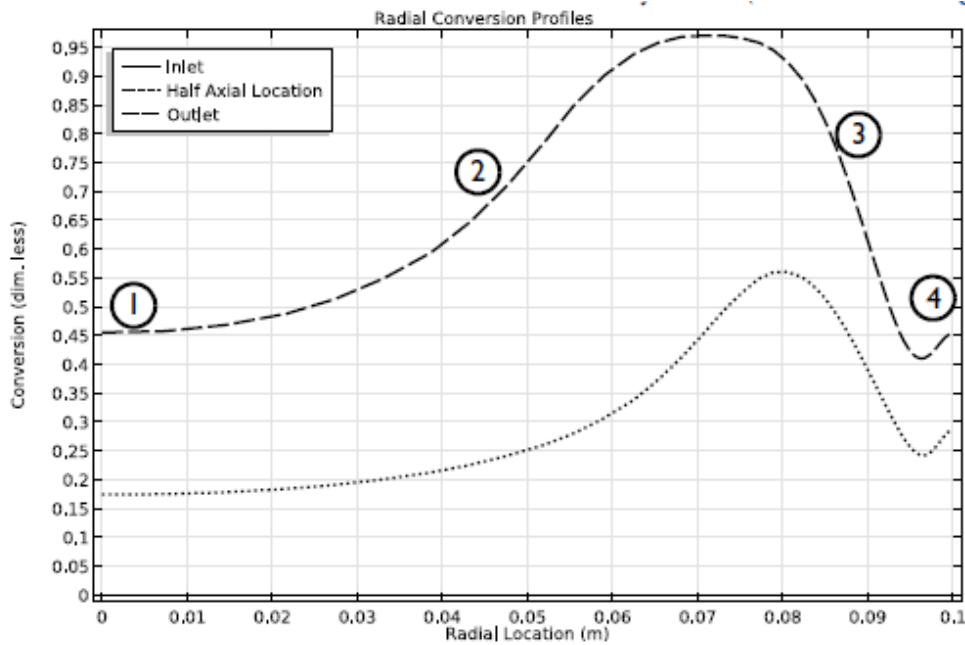


Figure 3: Cross-section plot of the conversion of A along the radius of the reactor and at different positions along the length. The conversion is 1 when all propylene oxide has been converted to propylene glycol at a give point.

Closer to the wall, the rate at which the fluid flows decreases, causing an increase in conversion. This is because the temperature remains relatively high farther away from the wall, which leads to a higher response rate (labelled as 2 in Figure 3).

However, as proximity to the wall increases further, conversion begins to decline due to the cooling effect of the jacket, which reduces the reaction rate (labeled as 3 in Figure 3 above).

At the reactor wall, the cooling is remarkably effective, which theoretically should further reduce conversion. Nevertheless, the conversion sees a marginal rise due to the absence of reactant movement at the wall. The residence time for the volume elements travelling along the wall is very long due to the absence of flow at the wall (referred to as 4). As a result, the reactants are more extensively depleted.

Sensitivity to Input Data:

A mathematical model is deemed well-posed when it is correctly defined [3]. A mathematically well-defined model has a single solution that consistently depends on the data of the problem. If a model does not possess this characteristic, it will be apparent in the numerical depiction, leading to difficulties in the process of finding a solution.

To evaluate the sensitivity of the numerical solution to input, we can do a parametric sweep. Upon analysing the model equations, it becomes evident that the reaction term demonstrates an exponential relationship with the activation energy, in accordance with the Arrhenius equation. This could potentially give rise to difficulties or obstacles. The diagram below demonstrates the variation in conversion along the length of the reactor as the activation energy changes. When visualised as a surface plot, the resulting profiles have a smooth and continuous appearance, mimicking an animation of an increasing response rate constant.

This discovery suggests that the numerical solution remains stable even when the Arrhenius expression contains a potentially troublesome parameter. An analogous examination is performed for the normalised temperature (T/T_0), demonstrating the seamless nature of the numerical solution with respect to the activation energy. In addition, a parametric sweep analysis of the heat of reaction reveals a minimal impact and a consistently smooth response of the solution.

