DYNAMIC SIMULATION OF CONTINUOUS POLYSTYRENE REACTOR USING PYTHON

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Dynamic Simulation of Continuous Polystyrene Reactor

Using Python

by

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TABLE OF CONTENT

LIST OF TABLES

LIST OF FIGURES

LIST OF SYMBOLS

Symbol	Description	Units
A_d	Frequency factor for initiator decomposition	h^{-1}
A_p	Frequency factor for propagation reaction	$L.mol^{-1}.h^{-1}$
A_t	Frequency factor for termination reaction	$L.mol^{-1}.h^{-1}$
D_0	Zeroth order moment of the dead polymer	
D_1	First order moment of the dead polymer	
D_2	Second order moment of the dead polymer	
E_d	Activation energy for initiator decomposition	K
E_p	Activation energy for propagation reaction	K
E_t	Activation energy for termination reaction	K
f_i	Initiator efficiency	
hA	Overall heat transfer coefficient	$J.K^{-1}.h^{-1}$
$-\Delta H_r$	Heat of polymerisation	$J.mol^{-1}$
[I]	Concentration of initiator	$mol.L^{-1}$
$[I_f]$	Concentration of initiator in feed	$mol.L^{-1}$
k_d	Reaction constant for initiator decomposition	h^{-1}
k_p	Reaction constant for propagation reaction	$L.mol^{-1}.h^{-1}$
k_t	Reaction constant for termination reaction	$L.mol^{-1}.h^{-1}$
M_m	Molecular weight of the monomer	$g.mol^{-1}$
M_w	Weight average molecular weight	
M_n	Number average molecular weight	
[M]	Concentration of monomer	$mol.L^{-1}$
$[M_f]$	Concentration of monomer in feed	$mol.L^{-1}$
[P]	Concentration of polymer	$mol.L^{-1}$
ρC_p	Mean heat capacity of reactor fluid	$J.K^{-1}.L^{-1}$
$\rho_c C_{pc}$	Heat capacity of cooling jacket fluid	$J.K^{-1}.L^{-1}$
Q_i	Flow rate of initiator	$L.h^{-1}$
Q_m	Flow rate of monomer	$L.h^{-1}$
Q_s	Flow rate of solvent	$L.h^{-1}$
Q_c	Flow rate of cooling jacket fluid	$L.h^{-1}$
Q_t	Flow rate of reactor	$L.h^{-1}$

T	Temperature of the reactor	K
T_c	Temperature of cooling jacket fluid	K
T_f	Temperature of the reactor feed	K
T_{cf}	Temperature of cooling jacket fluid feed	K
V	Volume of reactor	L
V_c	Volume of cooling jacket fluid	L
η	Intrinsic viscosity	

LIST OF ABBREVIATIONS

AIBN	Azobisisobutyronitrile
CFD	Computational Fluid Dynamic
CSTR	Continuous Stirred Tank Reactor
DEM	Discrete Element Method
DPM	Discrete Phase Model
FBR	Fluidised Bed Reactor
GA	Genetic Algorithm
GUI	Graphical User Interphase
IDE	Integrated Development Environment
LCA	Long Chain Assumption
MFI	Melt-flow Index
MWD	Molecular Weight Distribution
ODE	Ordinary Differential Equations
PD	Polydisperse Index
PI	Proportional Intergral
PVC	Polyvinyl Chloride
QSSA	Quasi-Steady-State-Approximation
TFM	Two-Fluid Model
VR	Virtual Reality

ABSTRAK

Wabak COVID-19 telah menyebabkan pergolakan global dalam beberapa cara dan dari pelbagai sudut pandangan. Salah satu bidang di mana senario ini mempunyai pengaruh yang besar ialah pendidikan. Ini disebabkan pelajar tidak lagi boleh berjumpa dengan profesor dan pensyarah secara peribadi. Amalan makmal Kejuruteraan Kimia tidak lagi dilakukan secara bersemuka dan secara manual. Untuk menangani isu ini, pendekatan alternatif yang membolehkan pelajar belajar dan menjalankan sesi makmal mereka sendiri adalah perlu. Akibatnya, simulasi komputer dianggap sebagai penyelesaian terbaik untuk masalah ini. Simulasi antara fasa pengguna model matematik ini mempunyai kelebihan tertentu kerana ia membolehkan pelajar menganalisis peralatan kos tinggi seperti reaktor polimer. Pelajar tidak didedahkan kepada teknologi kos tinggi di makmal biasa kerana sekatan pembiayaan. Mereka dapat memperoleh pengetahuan yang lebih baik tentang proses dan sifat yang berkaitan, walau bagaimanapun, dengan menggunakan simulasi. Proses utama dalam kerja ini ialah simulasi reaktor pempolimeran polistirena, dan penukaran monomer reaktor digunakan sebagai metrik penilaian utama. Tesis ini membentangkan pembinaan dan simulasi simulator reaktor pempolimeran larutan untuk polistirena dalam tangki kacau berterusan, CSTR, menggunakan Python 3.10. Penyelesaian berangka kepada persamaan pembezaan biasa, yang diekstrak daripada literatur, telah diselesaikan dengan mencipta modul yang digunakan bersama dengan modul NumPy, Scipy dan Matplotlib yang disertakan dalam Spyder, yang merupakan persekitaran pembangunan bersepadu (IDE) untuk Python. Python digunakan untuk menyediakan penyelesaian realistik yang mengambil kira kesan kinetik pempolimeran bukan linear yang dinyatakan dalam literatur. Penemuan mendedahkan bahawa pada keadaan yang dinyatakan, penukaran monomer maksimum kira-kira 73.97 peratus boleh dicapai pada masa operasi maksimum kira-kira 400 jam untuk menghasilkan polimer penyebaran poli dengan indeks 1.51, yang disahkan dengan nilai literatur dengan boleh diterima. peratusan ralat, iaitu di bawah 30%. Ia juga terbukti bahawa Python, seperti mana-mana bahasa pengaturcaraan lain, boleh digunakan untuk menjalankan eksperimen yang setanding dengan kejayaan yang sama. Kadar alir bendalir pemula, monomer dan jaket penyejuk telah ditetapkan sebagai pembolehubah dimanipulasi dalam simulator tersebutDalam tesis ini juga, kesan pembolehubah dimanipulasi ini pada reaktor polistirena juga dibincangkan menggunakan simulator reaktor pempolimeran polistirena berterusan, yang dicipta menggunakan Python. Telah diperhatikan bahawa penukaran monomer pempolimeran polistirena meningkat dengan

pembolehubah yang dimanipulasi, iaitu kadar alir isipadu pemula, monomer, dan cecair jaket penyejuk. Ia juga telah diperhatikan bahawa penukaran monomer pempolimeran mempunyai nilai tertinggi pada kadar alir pemula 150 L/j, kadar alir monomer 278 L/j, dan kadar alir bendalir jaket penyejuk 571.6 L/j. Kesan pengaliran bendalir pemula, monomer dan jaket penyejuk ke atas pembolehubah lain, seperti kepekatan monomer dan pemula, suhu reaktor dan jaket, kelikatan, berat dan nombor purata berat molekul, dan polidispersi, juga dikaji dalam tesis ini.

