

AI-ML-based model predictive control strategies for reactors

A Project Report submitted by

Ankush Gupta(B20CH006)
Divyanshu Pandey (B20CH015)
Sujal Gupta(B20ES015)

in partial fulfillment of the requirements for the award of the degree of

Bachelors in Technology in Chemical Engineering

&

Bachelors in Technology in Engineering Science



॥ त्वं ज्ञानमयो विज्ञानमयोऽसि ॥

Indian Institute of Technology Jodhpur

Department of Chemical Engineering

January 2024

DECLARATION

I hereby declare that the report presented in this Project Report titled **AI-ML-based model predictive control strategies for reactors** – has been submitted to the Indian Institute of Technology Jodhpur in partial fulfillment of the requirements for the award of the degree of BTech. and is a bonafide record of the research work carried out under the supervision of *Dr. Angan Sengupta*. The contents of this project report in full or in parts, have not been submitted to, and will not be submitted by me to, any other Institute or University in India or abroad for the award of any degree or diploma.

Ankush Gupta(B20CH006)

Divyanshu Pandey(B20CH015)

Sujal Gupta(B20ES015)

CERTIFICATE

This is to certify that the Project Report titled **AI-ML-based model predictive control strategies for reactors** submitted by *Ankush Gupta(B20CH006)*, *Divyanshu Pandey(B20CH015)*, *Sujal Gupta(B20ES015)* to the Indian Institute of Technology Jodhpur for the award of the degree of BTech is a bonafide record of the research work done by her under my supervision. To the best of my knowledge, the contents of this report, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

Signature
Dr. Angan Sengupta

ABSTRACT

Polymerization reactions combined with inadequate cooling systems can lead to thermal runaway. In our recent study, we examined the potential for thermal runaway in batch reactors during the thermally induced free radical polymerization of styrene. The study for polymerization in batch reactors already exists. We attempt to deploy the same polymerization reaction for the plug flow reactor and study its behavior for the same. In a PFR each element of fluid that enters the reactor follows the same path and is subjected to the same reaction conditions as it travels through the length of the reactor. We attempted to achieve the results using Ansys fluent software and Matlab.

1.1 INTRODUCTION

Polystyrene, one of the earliest recognized polymers, is derived from the styrene monomer via a thermal polymerization process. This affordable and durable plastic is widely utilized in various everyday applications, including packaging, insulation, disposable cups, kitchenware, and toys. The polymerization processes leading to the formation of polymers like polystyrene are intricate, typically exothermic, and characterized by a strong nonlinear relationship between the operational parameters and the resulting polymer properties. The industrial process of thermally initiating the polymerization of styrene to produce high molecular weight polystyrene typically occurs within a temperature range of 90°C to 200°C. The challenges arise from the need for high-temperature initiation, the exothermic nature of the polymerization, and poor heat dissipation due to the high viscosity of the reaction mixture, leading to localized hotspots. Thermal runaway in this complex styrene polymerization reaction occurs when the heat generated surpasses the cooling capacity of the system, causing a rapid temperature increase inside the reactor vessel. This poses a significant risk of explosion and other safety hazards. The use of an insoluble initiator adds another layer of complexity to the process. The "intricate" and non-linear dynamics associated with the exothermic polystyrene formation reaction introduce challenges in managing the reactor's behavior, particularly at different steady-state conversion points. These complexities underscore the need for sophisticated control strategies tailored to the specific operating conditions encountered in industrial settings. Implementing effective control measures becomes crucial not only for optimizing the production process but also for ensuring safety and preventing potential hazards such as reactor runaways. Therefore, a comprehensive understanding of the reaction kinetics and thermodynamics is essential for developing robust control strategies that can adapt to the dynamic nature of the process. Based on a thorough review of the literature on styrene polymerization, as previously mentioned, it is evident that managing this reaction within a batch reactor presents challenges due to the emergence of localized hotspots. The heat transfer from the reactor is hindered by the highly viscous nature of the reaction medium, particularly as the initiator concentration fluctuates, potentially resulting in a thermal runaway situation.

1.2 OBJECTIVE

The objective of this project was to comprehensively investigate the polymerization reaction of styrene within a plug flow reactor (PFR), focusing on understanding the dynamic trends in monomer and initiator concentrations, as well as the temperature variations over time. To achieve this, the project involved the utilization of advanced modeling techniques, particularly employing Ansys software to create a detailed PFR model. The derived equations governing the changes in concentration of the monomer and initiator, as well as the temperature profile with respect to time, were then solved using mathematical methods.