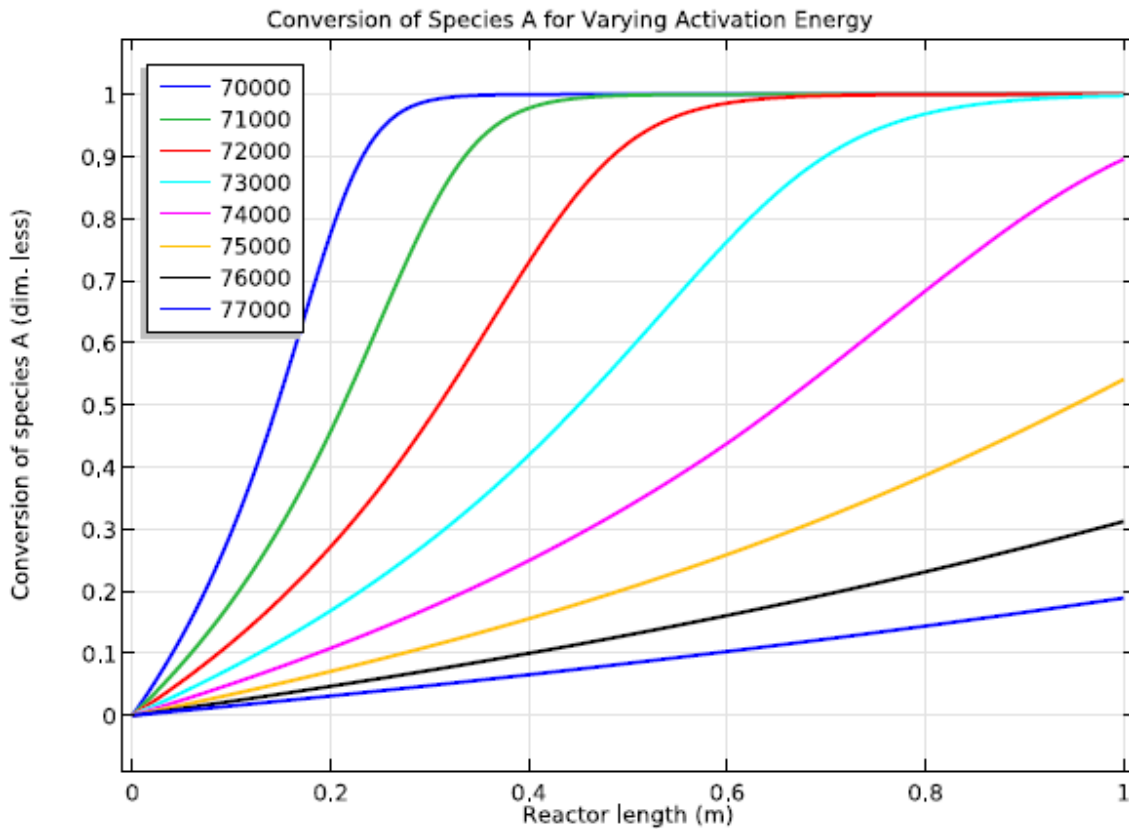


Figure 7: Conversion of species A for varying activation energy (J/mol).

Comparison with an Analytical Solution:

The equation describing the preservation of chemical species may be deduced under isothermal conditions and plug flow, providing a scenario that can be solved analytically [3]. This offers a distinct chance to compare the precise solution with both the mathematical model and the numerical solution. Comparisons between theoretical solutions and experimental results can be made for both laminar and turbulent flows, assuming that the radial diffusion is insignificant compared to the axial advection in the reactor's bulk.

By removing the radial dependency from the mass transfer equations, we obtain the following equation:

$$D_{\text{eff}} \frac{\partial^2 c_A}{\partial z^2} + \left(-U \frac{\partial c_A}{\partial z} \right) - k_f c_A = 0$$

Here, k_f denotes the rate constant (s^{-1}). The equation above has the following analytical solution:

$$c_A(z) = A_1 \exp(B_1 z) + A_2 \exp(B_2 z).$$

From the boundary conditions, the constants A_1, A_2, B_1 and B_2 can be determined as

$$\begin{aligned} A_1 &= \frac{c_{A0} B_2 \exp(B_2 L)}{B_1 \exp(B_1 L) - B_2 \exp(B_2 L)} \\ A_2 &= c_{A0} - A_1 \\ B_1 &= \frac{U}{2D_{\text{eff}}} - \sqrt{\left(\frac{U}{2D_{\text{eff}}}\right)^2 - \frac{k_f}{D_{\text{eff}}}} \quad , \\ B_2 &= \frac{U}{2D_{\text{eff}}} + \sqrt{\left(\frac{U}{2D_{\text{eff}}}\right)^2 - \frac{k_f}{D_{\text{eff}}}} \end{aligned}$$

When the reactor's length is denoted as L , employing identical parameters as those utilized in the preceding numerical solutions but with a consistent temperature set at 332 K yields the depicted plot in Figure 8 below (Deng W., 2019).