ABSTRACT

The COVID-19 epidemic has caused global upheaval in a number of ways and from a variety of viewpoints. One of the fields where this scenario has had a considerable influence is education. This is due to the fact that students can no longer meet with professors and lecturers in person. Chemical Engineering laboratory practise is no longer done face-to-face and manually. To address this issue, an alternative approach that allows students to study and conduct their own laboratory sessions is necessary. As a result, computer simulation is regarded as the best solution to this problem. This mathematical modelled user interphase simulation has certain advantages since it allows students to analyse high-cost equipment such as polymer reactors. Students are not exposed to high-cost technology in typical laboratories due to funding restrictions. They were able to obtain a better knowledge of the relevant processes and properties by using simulation. The primary process in this work is the simulation of a polystyrene polymerisation reactor, and the reactor monomer conversion is employed as the main evaluation metric. This thesis presents the building and simulation of a solution polymerisation reactor simulator for polystyrene in a continuous stirred tank, CSTR, using Python 3.10. The numerical solution to the ordinary differential equations, which was extracted from the literature, was solved by creating a module that was utilised in conjunction with the NumPy, Scipy, and Matplotlib modules included in the Spyder, which is an integrated development environment (IDE) for Python. Python was used to provide a realistic solution that takes into account the impact of the non-linear polymerisation kinetics stated in the literature. The findings revealed that at the stated conditions, a maximum monomer conversion of approximately 73.97 percent could be accomplished at a maximum operating time of about 400 hours to yield a poly-dispersion polymer with an index of 1.51, which is validated with literature values with acceptable error percentages, which is below 30%. It is also proved that Python, like any other programming language, can be used to conduct comparable experiments with equal success. The initiator, monomer, and cooling jacket fluid flowrates were set as manipulated variables in that simulator. In this thesis also, the effect of this manipulated variable on the polystyrene reactor is also discussed using the continuous polystyrene polymerisation reactor simulator, which was created using Python. It was observed that the monomer conversion of the polystyrene polymerisation increased with the manipulated variables, which are volumetric flowrate of initiator, monomer, and cooling jacket fluid. It has also been observed that the monomer conversion of polymerization has its highest value at 150

L/h initiator flowrate, 278 L/h monomer flowrate, and 571.6 L/h cooling jacket fluid flowrates. The effects of the initiator, monomer, and cooling jacket fluid flowrates on other variables, such as monomer and initiator concentration, reactor and jacket temperature, viscosity, weight and number average molecular weight, and polydispersity, were also studied in this thesis.

CHAPTER 1
INTRODUCTION

This chapter provides an overview of this study as well as the significance and importance of simulation of polymerisation reactors. In general, this chapter outlines the simulation research background, the problem statement, the objectives, and the scope of work for this final year project.

1.1 Virtual Laboratory for Polystyrene Polymerisation Reactor

The primary function of the engineering profession is to manipulate materials, energy, and information to benefit humanity (Feisel and Rosa, 2005). The overarching purpose of engineering education is to prepare students to perform engineering. Thus, instructional laboratory has been an integral element of undergraduate and, in some cases, graduate engineering education from their inception. Indeed, before the emphasis on engineering science, most engineering training may be considered to have taken place in the laboratory. The focus on laboratories has changed significantly over time.

The arrival of two phenomena in the last two decades, the digital computer and distant learning methods, notably through the Internet, has complicated laboratory instruction (Feisel and Rosa, 2005). The most difficult task for both universities and educators are determining how to integrate "actual" laboratories on the Internet (Balamuralithara and Woods, 2009). It is a challenging task to bring the laboratory learning environment online, but with the tremendous improvement of communication technology, it is getting simpler. Simulation environment lab, automated data acquisition, and online remote control of instrumentation are examples of new possibilities in the way lab sessions are accomplished (Balamuralithara and Woods, 2009; Feisel and Rosa, 2005).

There are two methods for conducting virtual laboratories online, which are simulation laboratories and remote laboratories. For explaining and reinforcing concepts, simulations have been proven to be identical to real-life laboratories. Even so, it only allows for a limited amount of exploration. The second option allows students to operate on real equipment and instrumentation that is remotely accessible through the Internet or online. Both approaches are

considered virtual laboratories since they do not involve any direct interaction of the user with the equipment.

These virtual laboratory programming often comprises the definition of the mathematical model as well as the virtual laboratory view. The user-to-model interface is the virtual laboratory view (Martin et al. 2008). Its purpose is to offer a visual representation of the model's dynamic behaviour and to make interactive operations on the model easier for the user. Model behaviour may be expressed in a variety of ways. Plotting the model variables against one other, for example, and using animated schematic representations of the system. There are plenty of programming software which could simulate and replicate the fundamental concept of actual world engineering works for study purpose such as MATLAB, Python, Tuner, Aloha, Anova, Aspens Plus and so on.

A component and example of numerous of these Industrial Revolution (IR) 4.0 concepts and technologies is computer simulation (Grodotzki et al., 2018). Computer simulation is used in hybrid modelling, simulation-based training, data analysis, developing connections such as network simulation, and simulation-based product design. Simulation is critical to achieving the objective of Industry 4.0 as well as the vision and purpose of the engineering profession. This is since learning in the engineering profession is significantly influenced by a variety of variables. Unfavourable and uncertain global conditions are one of the reasons. For instance, the Covid-19 epidemic has had a significant impact on engineering learning processes. It also has an impact on students' grasp of lessons and theories, particularly in laboratory sessions. As a result, computer simulation might be an option for this scenario, assisting students to study and continue their learning processes in the engineering field.

Ouyang et al. (2018) have briefly examined the principle of computer simulation. For chemical engineering students, a Unity3D-based virtual simulation was being constructed. This simulation is a virtual and integrated technical process landscape of practical learning. The goal of this simulation is to assist and improve the production practise of students in the chemical engineering profession. This virtual simulation based on Unity3D recreates genuine chemical plant sections. This simulation assists students in gaining an overview of structure demonstration, comprehension of fluid property and flow direction in pipeline, as well as operating principles of key plant equipment. This simulation fundamentally increases students' comprehension of chemical processes while also training their operational abilities. Aside from that, this Unity3D-based virtual simulation simulates virtual mishaps that might occur in a plant

and alternative solutions to such incidents. Eventually, this will raise students' safety production awareness and capacity to respond to such circumstances. According to the feedback from these chemical engineering students, this virtual simulation is quite successful in helping them grasp the chemical processes and equipment.

Since virtual laboratories would be the best option to substitute for high-end process equipment involved in experiments to avoid any safety and economic issues, the polymerisation process is chosen as a case study in this study. Polymerisation is a sort of chemical process that is widely utilized on an industrial scale all over the world to produce a wide range of lattices for use in the production of resins and solvent-free paints that are simple to use owing to their high fluidity. Styrene monomer is one of the petrochemicals intermediates whose demand is continually growing. It is most involved in the manufacturing of plastics, synthetic rubber, and lattices. Crystal (unmodified) polystyrene (GPPS), rubber-modified polystyrene (HIPS), styrene-acrylonitrile copolymer (SAN), and rubber-modified styrene-acrylonitrile copolymer (SAN) are the most common styrene plastics (ABS). The automotive, electronics, and packaging sectors all have major and rising markets for these polymers. The free-radical, anionic, cationic, and Ziegler processes could all be used to produce crystal polystyrene, but only the free-radical approach is of substantial economic significance(Chen, 1994).