In addition, Matlab was employed as a powerful computational tool to carry out the numerical solutions of the derived equations. The integration of both Ansys and Matlab facilitated a comprehensive analysis of the polymerization process within the PFR, allowing for the exploration of intricate interactions and dynamic behaviors during the reaction. The project aimed to contribute valuable insights into the kinetics and thermodynamics of styrene polymerization, providing a foundation for optimizing reaction conditions and enhancing the efficiency of polymer production processes.

1.3 LITERATURE SURVEY

Polystyrene, one of the earliest known polymers, is derived from the thermal polymerization of styrene monomers. This inexpensive and rigid plastic has widespread applications in everyday life, such as packaging, insulation, disposable cups, kitchen appliances, and toys. The polymerization reactions involved, similar to those forming polystyrene, are intricate, generally exothermic, and exhibit a nonlinear relationship between operating conditions and polymer properties.

In the industrial process of thermal-initiated polymerization, converting styrene into high molecular weight polystyrene occurs within the temperature range of 90°C to 200°C. However, challenges arise due to the need for high-temperature initiation, the exothermic nature of the reaction, and insufficient heat dissipation from the highly viscous reaction mixture, leading to local hotspots. This situation poses a risk of thermal runaway, where the heat generated by the reaction surpasses the maximum temperature for technical reasons (MTT) inside the vessel, potentially causing explosions and hazards.

The term "thermal runaway polymerization" describes a scenario in which the heat produced by the reaction is inadequately removed by the cooling system, resulting in a rapid temperature increase beyond the MTT. To comprehend the impact of temperature on the conversion rate of styrene in thermally initiated polymerization, early researchers developed theories on reaction kinetics for polystyrene formation. This understanding of reaction kinetics has since been employed by various research groups to design and develop industrial reactors for the thermal-initiated free radical formation of polystyrene. A thorough literature review on polystyrene formation and reactor studies provides insights into this complex process.

The investigation and comprehension of thermally initiated free radical polystyrene formation within different reactor setups, including batch reactors, tubular reactors, microreactors, and semi-batch reactors, under both steady and unsteady states, have been explored through a combination of experiments and mathematical modeling approaches. These studies reveal the non-linear dependence of various operating parameters and the impact of inhibitors on polymer properties and reactor stability.

Kim and Choi initially demonstrated the use of bifunctional free radical initiators, such as diperoxyesters, for polystyrene production and their influence on the stability of a continuous stirred-tank reactor (CSTR) through reactor stability analysis. Their findings indicated that higher molecular weight polystyrene could be achieved using bifunctional free radical initiators across a broad range of operating conditions, overcoming limitations observed with monofunctional initiators.

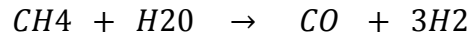
Additionally, Kotoulas and colleagues developed a comprehensive kinetics model considering the effects of both thermal and chemical initiation mechanisms on polystyrene formation. This model utilized dynamic molar balances of all quasi-state radical species to provide insights into the process.

Furthermore, the surface polymerization of styrene on silica was investigated to understand the impact of dissolved oxygen and free radical initiator solubility on kinetics, yield, and molecular weight of the resulting polystyrene. The study revealed that the presence of oxygen decreased the yield of high molecular-weight polystyrene, while water-soluble initiators led to the formation of higher molecular-weight polymers compared to their water-insoluble counterparts.

The intricate and non-linear dynamics of the exothermic reaction involved in polystyrene formation pose challenges in controlling reactor dynamics at various steady-state conversion points. In response to this complexity, there is a recognition of the need for effective control strategies to avert runaway conditions in reactors operating under specific industrial conditions. The authors employed a less computationally intensive Model Predictive Control (MPC) approach, demonstrating its efficacy in utilizing initiator concentration as a means to address various sources of modeling errors in the control of jacketed Continuous Stirred-Tank Reactors (CSTR).