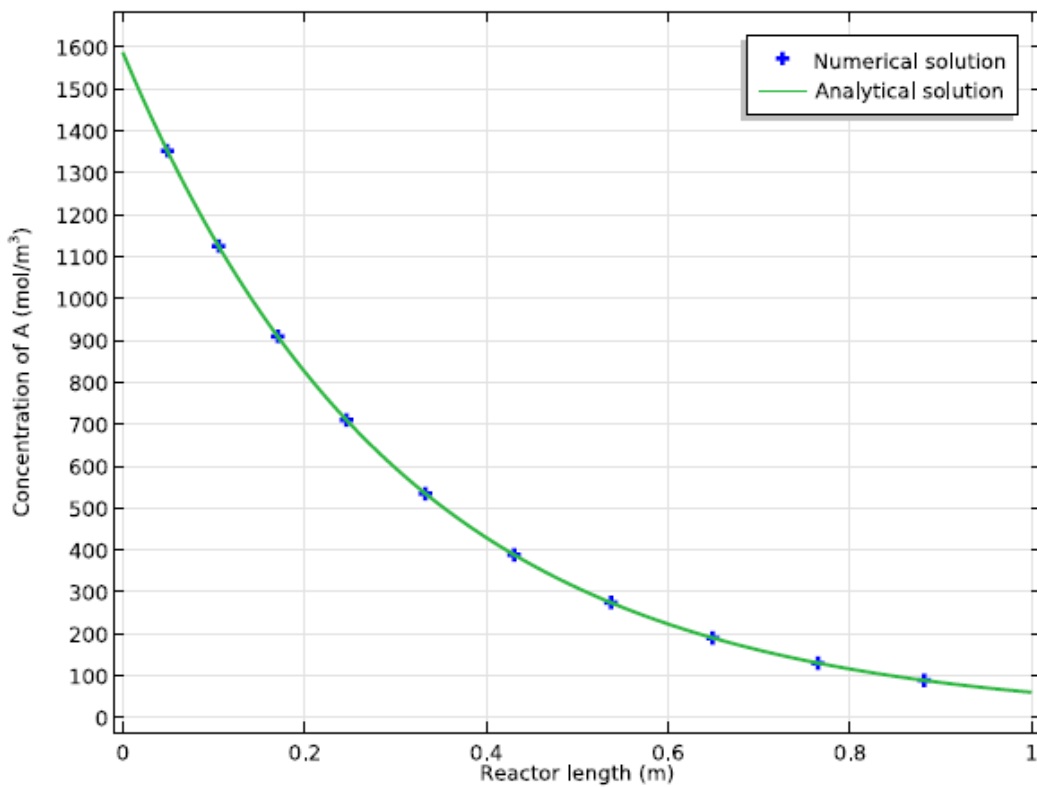


Figure 8: Concentration of species A along the length of the reactor computed using the numerical and analytical solution to the model equations.

The graph clearly demonstrates a significant level of agreement between the numerical and analytical solutions. These findings indicate that the numerical model is a reliable and accurate representation of the mathematical model, especially when the conditions are isothermal.

It is crucial to emphasise that the act of comparing with analytical answers is not universally applicable. These analogies are only applicable to certain situations, and any conclusions made based on them should be handled with caution.

RESULTS

Model of Propylene Glycol formation

Simulation models are highly valuable instruments for optimising and improving the operational efficiency of chemical industry processes, specifically in relation to the reactions occurring within reactors [10]. Aspen HYSYS, a process simulator mentioned in literature, enables the optimisation of process parameters, resulting in reduced operational time and costs. The production of propylene glycol in Continuous Stirred-Tank Reactors (CSTR) and Plug Flow Reactors (PFR) is simulated using Aspen HYSYS V11, assuming steady-state conditions. The Soave-Redlich-Kwong (SRK) equation is utilised to calculate physical properties. The simulation is performed using a set of predetermined assumptions, which are outlined below:

The reactor functions under stable circumstances throughout the reaction process.

The reactor volume for a single reactor is 5 litres, however for twin reactors, each reactor has a volume of 2.5 litres.

The reactors are positioned sequentially, with each having the same residence durations.

The reactor is configured in a parallel arrangement, where the incoming flow converges into a unified stream before being split into two streams of equal flow rates.

Regarding the reaction kinetics data, the Arrhenius equation is employed to determine the reaction rate of propylene glycol.

The value of the frequency factor is as follows:

$$k = 16.96 \times 10^{12} e^{\frac{-76000}{R.T}} \quad (2)$$

where R is the ideal gas constant, and T is the temperature.

Table 1. HYSYS Reactants Stream Simulation Data

Parameter	<i>Propylene Oxide</i>	<i>Air</i>
Temperature (°C)	23.89	23,89
Pressure (atm)	1.1	1,1
Mass Flowrate (kg/hr)	5000	5000

The CSTR mathematical model is as follows;

$$\tau = \frac{V}{v_o} = \frac{C_{A0} \cdot V}{F_{A0}} = \frac{C_{A0} \cdot X_A}{-r_A} \quad (3)$$

where τ is the residence time (hour), V is reactor volume (l), v_o is the flow rate (l/hour), C_{A0} is the initial concentration (mol/l), F_{A0} is the mass flow rate of fluid (kg/hour), X_A is the reaction conversion, and r_A is the reaction rate.

The reaction rate can be calculated using the following Eq. (4).

$$-r_A = -\frac{dC_A}{dt} = kC_A \quad (4)$$

where dC_A/dt is the change in concentration over a change in reaction time, C_A is the reactant remaining from the reaction products (mol/l), and t is the reaction time.

Impact of Reactor Design

The selection of reactor architecture has a substantial influence on the conversion of propylene oxide into propylene glycol products. For this study, two types of reactors were used: a Continuous Stirred-Tank Reactor (CSTR) and a Plug Flow Reactor (PFR), as shown in Figure 3.

Figure 3 illustrates the reactor setups employed in the HYSYS simulation to produce propylene glycol from propylene oxide and water. Figure 3 illustrates the process flows for CSTR (Figure 3(a)) and PFR (Figure 3(b)). The input stream is combined at the mixing point (MIX-100) prior to entering the reactor.