Styrene polymerizes easily into polystyrene through a simple free radical chain process. Polymerisation will begin with either heat or initiators. Thermal decomposition of initiators results in the formation of active free radicals that are efficient in initiating the polymerisation process. Benzoyl peroxide and di-tert-butyl per-benzoate are common initiators used in the suspension procedure. Styrene monomer will react with itself to produce a homopolymer in the presence of inert components. Styrene monomer reacts with several different monomers to generate a range of copolymers. Polystyrene is an odourless, tasteless, rigid thermoplastic. Pure polystyrene has the following structure:

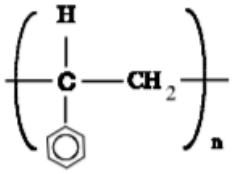

Figure 1 Polystyrene structure.

The polymerisation reactor plays an important role in the polymer and chemical engineering industries. Polymerisation reactor models have been extensively used to assess the efficacy of different control measures such as coolant inlet temperature, initiator concentration, and monomer concentration. Polystyrene polymerisation is a form of radical and solution polymerisation. Polystyrene polymerisation is an exothermic process that emits heat into the surrounding environment, which would be one of the major worries when this equipment is handled by students for educational purposes. This can be avoided by using a virtual laboratory since it is very safe environment. Polymerisation reactions are well-known as frequent sources of thermal runaway in fine chemical industries due to their high exothermicity and gel effect. Furthermore, unfavourable secondary reactions in polymerisation, such as chain transfer to monomer, increase the probability of heat runaway.

To avoid this scenario, proper monitoring and control mechanisms for the polymerisation reactor should be implemented. To get a proper monitoring and control system, some experiments and trials need to be done so that the reactor can operate at its optimum with good control systems. Since polymerisation reactors are designed to be operated under extreme conditions, the cost of the reactor and the whole setup is very costly, so by using a virtual laboratory setup, this cost can be cut off. Besides, this also cuts the cost of the raw material and catalyst purchase, plus students or users can do the experiments countless times since they are totally free and there is no time limit.

Thus, this thesis is primarily concerned with the dynamic simulation of a continuous styrene polymerisation reactor. Styrene is the monomer used in polystyrene polymerisation. The solvent was toluene, and the initiator was azo-bis-isobutyronitrile (AIBN). The process requires high-performance control of input variables such as volumetric flow rate of monomer, initiator, and cooling fluid due to the complexity of this process. This simulation will aid in viewing and monitoring the reactor. Python was chosen as the programming language and platform for simulating the polystyrene polymerisation reactor. Python was selected because it is open source and may be executed on any computer platform. Furthermore, it includes a vast library of modules such as NumPy, SciPy, Matplotlib, and Tkinter, which are required for building simulations of a polystyrene polymerisation reactor.

1.2 Problem Statement

This COVID-19 pandemic has caused worldwide disruption in a variety of ways and perspectives. Education is one of the sectors where this scenario has had a significant impact. This is because students can no longer attend face-to-face sessions with instructors and lecturers. Laboratory practise, as specified for Chemical Engineering, is no longer done face-to-face and manually. To solve this issue, an alternate solution is required in which students may still study and execute their individual laboratory sessions effectively. As a result, process simulation is considered the best option to solve this issue. Students can still perform their experiments virtually and be exposed to the ethics of traditional laboratory sessions by using process simulation. This process simulation offers certain advantages since simulation provides a platform for students to evaluate high-cost equipment. Due to financial constraints, students are not exposed to handling high-cost equipment in traditional labs. However, using simulation, they were able to gain a better understanding of the respective processes and characteristics. The modelling of a polystyrene polymerisation reactor is used as the major process in this study, and the reactor monomer conversion is used as the evaluating parameter. At the end of this research, it will show and discuss how this polymerisation reactor operates in a real plant, as well as examine the effect input flowrate of initiator, monomer, and cooling fluid to polystyrene polymerisation in continuous mode.

1.3 Research Objectives

1. To implement Python programming language on solving the ordinary differential equation of the polystyrene polymerisation reactor.
2. To build a dynamic simulator using a GUI for a continuous polystyrene polymerisation reactor using the Python programming language.
3. To study and investigate effect of volumetric flowrate of initiator, monomer, and cooling jacket fluid on the polystyrene polymerisation reactor simulator.

1.4 Scope of Thesis

The usage and demand of virtual labs has been rising over the past 2 years. This might be due to the distance learning system and also some hands-on experiments that require high-cost equipment, such as polymerisation. Thus, building virtual labs such as simulation labs would be the best way to solve this. The scope of this thesis is to build a simulator for a continuous polystyrene polymerisation reactor that could replicate the actual polymerisation plant's outcome. In order to build an effective training simulator, the Python programming language is used due to its wide availability.

The simulated results were compared and validated with literature values to ensure that the simulator produces the actual polystyrene polymerisation plant values. Then, the volumetric flowrate of initiator, monomer, and cooling jacket fluid were set as manipulated variables in the simulator. Thus, users can experience the changes in the simulated result due to the effects of manipulated variables. At the same time, users could understand more about the effects of manipulated variables on the responding variables: monomer and initiator; reactor and jacket temperature; monomer conversion; intrinsic viscosity; polydispersity index; number average molecular weight; and weight average molecular weight.

CHAPTER 2
LITERATURE REVIEW

The idea and concept of polystyrene polymerisation and the evolution of virtual laboratory in engineering disciplines were explored briefly in the earlier chapter. In Chapter 2, the different types of laboratories, different forms of simulation, simulation done for a polymerisation reactor, the value of Python, and how to use Python in engineering are discussed.

2.1 Traditional Laboratory VS Virtual Laboratory

The laboratory session also served as a platform for good engineering practise prior to working in an industrial facility. Basically, there are two types of laboratories which is traditional and virtual laboratory. Traditional laboratory, also known as instructional is described as a session in which the laboratory equipment must be physically set up and the students who do the laboratory are physically present in the lab. Traditional laboratory sessions assist students in learning more about the nature of a process and its design. When students practise engineering concepts and theories in a traditional laboratory, they will gain a better understanding of them. Furthermore, students will be able to compare the measurement and findings acquired with experimental data and will investigate the causes if the values of the results differ or diverge from each other.

As mentioned before, this traditional laboratory faces some challenges such as time constraint, need physical present of student which may be difficult to distant students and also most of academy institutions just let half of their student to enter the laboratory due to this Covid-19 pandemic, besides, some equipment is expensive, dangerous, sensitive and also requires huge space, of experimental infrastructure (Aşiksoy and Islek, 2017; Balamuralithara and Woods, 2009; Feisel and Rosa, 2005). To overcome these problems, instructors and institutions are tried to come up with virtual laboratory as an alternative. There are two types of virtual laboratory which are remote and simulation laboratories.