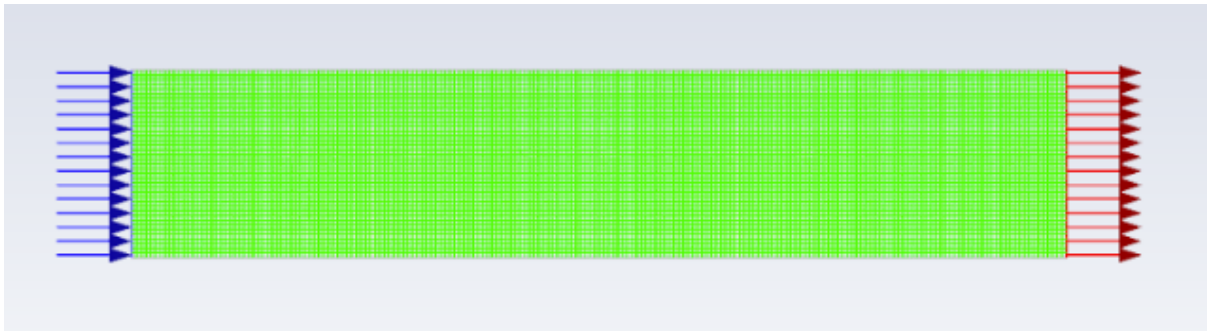
1.4 METHODS AND METHODOLOGY

At first, we employed a Plug flow reactor for a reaction. The reaction is represented by the equation:



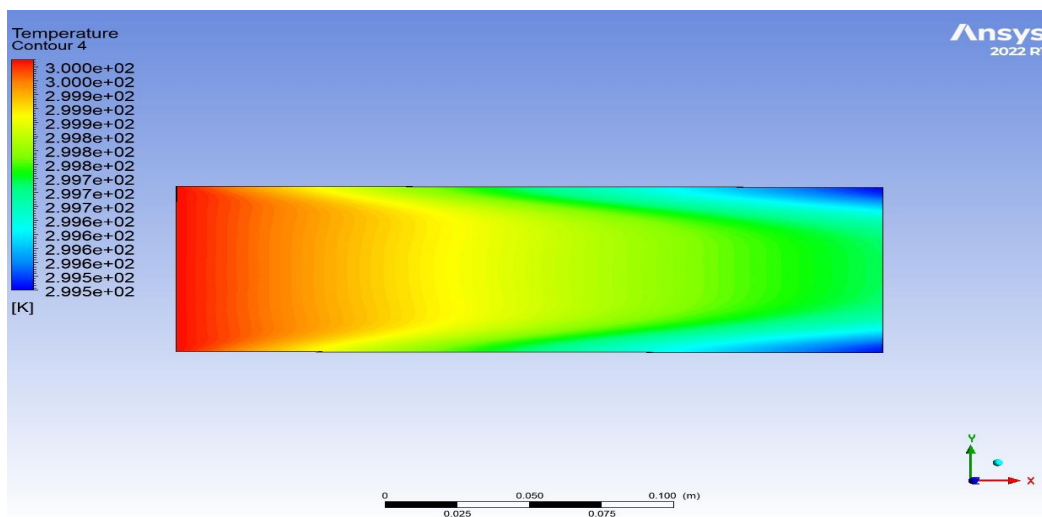
is called steam methane reforming. This reaction is highly endothermic, meaning it absorbs heat from its surroundings to proceed.

A simple PFR with a single inlet and outlet:

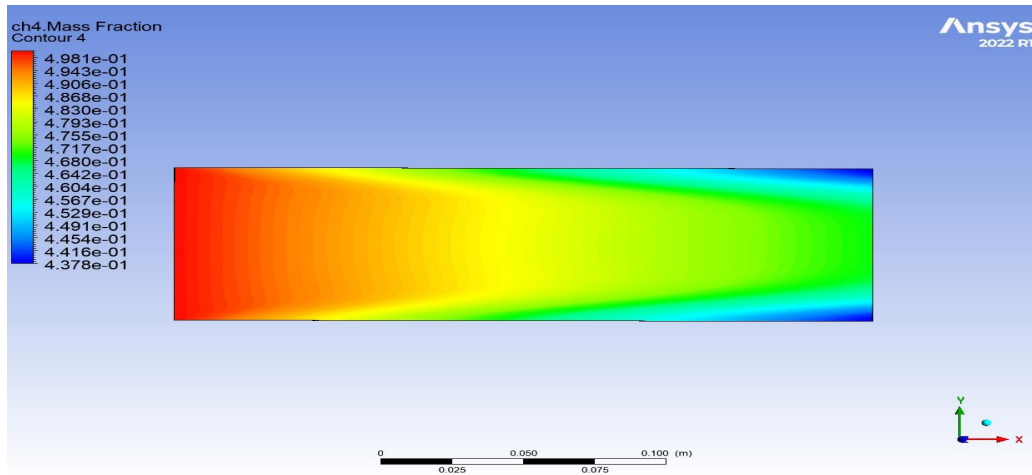


After complete reaction and simulating the results we got the following profiles:

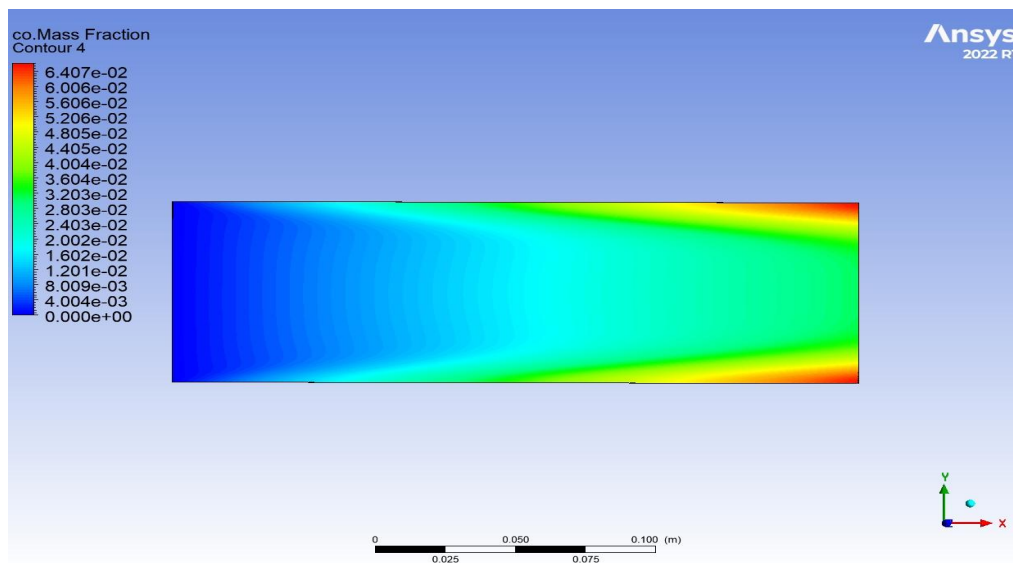
- 1) For a non-jacketed system with an input speed of 0.1m/s and initial mass fractions of CH_4 and H_2O is 0.5. Dimensions of PFR length 245mm and diameter 80mm:



Temperature profile

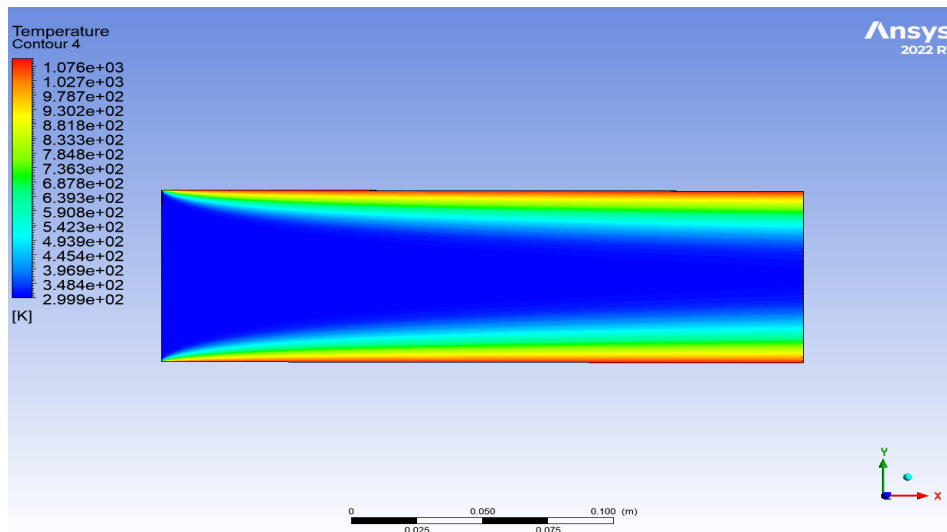


CH4 profile

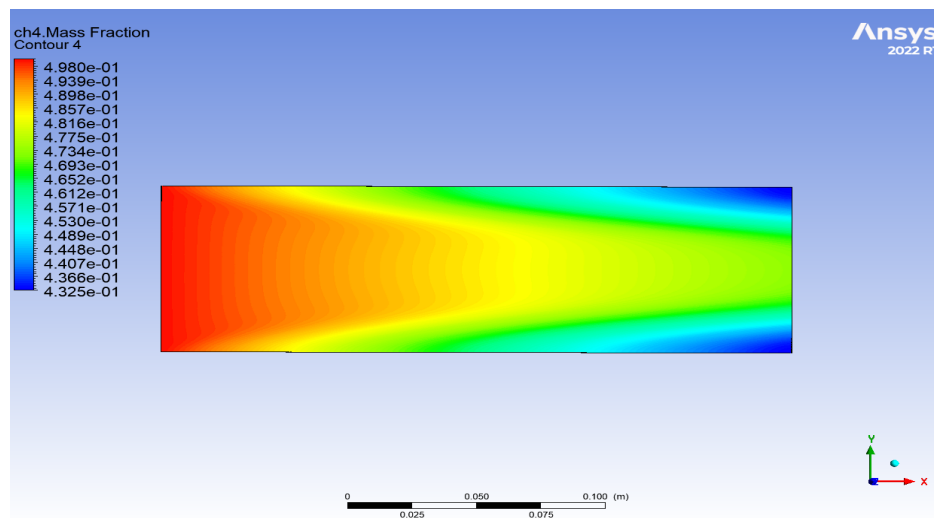


CO profile

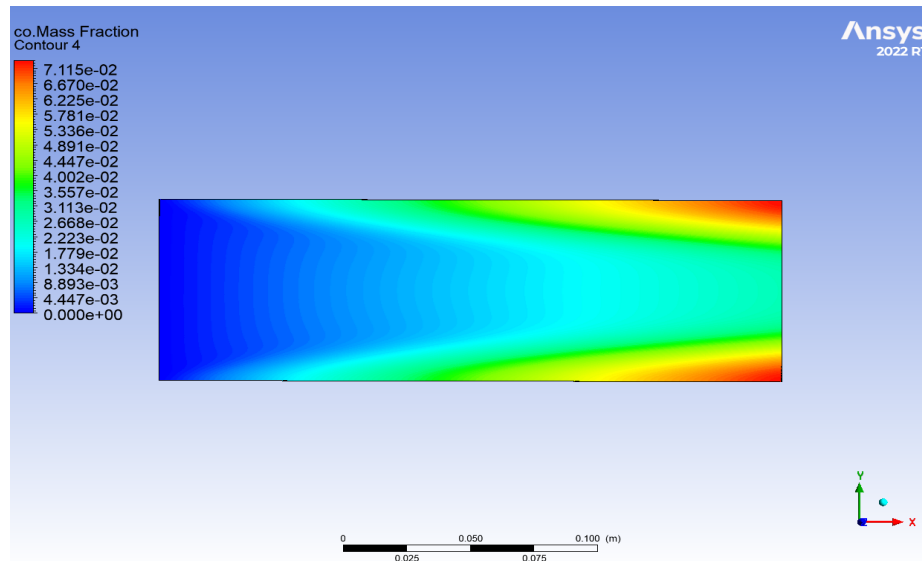
- 2) For a jacketed system with an input speed of 0.1m/s and initial mass fractions if ch4 and H2O is 0.5 and wall thickness 5mm Dimensions of PFR length 245mm and diameter 80mm Dimensions of PFR length 245mm and diameter 80mm:



Temperature profile

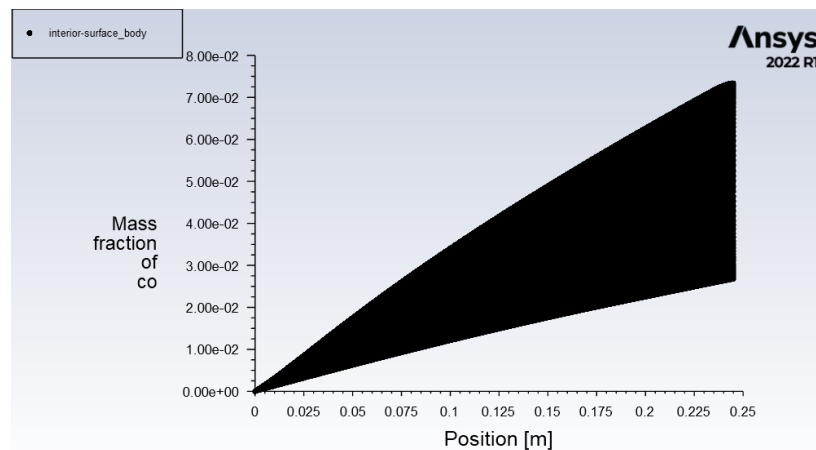
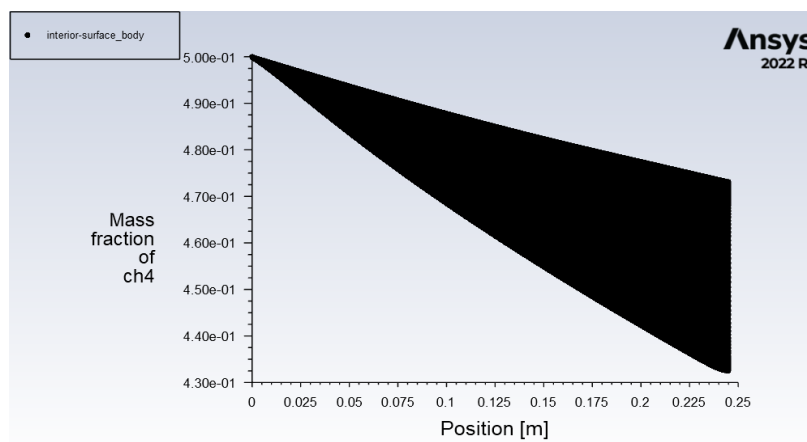


CH4 profile



CO profile

Graphs for the mass fractions of CH₄ and CO are attached below

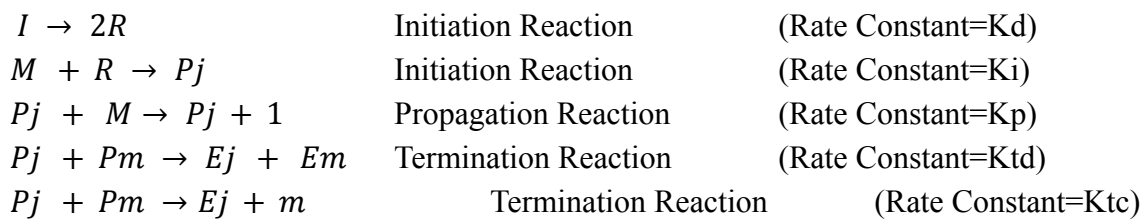


These graphs correctly depict the concentration of CH₄ and CO across different cross-sections of the PFR as at each cross-section the mass fraction of the species is also variable we get the following graphs. The increasing trend of mass fraction of CH₄ correctly matches with the contour of CH₄ and the decreasing trend of mass fraction of CO correctly matches with the contour of CO.

We intended to do the same for the polymerization reaction of styrene in PFR in Ansys fluent but the elements involving the reaction were missing from the fluent database due to which it became practically impossible. So we did further study using Matlab by deriving the equations and solving them in Matlab using Ode Solver.

Equations for the Model -

Steps for free radical polymerization reaction:



Now let's find the rate of change of concentration of initiator w.r.t to time

The general form of the mass balance equation for PFR is

$$\frac{dF_i}{dt} = R_i$$

F_i = Molar flow rate of species i

V = Volume of reactor

R_i = rate of reaction of species i

let's assume the initial concentration of I is C_{i0} and the concentration of I and R are C_i and C_r at any given point in the reactor

The rate of the given reaction can be written as:

$$R_i = - \frac{dC_i}{dt} = k_d * C_i$$

Since $I \rightarrow 2R$ the rate of formation of R is twice the rate of disappearance of I:

$$R_r = - \frac{dC_r}{dt} = 2k_d * C_i$$

Now the mass balance for species I in PFR is:

$$\frac{dF_i}{dV} = - R_i$$

Since $F_i = C_i * A * u$ (A = CSA of PFR and u is velocity)

$$\frac{d(C_i * A * u)}{dV} = - k_d * C_i$$

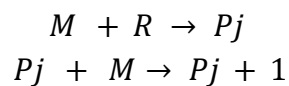
Since A and u are constant

$$A * u * \frac{dC_i}{dV} = - k_d * C_i$$

So Finally rearranging and solving we get

$$\frac{dC_i}{dt} = - \frac{k_d * C_i}{A * u}$$

So now let us consider equations



Now

$$R_{mr} = - \frac{dC_m}{dt} = - k_i * C_m * C_r$$

and

$$R_{pm} = - \frac{dC_m}{dt} = - k_p * C_{pj} * C_m$$

Now applying the mass balance for species M in PFR, we have:

$$A * u * \frac{dC_m}{dV} = R_{mr} + R_{pm}$$

Substituting the rate expression we get:

$$A * u * \frac{dC_m}{dV} = k_i * C_m * C_r + k_p * C_{pj} * C_m$$

Now we have $C_r = 2C_i$ and $C_{pj} = C_m$ So above equation becomes

$$A * u * \frac{dC_m}{dV} = k_i * C_m * 2C_i + k_p * C_m * C_m$$

Therefore

$$\frac{dC_m}{dt} = \frac{k_i * C_m * 2C_i}{A * u} + \frac{k_p * C_m * C_m}{A * u}$$

Let us derive the change in temperature of the reactor

General form of Energy Balance equation of PFR is

$$\frac{dT}{dV} = - \frac{\Delta H_r}{p * C_p} * r$$

So we have to consider the enthalpy of each reaction as $\Delta H_{r1}, \Delta H_{r2}, \Delta H_{r3}$.

Now the total rate of reaction in PFR is given by the sum of individual rates

$$r = k_d * C_i - k_i * C_m * C_r + k_p * C_{pj} * C_m$$

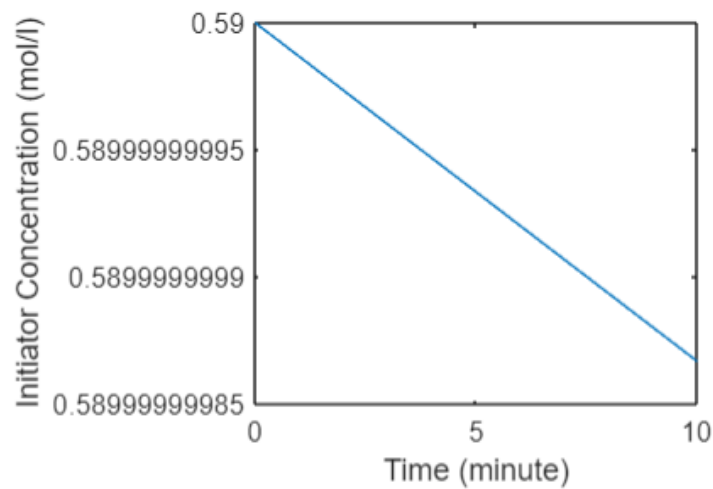
So by substituting these values in the energy balance equation

$$\frac{dT}{dt} = - \frac{\Delta H_{r1}}{p * C_p} * (k_d * C_i) - \frac{\Delta H_{r2}}{p * C_p} * (k_i * C_m * C_r) - \frac{\Delta H_{r3}}{p * C_p} * (k_p * C_{pj} * C_m)$$

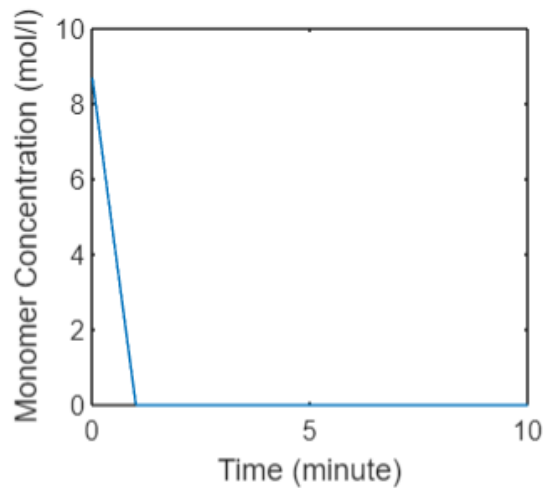
So we have solved the equation using 3rd order runge kutta method using ODE45 Solver in MATLAB using the following parameters.