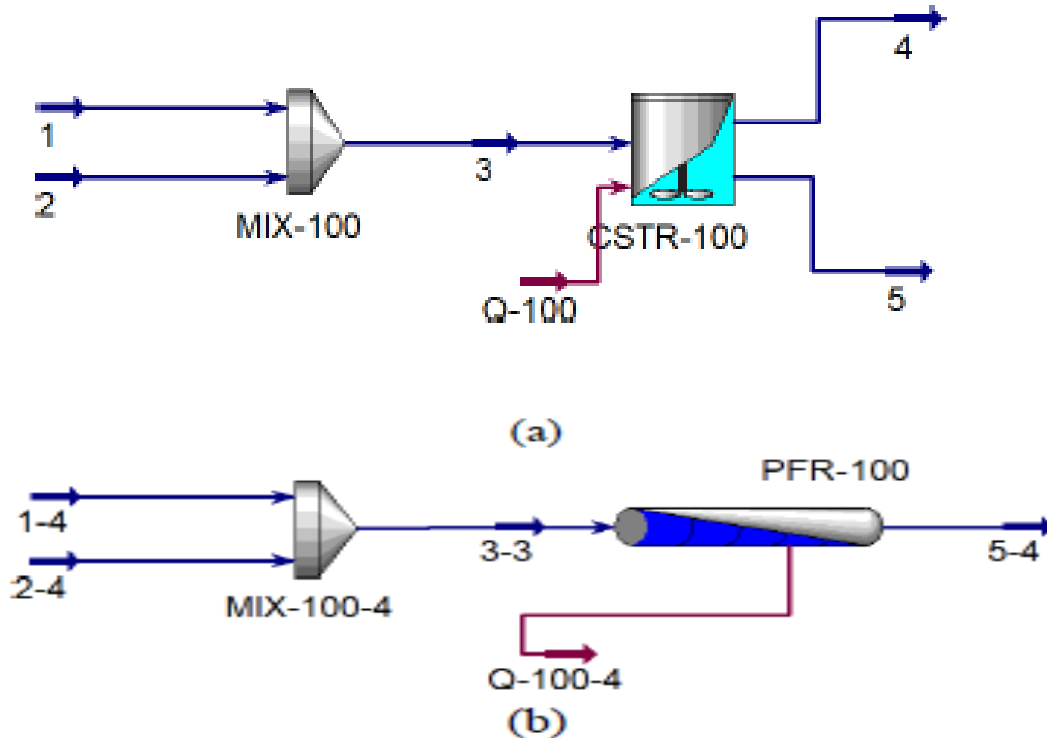


Figure 3. Flow Diagram HYSYS Simulation (a) CSTR; (b) PFR.

Table 2. HYSYS Simulation Results of 2 Reactor Types

Reactor Type	Conversion (%)
CSTR	60.53
PFR	82.30

Table 2 shows that the Plug Flow Reactor (PFR) outperforms the Continuous Stirred-Tank Reactor (CSTR) in terms of conversion. The CSTR is estimated to have a conversion rate of 65%, while the PFR is estimated to have a conversion rate of 82.30% according to HYSYS. The reduced conversion seen in the CSTR simulation is attributed to the occurrence of back-mixing, which involves the interaction of reactants with

unreacted components (Ariyanto et al., 2024). Nevertheless, the continuous stirred-tank reactor (CSTR) provides the benefit of generating a homogeneous product, which is simpler to control and more suitable for industrial-scale production.

A Plug Flow Reactor (PFR) is a type of reactor where reactants are continually fed into a pipe, allowing reactions to occur at different speeds along the length of the pipe. The lack of back-mixing in the Plug Flow Reactor (PFR) allows reactants to have a longer residence period for reactions compared to the Continuous Stirred-Tank Reactor (CSTR). Figure 4 illustrates the results of the HYSYS simulation for both the Continuous Stirred Tank Reactor (CSTR) and the Plug Flow Reactor (PFR) volumes.

Impact of Reactor Configuration

The configuration of reactors has a substantial impact on the transformation of propylene oxide into propylene glycol [10]. The HYSYS simulation, as depicted in Figure 5, was performed using reactors with a volume capacity of 2.5 L each. Figure 5(a) illustrates a series reactor setup, whereas Figure 5(b) depicts a parallel reactor layout where the feed is divided into two streams (streams 9 and 10) with identical flow rates. The temperature and pressure in both reactors were adjusted to 23.9°C and 111.5 kPa, respectively. Figure 6 presents the simulated dimensions of the Continuous Stirred-Tank Reactor (CSTR) in HYSYS.

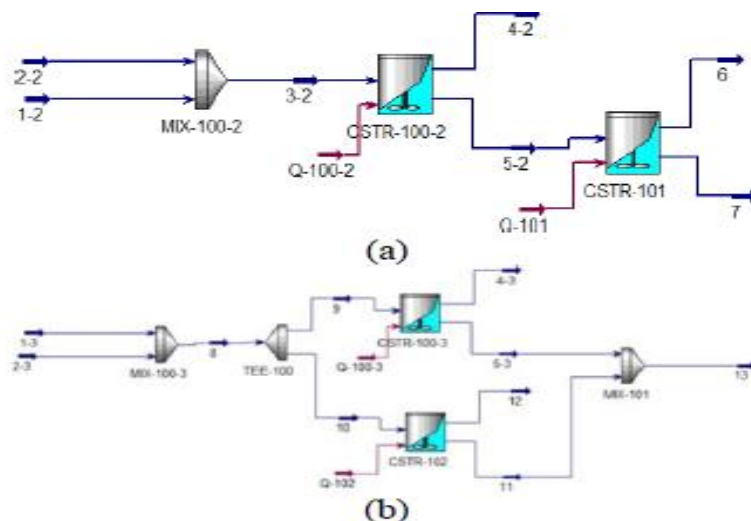


Figure 5. Reactor configuration in the HYSYS simulation (a) Series; (b) Parallel.