The remote lab implements the technologies of distance learning. In other words, a remote lab is a sort of system that utilises a computer-based technology to allow students to engage with a physical laboratory by providing access to the real equipment in the laboratory

through the Internet (Mosterman et al., 1994). This sort of lab allows students to transmit commands that are pre-processed on their end. The experiment will then be run through the server and executed in the physical lab on real equipment. The generated findings of the experiment will be displayed to the learner. The sole difference between a remote lab and a typical lab is the distance between the experiment and the person carrying out the experiment. The remote lab allows students or users to conduct experiments from anywhere as long as their computer attach with the physical lab server.

Simulation labs are digital representations of real-world investigations that take place in real laboratories. All the information and inputs needed for laboratories are simulated in computers using various simulation tools and computer programming languages such as MATLAB, Aspen Plus, Tuner, Aloha, Anova, and Python (Martínez et al., 2011). Simulation labs can deal with the high expenses and costs associated with regular laboratories. Simulation labs help reduce the amount of time required to conduct out experiments and understand the results of such experiments. Furthermore, simulation laboratories establish a pathway for active learning, which eventually increases students' experiment performance. The benefits of simulation labs to students and schools include portability, simplicity of use and handling, simple accessibility, and cost efficiency.

As conclusion, simulation labs and remote labs are alternatives to regular labs. However, in terms of cost effectiveness and equipment requirements, the simulation lab outperforms the remote lab. In this study, a simulator of a polymerisation reactor for polystyrene polymerisation in continuous mode will be built, which will help the simulation lab.

2.1.1 Comparison between Traditional and Virtual Laboratories

Due to the general rising expense of hands-on laboratories and the rise in distance education, the use of virtual laboratories in scientific laboratories has become an increasingly important problem. Recent studies have looked at the use of virtual laboratory tools to enhance traditional hands-on labs, however many virtual tools have not been employed as substitutes. Here are the detailed comparison between traditional and virtual laboratories.

2.1.1.1 Accessibility

In simulation labs, students or users can interact with the material and conduct experiments at any time. The accessibility of materials and the ability to conduct an experiment in remote laboratories is the same as in simulated labs, although it is largely dependent on the timetable. Traditional laboratories, on the other hand, limit students to using equipment and doing experiments in 2-3 hours weekly lab sessions. In remote and simulation labs, users can work with equipment and experiment for longer periods of time than in usual 2–3 hours weekly lab sessions. When compared to regular laboratory sessions, remote and simulation laboratories allow access to persons with physical and psychological limitations.

2.1.1.2 Student-Instructor contact time

Simulation labs and remote labs reduce the amount of time students and instructors interact among each other. In other words, simulation and remote labs are asynchronous and reducing student-instructor communication. Furthermore, this is becoming an impediment to students asking questions about the experiment to the instructor. However, this benefits students since they can learn and obtain information independently. They can learn more about the principles and procedures of the experiments by doing themselves.

2.1.1.3 Growth Potential

Due to facility limitations, students in traditional labs are unable to handle all equipment in the lab. This difficulty could be solved in simulation and remote labs since students will have a clear idea of how to utilise the equipment through video lessons, animation, and lab instructions. Furthermore, conventional labs have restricted space due to inadequate facilities. However, simulation and remote lab would provide a platform for students to conduct numerous experiments while having access to varied equipment. Late Nite Labs, for example, is a start-up that provides virtual lab settings with over 100 experiment alternatives.

2.1.1.4 Safety

Traditional laboratories focus not just on conceptual learning but also on procedural abilities. In other words, when students do hands-on experiments with

equipment, safety is an important factor to consider in conventional laboratories. To control hazards, every experiment and piece of equipment in a typical lab must follow Safety Operation Procedure (SOP). Given this, standard lab research may be limited, and schools may need to spend more money on safety. However, safety difficulties can be solved in simulation and remote laboratories since students do the experiment digitally and from a safer distance than in traditional labs.

2.1.1.5 Cost

The cost of a laboratory varies depending on the institution. For traditional laboratories, students must pay lab fees and acquire a lab manual in certain scenarios, although other institutions do not charge lab costs. Maintenance and safety equipment are two factors that highlight laboratory costs. When students execute the experiment manually in a typical lab, the university must spend more money on equipment service. Furthermore, institutions must invest in additional safety equipment to safeguard the safety of students in conventional labs. Since the studies are frequently done digitally by students in remote and simulation labs, these problems may be addressed.

2.2 Types of Simulation

A computer simulation (or "sim") is an attempt to replicate a real-life or theoretical system on a computer so that the system can be investigated. Simulation is the concept of utilising mathematical modelling as the theoretical basis for specific chemical processes. This simulation is then designed to solve the equations associated with the processes, allowing us to gain the necessary information about the performance and parameters involved in specific chemical processes. Process simulation, also known as process flow sheeting, refers to the use of computer tools to conduct in steady-state and dynamic mode (unsteady-state), mass balance, momentum balance, energy balance, sizing of unit activities, and costing calculations for a chemical process (Skorych et al., 2017). Process simulation is typically used in chemical plants for the following purposes: modelling of process behaviour, sensitivity and economic analysis, process optimization, and process control.

Nowadays, simulation is regarded as the finest option and alternative to traditional and remote laboratories. This is because simulation helps students boost data analysis abilities as well as analyse experimental data (Balamuralithara and Woods, 2009). Simulation is an

effective tool for assisting students in designing and doing experiments in a systematic manner in the least amount of time to decrease operational expenses while maintaining the accuracy of results. One of the most important learning outcomes in undergraduate education is the capacity to act autonomously, and its level is closely proportional to confidence earned while studying. Aside from that, students can use simulation tools such as MATLAB, Aspen Plus, Tuner, Aloha, Anova, Python, and others. Simulation may be classified into three types. That are live simulation, virtual simulation, and constructive simulation.

2.2.1 Live Simulation

The live simulation is a real-life adventure brought into the classroom using distant learning technology. These live simulations are often held in their respective locations using the internet and video conferencing technology. The learning method is a student-cantered, team-based, interactive educational experience that encourages students to solve issues using scientifically correct facts (Dyrberg et al., 2017). A live simulation performed by the flight director and students from Wheeling Jesuit University's Challenger Learning Centre. Teachers conduct a pre-mission preparation for their students prior to the live simulation, which encompasses all mission materials required for the ultimate "live" event. On the mission day, students assemble emergency response teams. Teams communicate with a flight director at mission control in Wheeling using the Internet and video conferencing technology. While the event is unfolding, the emergency response teams collaborate and communicate with mission control to tackle a "live" problem. New data is provided to the classroom every few minutes. Student’s compute, draw graphs, appraise the scenario, and make judgments based on their data analysis.

2.2.2 Virtual Simulation

Immersive multimedia or a computer-simulated environment that may imitate physical activity in places in real or projected circumstances are examples of virtual simulation (Padilla et al., 2018). In chemical engineering, virtual simulation is used to simulate and visualise genuine industrial processes on computers by using numerical techniques to solve the

mathematical equations of physical models. This enables chemical engineers to develop, scale-up, optimise, or regulate processes online and in real time, eliminating the need for repeated experiments in various phases including trial and error. Students at the University of Southern Denmark, for example, utilise a virtual simulation software called 'Labster' (Padilla et al., 2018). Students from the University of Southern Denmark used virtual simulation to execute High-Performance Liquid Chromatography (HPLC) to analyse chemically diverse chemicals using various column combinations. They utilized virtual simulation parameters such as phase, solvent type, and temperature. In a real laboratory, each modification of a component would need minutes to hours of system equilibration before it was ready for the next investigation.