Process Parameters		
Input Parameters	Values (units)	Reactor Condition
Volume of reactor (V)	3000 (l)	Adiabatic, Non-adiabatic
Volume of cooling jacket (V_c)	3312.4 (l)	Non-adiabatic
Volumetric flow rate of coolant (Q_c)	7.86 (l/min)	Non-adiabatic
Inlet temperature of coolant (T_{ci})	300 K	Non-adiabatic
Arrhenius pre-exponential constant for initiator decomposition (A_d)	5.95×10^{13}	Adiabatic, Non-adiabatic
Arrhenius pre-exponential constant for chain propagation (A_p)	1.06×10^7	Adiabatic, Non-adiabatic
Arrhenius pre-exponential constant for chain termination (A_t)	1.25×10^9	Adiabatic, Non-adiabatic
Activation energy for initiator decomposition (E_d)	14,897 (K^{-1})	Adiabatic, Non-adiabatic
Activation energy for chain propagation (E_p)	3557 (K^{-1})	Adiabatic, Non-adiabatic
Activation energy for chain termination (E_t)	843 (K^{-1})	Adiabatic, Non-adiabatic
Heat of reaction (ΔH_r)	-16700 (J/mol)	Adiabatic, Non-adiabatic
Initiation efficiency factor (f)	0.65	Adiabatic, Non-adiabatic
Overall heat transfer coefficient (in terms of UA)	50, 60, 70 (J/min/K)	Non-adiabatic
Initial Conditions		
Initial initiator concentration (C_{i0})	1.4×10^{-4} , 0.14, 0.2, 0.59 (mol/l)	Adiabatic, Non-adiabatic
Initial monomer concentration (C_{M0})	8.69, 9.5 (mol/l)	Adiabatic, Non-adiabatic
Initial reactor temperature (T_0)	360.15, 373.15 (K)	Adiabatic, Non-adiabatic
Initial coolant temperature (T_{c0})	300 (K)	Non-adiabatic

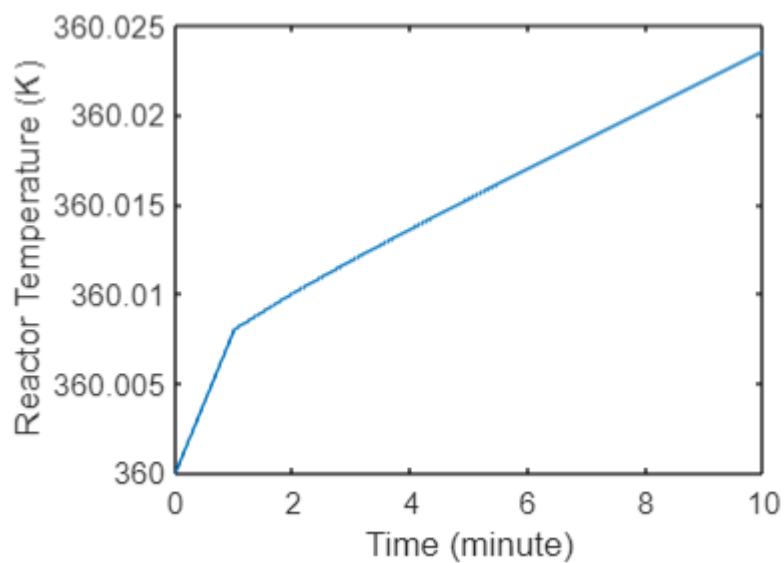
1.5 RESULTS



Initiator Concentration v/s Time



Monomer Concentration v/s Time



Reactor Temperature v/s Time

1.6 CONCLUSION

The reactor temperature increases to infinity after a certain point of time due to the fact that the monomer concentration reduces to null. The initiator concentration shows a linear relationship with time. The temperature profile is dependent on the initial values of reactors. The 4th order runge kutta method was also tried but the temperature reached infinity after some point of time proving some sort of errors in calculation. Since PFR does not have any

accumulation of substance hence the monomer gets depleted after a certain time. The temperature profile kept on increasing as long as we left the reactor on and ran the equation for further minutes.

1.7 FUTURE WORK

In the present work we found out the reaction and temperature profiles in a PFR for a styrene polymerization reaction. We further aim to develop a strategy to prevent the temperature profile to keep on increasing after the monomer depletion. We also aimed to solve these equations using the fourth-order runge kutta method and found out the difference between the results obtained.

Also in the future, if the polymerization reaction reactants and mechanism is added in Ansys Database then the reaction can be simulated in Ansys similar to the above reaction resulting in better visualisations and analysis.

1.8 REFERENCES

- [1]. Angan Sengupta (2022) “A Case Study of Online Estimation of Polystyrene Formation Runaway Reaction Process Parameters”, Journal of Loss Prevention in the Process Industries, 80.
- [2]. Brooks B.W (1979) Chemical Engineering Science. 1979 34 1417.
- [3]. Brooks B.W (1980) “Dynamic Behaviour of Continuous Flow polymerization Reaction”, Chemical Engineering Science, 36 pp. 589-593