Table 3. HYSYS Simulation Results on the CSTR Configuration

Reactor Configuration	Conversion (%)	
	Reactor I	Reactor II
Series	43.38	31.09
Parallel	60.53	60.35

The results of the simulation indicating that the Continuous Stirred-Tank Reactor (CSTR) operates in parallel rather than series demonstrated a greater conversion rate of 60.53 percent for propylene oxide. Nevertheless, the average conversion rate for the parallel reactors remains unchanged at 60.53%. In contrast, the series configuration comprising two reactors calculates the conversion rate by aggregating all individual conversions that take place within those two reactors. It was determined that the two reactors in series achieved an aggregate conversion rate of 74.44%. The CSTR exhibited a higher conversion rate in series configuration, with outcomes comparable to those of the Plug Flow Reactor (PFR).

Impact of Reactor Temperature

The conversion of reactions is significantly impacted by the temperature of the reaction, as it dictates the kinetics and equilibrium of chemical processes [10]. In general, an increase in the temperature of the reaction results in a corresponding acceleration of the

reaction rate, which in turn enhances the conversion efficiency of the reaction. The outcomes of HYSYS simulations performed at different temperatures for CSTR and PFR reactors are displayed in Table 3.

Table 4. HYSYS simulation results with various reactor temperature

Temperature (°C)	Conversion (%)	
	CSTR	PFR
23.89	60.53	82.30
30	73.84	90.73
35	83.04	95.52
40	87.91	98.26

Table 4 demonstrates that increasing the temperature can enhance the conversion of propylene oxide in both reactors. Elevated temperature enhances the molecular kinetic energy, hence increasing the frequency of molecular collisions and aiding the breaking of chemical bonds, ultimately encouraging chemical processes. Thus, adjusting the reaction temperature can efficiently increase both the rate of reaction and conversion.

Impact of Reactant Ratio

The reactant ratio refers to the mole-to-mole proportion of any two chemicals participating in a balanced chemical reaction. Changes in the ratio of reactants can have an impact on both the speed and extent of chemical reactions. The results of HYSYS simulations performed on both types of reactors with different reactant ratios are presented in Table 5.

Table 5. HYSYS simulation results on various in reactant ratios

Reactant Ratios (H ₂ O : C ₃ H ₆ O)	Conversion (%)	
	CSTR	PFR
1:1	71.84	94.02
2:1	67.07	89.61
1:2	70.91	54.31

Table 5 demonstrates that the ratio of reactants has a substantial influence on the conversion of propylene oxide [16]. A rise in the ratio of H₂O to C₃H₆O is associated with a decrease in propylene oxide conversion in both types of reactors. The ratio of reactants can influence the tendency of reactants to interact and produce products. Suboptimal reactant ratios can lead to inefficient chemical reactions. Inadequate amounts of reactants below stoichiometric levels might hinder the production of products, resulting in reduced conversion. On the other hand, high concentrations of reactants can impede reaction rates because of competition amongst molecules, which is referred to as diffusion barriers.

Increasing the concentration of C₃H₆O with a reactant ratio of 1:2 resulted in a decreased propylene oxide conversion yield of 54.31% in the Plug Flow Reactor (PFR), compared to 70.91% in the Continuous Stirred-Tank Reactor (CSTR). The increased conversion rate in the Continuous Stirred Tank Reactor (CSTR) can be due to the agitation process, which guarantees homogeneous reactant concentrations over the whole reactor. As a result, the reaction can continue until it reaches a state of equilibrium. During propylene glycol manufacturing, surplus propylene oxide has a reaction with H₂O until a state of equilibrium is reached, resulting in high rates of conversion.

Conversely, in a Plug Flow Reactor (PFR), the reactants flow through the reactor in a single pass without undergoing continuous mixing during the reaction. As a result, any surplus propylene oxide has a short reaction with H₂O before leaving the reactor as a mixture of unreacted product and ethylene glycol. Due to the absence of equilibrium in reactions, the conversions in the PFR are reduced.

On the other hand, increasing the amount of H₂O can potentially improve the conversion of propylene oxide in the PFR. According to the data presented in Table 5, a rise in the H₂O ratio leads to a substantial improvement in conversion, increasing it from 54.31%

to 89.61%. However, the use of a continuous stirred-tank reactor (CSTR) leads to a drop in conversion. The observed disparity is attributed to the duration that the reactants reside in the plug flow reactor (PFR). By reducing this period, the reactants can undergo efficient reactions and achieve higher conversion rates.

In conclusion:

The results of a HYSYS simulation examining the production of propylene glycol from propylene oxide and water clearly demonstrate that the selection of reactor type, reactant ratio, reaction temperature, and reactor configuration have a substantial impact on the conversion of the reaction [10].