2.2.3 Constructive Simulation

Constructive simulation is a simulation in which simulated individuals interact with simulated systems. Real individuals may provide feedback, but they will not be involved in selecting the simulation's outcomes. Constructive simulation will assist users in predicting probable simulation outcomes, analysing corresponding ideas, taking appropriate measurements, generating data and statistics, and performing analysis. In land force operations, an example of constructive simulation is employed. Selvaag et al., (2017), created an easy-to-use web-based graphical user interface (GUI) framework for manipulating Virtual Battle Space, VBS simulated constructive elements. They created capabilities to control indirect fire entities as well as manoeuvring entities. Since simulations are solely used for testing and analysis, the system has been designed to require least amount input from the operators as possible.

2.3 Simulation for Polymerisation Reactor

Polymerisation experiments are more likely to be carried out using simulation than traditional laboratory methods. This is due to the fact that the cost of raw materials that would be used in polymerisation is high. By doing so, virtually it can be neglected. Besides, the operating conditions of polymerisation are very extreme, which may require some experts or technicians to be on site while a student or researcher is conducting their experiment. By doing

this in simulation, the safety of them is ensured. Furthermore, the cost of the equipment itself is very costly. Thus, some institutions cannot afford to prepare that set up for polymerisation. So, as a solution to these criteria and scenarios, the simulation laboratory takes place.

Reginato et al., 2003 developed dynamic mathematical model and simulation for a liquid-phase propylene reactor. This simulation done for a non-ideal continuous stirred tank reactor model (CSTR). Nonlinear hydrogen influence on polymerisation rate and non-idealist produced by polymer segregation are both considered for dynamic modelling to produce good simulation results. Besides, the simulation results were compared to plant data from OPP Qu'mica S.A for parameter estimation and model validation. For a better output result, several dynamic factors like as molecular weight distribution (MWD) and melt-flow index (MFI) are added in this model. Finally, the simulation was developed using MATLAB and SIMULINK with the language C in S-functions (Reginato et al. 2003).

Almeida et al., (2007) constructed a mathematical model to predict the steady-state and dynamic behaviour of a continuous process involving free radical polymerisation of styrene. The kinetic and thermodynamic models receive special attention, with the most sensitive parameters evaluated utilising data from an industrial plant. The thermodynamic model is derived on a cubic equation of state as well as a mixing rule applied to the low-pressure vapor-liquid equilibrium of polymeric solutions, and it is suitable for modelling auto-refrigerated polymerisation reactors that use the vaporisation rate to remove reaction heat from exothermic reactions. When compared to plant data, the simulation results demonstrate that the proposed model has a strong predictive potential for conversion, average molecular weights, polydispersity, melt flow index, and thermal properties for various polymer grades. (Almeida et al., 2007.).

Bhat et al., (2004) simulated and optimised the continuous tower method, a prominent industrial polystyrene production method. A kinetic model for the thermal polymerisation of styrene was developed, which takes into consideration the Trommsdorff effect and the volume change associated with the process. This was used to develop model equations for the tower's continuous flow stirred tank reactor (CSTR) and plug flow reactor. Under defined operating parameters, the model can estimate monomer conversion, number-and weight-average molecular weights, polydispersity index (PD), and temperature at various places in the unit. This approach was additionally optimised for multiple goals using an application of a genetic algorithm (GA). The two goals were to maximise the final monomer conversion and minimise

the product's PD. The CSTR conversion was confined to occurring within a particular range, and a polymer with a defined number-average molecular weight was to be created (Bhat et al., 2004).

Okullo et al., (2017) used Python 3.5 to model and simulate a suspension polymerisation in an isothermal reactor for methyl methacrylate to yield poly methyl methacrylate. The numerical solution to the ordinary differential equations was achieved by creating a custom module that was utilised in conjunction with the NumPy and matplotlib modules. Python was used to create a realistic solution that takes into account the gel, glass, and cage effects that affect the non-linear polymerisation kinetics stated in the literature. The findings revealed that at the stated conditions, a maximum monomer conversion of about 92.8 percent could be accomplished at a minimum batch time of about 2.2 hours to generate a polydisperse polymer with an index of 27 (Okullo et al., 2017).

Schneiderbauer et al., (2017) used Lagrangian-Eulerian hybrid model for olefin polymerisation fluidized beds. The Lagrangian-Eulerian hybrid model is made up of the Lagrangian discrete phase model (DPM) and a coarse-grained two-fluid model (TFM). On the one hand, the DPM model provides information like the local particle size distribution. TFM provides information on inter-particle stresses. This hybrid technique also permits efficient particle-level assessment of gas-solid processes. This hybrid model aids in understanding olefin polymerisation in terms of catalyst profile, pressure-driven polymer particle solubility, particle crystallinity, and the accompanying reaction masses and reaction heat. Furthermore, the model can forecast particle development in a fluidized bed reactor as well as its influence on the bed's hydrodynamics. The findings also provide more information regarding the temperatures and crystallinity of the polymer particles. CFD-DEM (CFD: computational fluid dynamics; DEM: discrete element method) simulation was utilised for this model (Schneiderbauer et al., 2017).

Lee et al., (2018) developed a dynamic simulation model with mass balance, energy balance, and complex polymerisation kinetics for commercial scale batch reactor. As compared to reference data, simulation results were validated with less than 10% marginal error. To study the effect of monomer initial concentration, the simulation was run with eight different initiator and monomer starting concentrations. The simulation findings aided in predicting the operating conditions for the targeted product. The results were compared to other reference data and found to be in good agreement. According to the findings, the approach and results of this study

may be utilised to scale up a polymerisation batch reactor from the early stages of design (Lee et al., 2018).

Herrera et al., (2019) developed semi-batch reactor that consists of highly nonlinear equations and functions. The model's input control variables were set to coolant, monomer, and initiator feed flow. The simulation was built as the monomer was initially fed into the reactor, followed by initiator feeding after two hours. This is done to guarantee that an initial polymer chain is generated, and that the polymerisation rate remains consistent. As a consequence of the simulation, the reactor temperature remained nearly constant at 345 K after the heating procedure was completed. This simulation shows that the reactor temperature tends to decline near the completion of the reaction due to monomer build up. The simulation output was then compared to industry data while taking viscosity and solid content into consideration (Herrera et al., 2019).

El-Helw et al., (2019) choose PVC polymer reactor as case study and mainly the heat transfer in polymer reactors has been investigated. The simulation was based on energy balance equations. The investigation of various ways of heat transmission in jacketed agitated vessels, as well as the effect of changing agitators on heat transfer, is suggested. For each scenario, a computer programme is developed to measure the heat transmission parameters and the heat duty required. As the first phase, an energy balance model was developed and implemented in Microsoft Excel to calculate heat transport behaviour. The model was then simulated using the VISIMIX simulation software version turbulence SV. In addition, Aspen HYSYS V8 is used to simulate the chemical process (El-Helw et al., 2019).