Out of the different types of reactors, the Plug Flow Reactor (PFR) exhibits higher conversion rates in comparison to the Continuous Stirred-Tank Reactor (CSTR). Based on the HYSYS models, the Continuous Stirred-Tank Reactor (CSTR) achieves a conversion rate of 65%, while the Plug Flow Reactor (PFR) achieves a higher conversion rate of 82.30%. Furthermore, the reaction temperature is crucial, as greater temperatures result in increased conversion rates.

The highest level of conversion is obtained when the reactant ratio is 1:1. This results in conversion rates of 71.84% for the CSTR and 94.02% for the PFR. On the other hand, when the ratio of reactants is increased, it is associated with a fall in conversion rates. In comparison to a parallel design, a series arrangement of CSTR reactors results in greater conversion rates. The overall conversion rate for the two reactors in series is 74.44%.

These findings can be practically applied to optimise propylene glycol production by guiding the selection of reactor type, setup, temperature control, and reactant ratios. Furthermore, this study establishes a foundation for future research focused on improving the effectiveness and long-term viability of propylene glycol production methods.

CHAPTER 4

OPTIMIZATION STRATEGIES

An amalgamation of optimisation strategies, enhanced design, and operational considerations are utilised to increase the output and performance of a reactor [17]. The following is a synopsis of essential approaches to achieve these objectives:

1. Reaction Kinetics and Mechanism:

- Understanding Reaction Pathways:
 - Investigate and comprehend detailed reaction pathways, kinetics, and mechanisms to optimize conditions for the desired product formation.

1.2 Catalyst Selection and Optimizations:

- Select or create catalysts that enhance the speed of chemical reactions, the degree of selectivity, and the overall effectiveness. Optimise catalyst parameters such as concentration, particle size, and distribution.

2. Reactor Design and Configuration:

2.1 Tubular Reactor Optimization:

- Optimise the shape, length, and diameter of tubular reactors to achieve effective mixing, ideal distribution of residence time, and homogeneous temperature profiles.

2.2 Flow Patterns and Mixing:

- Utilize methods to optimise fluid dynamics, promoting efficient blending and minimising differences in concentration. Investigate baffles, static mixers, or enhanced reactor designs to promote homogeneous distribution of reactants.

2.3 Heat Integration:

- Adopt effective heat integration strategies to maintain ideal temperature profiles. Consider utilizing heat exchangers or regulating heat transfer rates to boost energy efficiency.

3. Operational Conditions:

3.1 Temperature and Pressure Control:

- Ensure precise regulation of temperature and pressure to maximise reaction rates and achieve optimal equilibrium conditions. Avoid excessive circumstances that may induce undesired side reactions or catalyst deactivation.

3.2 Flow Rates and Residence Time:

- Adjust the rates at which substances flow and the amount of time they spend in a system to maximise the efficiency of converting them into desired products and the amount of product obtained. Ensure sufficient duration for reactions to fully occur without generating unwanted by-products.

4. Process Monitoring and Control:

4.1 Real-time Monitoring:

- Introduce real-time monitoring of critical parameters such as temperature, pressure, and concentration. Deploy sensors and feedback control to uphold optimal conditions.

4.2 Advanced Process Control (APC):

- Employ sophisticated process control strategies to flexibly adjust operating parameters, counteracting fluctuations and disruptions, and guaranteeing consistent reactor performance.

5. Experimental Analysis and Validation:

5.1 Continuous Improvement:

- Regularly perform empirical investigation to verify and improve theoretical models. This iterative technique promotes continuous enhancement in comprehending and optimising reactor behaviour.

6. Safety and Environmental Considerations:

6.1 Safety Protocols:

- Emphasize safety in reactor design and operation to prevent accidents and safeguard personnel well-being.

6.2 Environmental Impact:

- Evaluate the environmental impact of the process. Fine-tune reactor design and conditions to minimize waste generation and energy consumption.

7. Computational Modeling and Simulation:

7.1 Numerical Simulations:

- Employ computational modelling methods to replicate reactor behaviour across various situations. This facilitates the prediction of the effects of design alterations and the optimisation of operational variables.

7.2 Sensitivity Analysis:

- Perform sensitivity analyses to pinpoint key parameters influencing reactor performance, directing optimization efforts.

By employing a customised blend of these tactics, taking into account the distinct attributes of the response and reactor setup, industrial operations might attain substantial enhancements in performance, output, and general effectiveness.

ECONOMIC CONSIDERATIONS IN REACTOR DESIGN AND OPERATION

Effective reactor design and operation necessitate a comprehensive understanding of economic considerations to ensure sustainability and profitability.

1. Construction and Material Costs:

- Optimize material selection and construction techniques to strike a balance between durability and cost-effectiveness.

2. Energy Consumption and Efficiency:

- Assess and reduce energy consumption during operation to enhance overall process efficiency and cut down operational costs.

3. Catalyst Costs:

- Evaluate the cost-effectiveness of catalysts, taking into account factors such as lifespan, activity, and selectivity.

4. Operational Costs:

- Manage utility and maintenance expenses by implementing strategies to optimize resource consumption and facilitate straightforward maintenance.

5. Process Yield and Product Value:

- Maximize product yield and gauge the market value of the end product to offset operational costs.

6. Waste Management and Environmental Compliance:

- Consider costs linked with waste treatment and regulatory compliance, aligning with economic and environmental objectives.

7. Scale-Up and Production Volume:

- Explore economies of scale and design adaptability for efficient scale-up or downscaling based on market demand.