Sbaaei et al., (2020) used Polymers Plus v.9 as software to simulate the gas-phase propylene homopolymerisation to create a model for an existing fluidized bed reactor, FBR. However, hydrodynamic parameters were considered in this simulation to produce more realistic findings. The hydrodynamic characteristics, which describe the real fluidization condition of the plant FBR, were included in this model. Data from the industrial homopolymerisation unit under examination was gathered to create and validate the FBR model to match the plant's FBR performance (Sbaaei et al., 2020).

Muhammad et al., (2021) investigated on melt Flow Index and reactor temperature are most focusing control objective on LDPE tubular reactor. For most cases, the initiator flow rate or jacket flow rate will be controlled as a variable in temperature control to keep the reactor temperature stable and prevent temperature runaway. Flow rates of initiator one and initiator

two are chosen as manipulated variables MV1 and MV2) in this article to regulate maximum reactor temperature in zones three and five (CV1 and CV2). To validate the model, the needed data was extracted from the original case study and compared to the results of the simulation run. MATLAB Simulink was the programme used to simulate the LDPE tubular reactor (Muhammad et al., 2021).

Mokhtarname et al., (2021) done a dynamic model and controlled an existing industrial continuous bulk free radical styrene polymerisation process to test the performance of auto refrigerated CSTRs. Controlling the high viscosity reactor contents and heat removal is one of the most challenging ones in polymerisation processes. Temperature control of an auto refrigerated CSTR is performed in this work employing an alternate control technique that takes use of a vacuum system connected to the condenser. The created model is then validated using experimental data from a real-world operating plant. A popular control method employed in some earlier research is also simulated to demonstrate the heat removal capabilities of this control system. The simulation findings illustrate which control system has quicker dynamics and greater performance. Furthermore, for the polymerisation process under investigation, a nonlinear model predictive control (NMPC) is designed to give improved temperature control while maintaining the input/output and heat exchanger capacity limitations on heat removal. Then, using some typical tuning principles, a comparison with the standard proportional-integral (PI) controller was done. Some simulations are also used to perform robustness and stability studies of the control methods under consideration. MATLAB is the simulation programme utilised in this work (Mokhtarname et al., 2021).

2.3.1 Simulation in Other Fields

Yuniarti et al., (2017) developed a Virtual Laboratory based on interactive multimedia on the sub material of planting and painting bacteria. Knowing the media's eligibility and the student's response that has been taught of utilising Virtual Laboratory. The research approach used in this study is development research. This study is divided into two stages: preliminary (planning and design) and formative assessment (self-evaluation, expert reviews, small group, and fields test). Questionnaires and tests were utilized to collect data for this study. This study's participants include 37 students. Virtual Laboratory is classified as valid based on the validation results from the validator expert. This value is acquired because Virtual Laboratory

can be installed on a variety of hardware and software, is simple to use, the application works well, and Virtual Laboratory has a distinctive shape, interactive features, and good animation. Meanwhile, students answer positively, indicating that they may use Virtual Laboratory to operate and mimic the experiment of planting and painting bacteria, allowing them to better comprehend the material of planting and painting bacteria. As a result, it is possible to infer that Virtual Laboratory is legible for use as a learning medium (Yuniarti et al., 2017).

Ismail et al., (2016) developed a STEM-based virtual lab as an alternate media for enhancing scientific literacy in junior high school pupils on the topic of water pollution. Define, Design, Develop, and Disseminate are the 4 Ds used in development. Following implementation, the efficacy in enhancing scientific literacy was assessed using a one-group pretest-posttest approach. PISA 2012 describe stage difficulties, KDs, and STEM features were examined. During the design process, flowcharts, storyboards, and user interfaces were created. The development phase comprises the design of virtual labs as well as validation by a media specialist and a scientific instructor. The dissemination phases of this research will be confined to two classes of junior high school students. The results of media expert validation and scientific teacher validation demonstrate that STEM-based virtual laboratories that have been constructed perform very well in the feasibility study, with a percentage of 86.24 percent for media experts and 82.71 percent for science instructors. The results demonstrate that implementing the STEM-based virtual lab that has been built will improve students' scientific literacy with a substantial increase (N-gain) in class 7B of 0.46, which falls into the medium category, and class 7D of 0.29, which falls into the medium category (Ismail et al., 2016).

2.4 Importance of Python

Python is a great general-purpose, high-level programming language with simple syntax (Rashed and Ahsan, 2012). Python is a programming language that emphasises code readability, lowering the cost of system maintenance. Python is the only major programming language that uses indentation to create code blocks. Python has many built-in data types such as strings, lists, and dictionaries, as well as modules, classes, exception handling, automated memory management, multiprocessing, and parallel computing capabilities. Python is a dynamic typing and binding programming language since variables are not assigned a type in Python where dynamic typing postpones determining the class to which an object belongs until

the programme is running while, dynamic binding postpones determining which method to invoke on an object until programme execution time. Instead, it accepts the type of the object that is presently allocated to it.

As compared to other programming languages such as Java, C++, and FORTAN, Python always has an advantage due to its capabilities and countless benefits (Holkner and Harland, 2009). In contrast to other programming languages, Python emphasises the simplicity of scripting paradigm and the convenience of code reuse. Furthermore, Python provides advantages such as unrestricted type checking, an abundance of flexibility, reliance on global data, and the availability of a low-cost compiler. The sole problem of Python is that it is an interpreted language, which causes it to be sluggish.

Additionally, Python may use as an extension language for existing modules and programmes that enable a programmable interface. It supports a wide range of programming paradigms, including object-oriented, imperative, and functional programming approaches. Python includes all main scientific libraries, either as part of the standard library or as a third-party open-source library. The following are the most often used Python libraries or modules for scientific computing; SciPy, NumPy, SymPy and Matplotlib. SciPy is an open-source algorithm and mathematical tool library for the Python programming language. It includes modules for optimization, linear algebra, integration, interpolation, special functions, Fast Fourier Transformation, signal and image processing, ODE solvers, and other typical scientific and engineering activities. NumPy is a module that adds more math skills that supports multidimensional. It introduces new data types such as long integers of infinite length and complex numbers. It also contains a new array data type that encourages the creation of vectors and matrices. SymPy is an open-source library for symbolic computation. It can perform computer algebra. Matplotlib is a plotting library for Python and its numerical mathematics extension NumPy.

Python has several graphical user interface (GUI) frameworks, ranging from the native Tkinter to several cross-platform alternatives such as GTK, Qt, Tk, and wxPython. GUI programming in Python entails adding cross-platform GUIs to a scientific application, which is a fast procedure that takes far less code than any other programming language. Python is important in computer science with its high level of code reuse as well as capacity to solve big scale complicated engineering problems. Python has become a key aspect of systems engaged

in the computing and processing of scientific data due to the higher speed, productivity, and availability of tools such as Scientific Python and Numeric Python.

2.5 Gaps in Knowledge

Simulation laboratory methods enable students to gain a better understanding of the concepts and theory of a phenomenon, in this case, polymerisation. This statement is also proven by most researchers by doing surveys on it. However, there is also a loophole in this statement that has been identified where the students who are doing their lab via virtual lab or simulation lab may encounter some problems in applying their skills and concepts to real-built-in equipment. Based on the latest survey that was conducted in Saudi Arabia, they found that 60% of students who were doing virtual simulation labs had difficulty in applying and understanding skills and concepts to actual equipment (Aljuhani et al., 2018). This is because when the simulations are programmed, they are assumed to work in an ideal environment and without any disturbance, which is something that could not happen in real life. Besides, some of this simulation lab's equipment did not show or provide exact size and dimension of equipment. This made students struggle to handle it, where in simulations the equipment is easy to handle; you just need to key in the values of input, but in reality, it is totally different. To overcome this, some researchers and institutions already work on actual reality and virtual reality labs that duplicate the exact equipment sizes and dimensions. This method also needs to be improvised with some advanced technology tools like VR headsets or holograms in future studies. So, that student will be able to figure out the actual size and dimensions.

CHAPTER 3
METHODOLOGY

This chapter mainly explains about methodology of the research work that was done to develop the simulation of continuous polystyrene polymerisation reactor using Python.

3.1 Research Flow

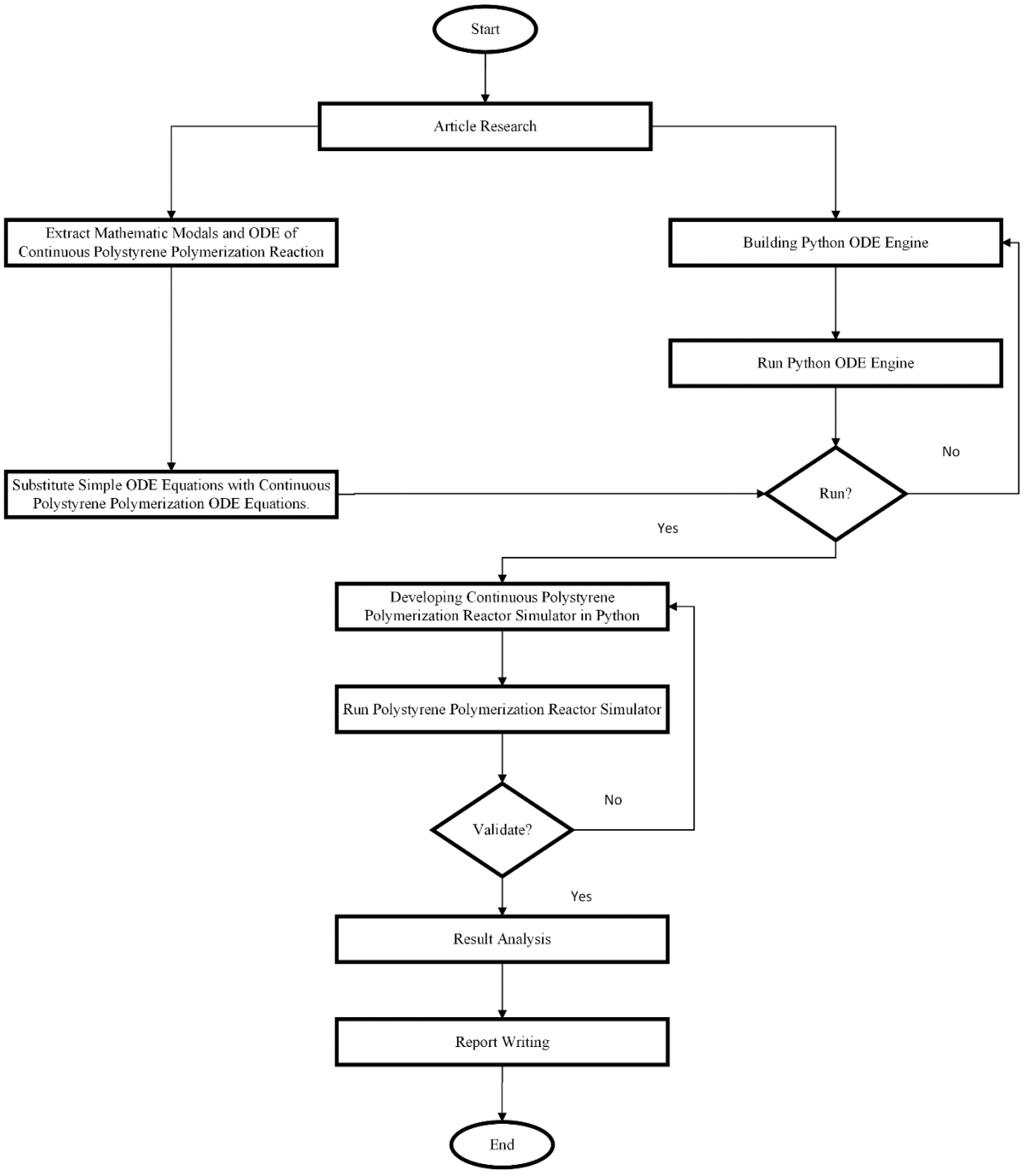

Figure 2 Flow diagram of this research work

Figure 2 shows the flow diagram for this research project, which is creating a simulator of continuous polystyrene polymerisation. Countless articles have been read and reviewed in order to comprehend the ideas of virtual learning and simulation. Furthermore, this stage will provide an overview and comprehension of modelling and simulation of various types of reactors as well as polymerisation kinetic reactions. Furthermore, the significance of Python in simulation also has been investigated. Then, using simple ODE equations, the ODE engine is created. This step is crucial to achieving that Python can replicate values that are identical to those found in the literature. This will also guarantee that the styrene polymerisation simulator can simulate the expected outcomes. Meanwhile, mathematical models for the continuous polystyrene polymerisation reactor simulator were extracted in order to derive the ODE equations required for simulation. Then, after successfully running and validating the Python ODE Engine, the ODE equations from mathematical models were utilised to develop the continuous polystyrene polymerisation reactor simulator. Once the simulator's simulated outcomes were successfully run and verified with literature, the procedure moved on to sensitivity and result analysis. Then, a report has to be written to complete the thesis.

3.2 Extracting Mathematical Models and ODE of Continuous Polystyrene Polymerisation Reaction from Literature

The polymerisation reactor is often at the core of the polymerisation process, and its operation can be challenging due to exothermic reactions, variable reaction kinetics, and high viscosity. The current study looks upon free-radical solution styrene polymerisation in a jacketed continuous stirred tank reactor, CSTR. Solution polymerisation is chosen due to better reactor temperature control and minimal requirement of initiator which could cut the cost in real industry. The CSTR contains three feed streams, as demonstrated in Figure 3: pure styrene monomer, 2,2'-azoisobutyronitrile (AIBN) initiator dissolved in benzene, and pure benzene solvent. Polymer, unreacted monomer, initiator, and solvent are all present in the exit stream.