8. Research and Development Costs:

- Allocate resources for innovation and upgrades, recognizing the long-term cost savings and competitive advantages they offer.

9. Lifecycle Analysis:

- Factor in the total cost of ownership over the reactor's lifecycle, encompassing initial costs, operational expenses, maintenance, and potential upgrades.

10. Risk Management:

- Implement contingency plans to mitigate unexpected events and maintain economic stability.

CHAPTER 5

FUTURE TRENDS AND SUSTAINABILITY IN PROPYLENE GLYCOL

Various innovative technologies and research areas are now reshaping the propylene glycol industry. These advancements have the goals of enhancing production efficiency, expanding the range of uses, and addressing environmental issues [18, 19, 20]

1. **Methods for environmentally friendly synthesis:** Research is currently focused on developing sustainable and eco-friendly approaches for synthesising propylene glycol. This involves investigating bio-based precursors and employing new catalytic techniques to reduce the environmental footprint.
2. **Biotechnological approaches** refer to the use of microorganisms or enzymes to convert renewable feedstocks into propylene glycol, hence satisfying the growing need for bio-based products.
3. **Catalyst Development:** Ongoing research focuses on developing and improving catalysts to increase the speed and efficiency of reactions, the ability to choose specific products, and the overall effectiveness of propylene glycol synthesis. The goal is to create processes that are both more affordable and environmentally sustainable.
4. **Advanced separation and purification techniques** are being investigated to enhance downstream processing, enhance the quality of propylene glycol, and minimise energy usage in the production process.
5. **Application diversification** involves the identification of novel uses for propylene glycol, including in innovative materials, pharmaceuticals, and energy storage systems. This broadens the market potential of propylene glycol beyond its conventional applications.
6. **Process intensification** refers to the efforts being made to enhance industrial processes by implementing novel reactor designs, flow chemistry, and continuous processing. The goal is to increase productivity and decrease production costs.

7. Quality control and analytics in propylene glycol manufacturing involve the development of advanced analytical techniques and real-time monitoring systems. These tools provide precise control over reaction conditions and product properties, ensuring high-quality production.
8. Waste Valorisation: Research is focused on reducing waste and maximising its value by efficiently utilising by-products or transforming them into chemicals that have additional value, in accordance with the concepts of a circular economy.
9. Intelligent Manufacturing and Industrialization 4.0 Integration: The incorporation of Industry 4.0 technology, such as Internet of Things (IoT) sensors and data analytics, is enhancing process control in propylene glycol manufacture. This enables real-time modifications, predictive maintenance, and optimised utilisation of resources.
10. Emphasis is placed on adhering to ever-changing regulatory standards and sustainability criteria, which motivates the investigation of methods that reduce environmental harm and conform to progressively rigorous rules.

SUSTAINABILITY AND ENVIRONMENTAL CONSIDERATIONS IN REACTOR DESIGN AND CHEMICAL PROCESSES

Integrating sustainability and environmental factors into the design of reactors and chemical processes is an essential component of modern industrial practices [21, 22].

1. Principles of Green Chemistry: Reactor designs and chemical processes are developed in alignment with the principles of green chemistry, with a focus on minimising or eliminating the use of harmful compounds, reducing waste generation, and maximising energy efficiency.

2. Transitioning to renewable feedstocks involves a significant change that seeks to lessen dependence on fossil fuels and minimise the environmental impact of chemical operations.
3. Sustainable Catalyst Development: Catalysts are specifically engineered and enhanced to increase the speed and efficiency of chemical reactions, while also reducing their negative effects on the environment. This involves investigating catalytic systems that are both more environmentally friendly and more efficient.
4. Energy Efficiency and Heat Integration: Reactor designs prioritise the optimisation of energy usage, emphasising the implementation of heat integration technologies to efficiently capture and recycle energy. This approach aims to minimise overall energy consumption and mitigate greenhouse gas emissions.
5. Waste minimization and valorization are focused on reducing waste generation and finding effective techniques for treating, recycling, or extracting value from by-products.
6. Life Cycle Assessment (LCA): It is essential to take into account the complete life cycle of chemical processes, starting with the extraction of raw materials to the disposal of the final product. Life cycle assessments provide information that helps make decisions to optimise processes in order to minimise their environmental impact.
7. Regulatory Compliance and Certification: Our reactor designs and chemical processes consistently meet and surpass regulatory standards. We actively seek certifications in safety, environmental management, and sustainability to showcase our dedication to responsible practices.
8. Smart manufacturing and digital technologies allow for real-time monitoring and control, which enables exact modifications to optimise resource utilisation, minimise emissions, and improve overall sustainability.
9. Water and Resource Management: Efficient water utilisation is prioritised, and sustainable strategies for managing water resources are adopted. Moreover,

the optimal utilisation of alternative resources, such as primary substances and dissolving agents, is a crucial factor to take into account.

10. **Environmental Impact Assessments:** Thorough environmental impact assessments are carried out to identify possible environmental hazards and formulate plans for minimising their effects. This proactive strategy guarantees the implementation of responsible and sustainable practices.

11. **Public and Stakeholder Engagement:** The importance of being transparent and involving the public and stakeholders is highlighted. This promotes consciousness, responsibility, and cooperative endeavours to tackle environmental difficulties linked to reactor design and chemical processes.