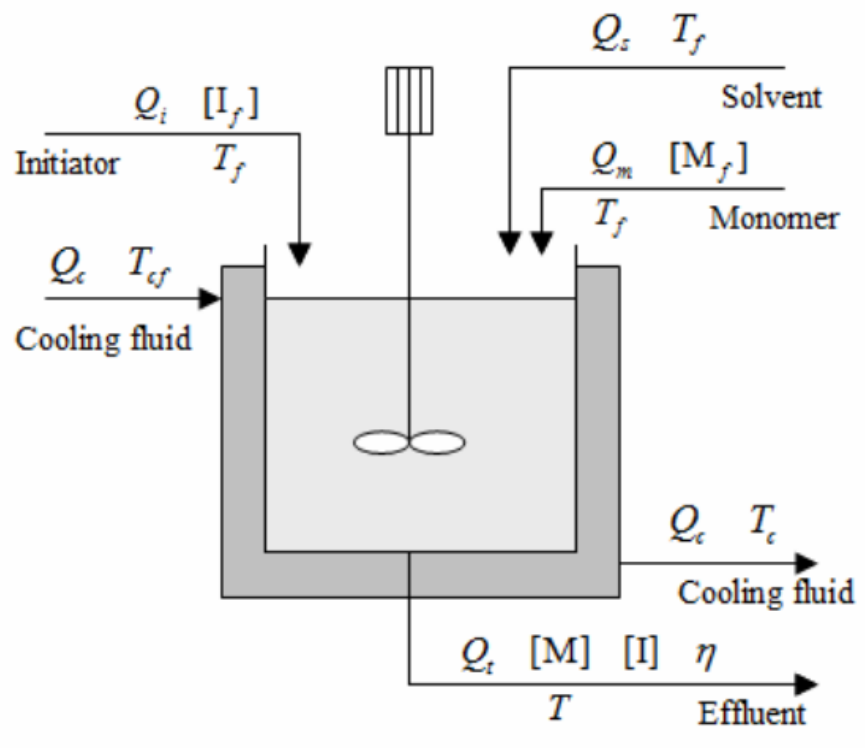

Figure 3 Process diagram for the styrene polymerisation.

The following stages outline the kinetic mechanism adopted for this homopolymerisation process (Alvarez and Odloak, 2011).

$I \xrightarrow{f_i,k_d} 2R$ (initiator decomposition) (1)

$M + R \xrightarrow{k_i} P_1$ (chain initiation) (2)

$P_n + R \xrightarrow{k_p} P_{n+1}$ (propagation) (3)

$P_n + P_m \xrightarrow{k_{td}} T_n + T_m$ (terminated by disproportionation) (4)

$P_n + P_m \xrightarrow{k_{tc}} T_{n+m}$ (terminated by combination) (5)

The decomposition of initiator *I* produces radicals *R*, which react with the monomer molecules M to produce new living (radical) polymer chains P_1. During the propagation stage, monomer molecules M are added to the live-polymer chains P_n (n≥1) one at a time. The chain growth stops when the propagating radicals lost their activity due to any termination reaction, resulting in dead-polymer chains, T_n (n≥1) (Alvarez and Odloak, 2011). There following assumptions was made by Alvarez and Odloak, (2011) to define the reactor mathematical model.

- By comparison to other system time constants, the lifespan of the polymer radical species is relatively short. Then, for R and P_n, the quasi-steady-state approximation (QSSA) is considered.
- The monomer consumption is mostly caused by propagation, which results in the Long Chain Assumption (LCA).
- The chain transfer reactions to monomer and solvent are not taken into account.
- Monomer thermal initiation does not occur since this reaction is only influential at temperatures over 373K. The reactor temperature evaluated in this research is below this limit.
- The total chain termination rate constant, k_t, is made up of contributions from both combination, k_{tc}, and disproportionation, k_{td}. Experiment findings for styrene in solution revealed that chain termination happens entirely through combination. Then termination by disproportionation is ruled out.
- The propagation rate is substantially faster than the termination rate.
- The initiation and termination heat are insignificant in comparison to the heat of polymerisation.

The continuous styrene polymerisation reactor is defined as follows (Alvarez and Odloak, 2011):

$$\frac{d[I]}{dt} = \frac{(Q_i[I_f] - Q_t[I])}{V} - k_d[I] \tag{6}$$

$$\frac{d[M]}{dt} = \frac{(Q_m[M_f] - Q_t[M])}{V} - k_p[M][P] \tag{7}$$

$$\frac{dT}{dt} = \frac{Q_t(T_f - T)}{V} + \frac{(-\Delta H_r)}{\rho C_p} k_p[M][P] - \frac{hA}{\rho C_p V}(T - T_c) \tag{8}$$

$$\frac{dT_c}{dt} = \frac{Q_c(T_{cf} - T_c)}{Vc} + \frac{hA}{\rho_c C_{pc} V_c}(T - T_c) \tag{9}$$

where,

$$[P] = \left[\frac{2f_i k_d[I]}{k_t}\right]^{0.5} \tag{10}$$

$$k_j = A_j \exp\left(\frac{-E_j}{T}\right), \quad j = d, p, t \tag{11}$$

$$Q_t = Q_i + Q_m + Q_s \tag{12}$$

Q_i, Q_m, Q_s, and Q_c represent volumetric flowrate of initiator, monomer, solvent, and cooling jacket fluid, respectively. V is reactor volume while V_c is cooling jacket fluid volume. $[I]$ and $[M]$ represent the concentration of initiator and monomer, respectively. $[I_f]$ and $[M_f]$ represent the feed concentration of initiator and monomer, respectively. T and T_c represent the temperature of reactor and cooling jacket fluid, respectively. T_f and T_{cf} represent the feed temperature of reactor and cooling jacket fluid, respectively. $-\Delta H_r$ represents heat of polymerisation while hA represents overall heat transfer coefficient. ρCp and $\rho_c Cp_c$ represent mean heat capacity of reactor fluid and cooling jacket fluid, respectively. k_d, k_p, and k_t are represent kinetic rate constant. A_d, A_p, and A_t are frequency factor. E_d, E_p, and E_t are activation energy. The f_i is initiator efficiency.

The dead polymers' moment equations are follows (Alvarez and Odloak, 2011):

$$\frac{dD_0}{dt} = 0.5k_t[P]^2 - \frac{Q_t D_0}{V} \tag{13}$$

$$\frac{dD_1}{dt} = M_m k_p[M][P] - \frac{Q_t D_1}{V} \tag{14}$$

$$\frac{dD_2}{dt} = 5M_m k_p[M][P] + 3M_m \frac{k_p^2}{k_t}[M]^2 - \frac{Q_t D_2}{V} \tag{15}$$

D_0, D_1, and D_2 denote the dead polymer's zero, first, and second order moments, respectively. M_m denote the molecular weight of monomer.

The weight-average molecular weight, M_w and number-average molecular weight, M_n are follows:

$$M_w = M_m \frac{D_2}{D_1} \tag{16}$$

$$M_n = M_m \frac{D_1}{D_0} \tag{17}$$

The polydispersity index (PD) is a characteristic of the dead polymer's molecular weight distribution that is defined as:

$$PD = M_m \frac{D_2 D_0}{{D_1}^2} \tag{18}$$

Based on all this ordinary differential equations, the monomer conversion, X can be defined as:

$$X = \left(1 - \frac{[M]}{[M_f]}\right) \times 100\% \tag{19}$$