THE EVOLVING ROLE OF NON-IDEAL REACTOR MODELS IN SHAPING FUTURE DEVELOPMENTS

The utilisation of non-ideal reactor models is becoming increasingly vital in influencing the future trajectory of chemical engineering and industrial processes [18, 19]

1. **Importance of Precision in Process Optimization:** Utilizing non-ideal reactor models provides a more precise depiction of the complexities seen in real-world scenarios, enabling accurate process optimisation. Gaining insight into variables such as mixing, heat transfer, and mass transfer discrepancies results in the development of more efficient and economically feasible systems.

2. **Improved Predictive Accuracy:** As models progress, they become more accurate in predicting outcomes by taking into account complex processes such as radial mixing, axial dispersion, and irregular fluid dynamics. This improvement helps to reduce differences between theoretical predictions and actual experimental outcomes.

3. **Customising Design for Heterogeneous situations:** The advancing models empower engineers to customise reactor designs for heterogeneous situations. This is essential in situations when the reactants or temperature profiles change

throughout the reactor, enabling the optimisation of conditions at different locations to achieve maximum efficiency.

4. **Minimization of Undesirable By-products:** Comprehending non-ideal behaviour aids in minimising the creation of undesirable by-products. Models that incorporate variables like as side reactions and incomplete conversions provide guidance for minimising waste production, hence promoting more sustainable and ecologically sensitive practices.

5. **Enhanced Safety Protocols:** The application of non-ideal reactor models also encompasses safety issues. These models help identify potential safety concerns by precisely detecting deviations from ideal behaviour. This leads to the creation of strong safety protocols and measures to reduce risks.

6. **Integration with modern Technologies:** Non-ideal reactor models are becoming essential elements of modern technologies, such as computational fluid dynamics (CFD) and artificial intelligence. This integration enables the use of more advanced simulations, which assist in the design and optimisation of reactors under various conditions.

7. **Comprehending Complex Kinetics:** Non-ideal models are crucial in deciphering intricate kinetics, particularly in complex reactions. Possessing this comprehension is vital for industries engaged in pharmaceuticals, specialty chemicals, and sophisticated materials, since it is imperative to have accurate management of reaction pathways.

8. **Progress in Renewable Energy Production:** Within the realm of renewable energy, the utilisation of non-optimal reactor models plays a significant role in the advancement of sophisticated systems for converting and storing energy. Gaining insight into the non-ideal behaviours exhibited by reactors utilised in renewable energy processes improves the overall efficiency of the system.

9. **Satisfying Rigorous Environmental Standards:** The changing role of non-ideal models corresponds with the industry's dedication to satisfying strict environmental standards. Industries can achieve sustainability benchmarks and

regulatory requirements by making precise predictions and effectively dealing with non-idealities in their processes.

10. Iterative Improvement through Experimentation: Non-optimal reactor models provide a continuous improvement process through experimentation. By validating models with real-world data, the insights obtained from the comparison guide ongoing refinement and optimisation, influencing the direction of future advances.

CONCLUSIONS

The study's findings about non-ideal tubular reactor models for propylene glycol synthesis signify a significant progress in the quest for enhanced efficiency, sustainability, and safety in the field of chemical engineering.

1. Enhanced Precision and Insight: The research improves the accuracy and depth of comprehension about intricate phenomena in tubular reactors. Gaining knowledge about non-ideal behaviours, such as the dynamics of mixing and variations in heat transmission, provides a deeper comprehension of the complexities involved in real-world reactor operations.
2. Efficiency Optimisations: Insights from the non-ideal reactor models offer a straightforward approach to optimising operational parameters. This optimisation directly improves the efficiency of the reactor, resulting in a more cost-effective and resource-efficient production of propylene glycol.
3. Environmental and Economic Impact: The study's consequences extend beyond technical concerns, including environmental and economic factors. The research aims to mitigate non-idealities, thereby advocating for sustainable methods, minimising waste generation, and enhancing the economic feasibility of propylene glycol production.
4. Enhanced Safety Protocols: The study reinforces safety protocols by identifying potential hazards linked to suboptimal reactor conditions. This

comprehension aids in the creation of resilient safety protocols, improving the safeguarding of individuals, and guaranteeing adherence to safety standards within the sector.

5. Incorporating sophisticated technology, such as computational fluid dynamics (CFD) and artificial intelligence, into non-ideal reactor models demonstrates a progressive approach. Engineers are provided with potent tools for designing, simulating, and optimising reactors through this combination.

6. Ongoing Enhancement via Validation: Iteratively validating non-ideal models against experimental data displays a dedication to ongoing enhancement. The iterative feedback process enhances current models and stimulates innovation, paving the way for future progress in propylene glycol manufacturing.

7. Driver of Industrial Progress: The collective research on non-ideal tubular reactor models greatly contributes to the advancement of the chemical industry. Researchers and engineers are addressing the difficulties presented by non-idealities to steer the sector towards resilience, sustainability, and technological progress. The simulations further validate that utilising a PFR configuration, sequential CSTR design, higher reactor temperatures, and ideal reactant ratios will significantly improve the efficiency of propylene glycol production, making it the most effective option to implement.

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