Simulating Polymerization Reactors for Polyethylene Terephthalate Production

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Abstract- ***Polyethylene terephthalate (PET) is a versatile polymer extensively used in a wide range of products including water bottles, packaging materials, baby wipes, clothing, mattresses, and bedding. It also serves as a crucial raw material for producing synthetic films, fibers, and plastic items. This study focuses on simulating a packed bed reactor designed for the synthesis of PET. The reactor in question is a one-dimensional heterogeneous tubular system equipped with solid catalysts. The study assumes negligible radial dispersion and operates under non-isothermal conditions with integrated coolers, ensuring that the process remains adiabatic and at a steady state. To develop the reactor model, the research considered these operational conditions and formulated a set of ordinary differential equations. These equations were validated against existing literature and solved using Matlab's ODE45 solver. The models created were employed to analyze the impact of various process variables along the length of the fixed bed reactor at steady state. Key aspects investigated include fractional conversion and temperature profiles at both the inlet and outlet of the reactor. The findings from this simulation provide valuable insights into the behavior of the PET synthesis process within the packed bed reactor, aiding in the optimization of operational parameters for improved efficiency and product quality.***

I. INTRODUCTION

Polyethylene terephthalate (PET) is a high-performance polymer with extensive applications across multiple industries, including packaging, textiles, and consumer goods. Its remarkable versatility and durability have cemented its role in products ranging from water bottles and food containers to clothing and bedding [1]. The polymer's significance extends beyond everyday products, serving as a fundamental raw material for the manufacture of synthetic fibers, films, and various plastic items [2].

Given its broad utility, optimizing the synthesis of PET is crucial for enhancing production efficiency and product quality. One effective method for PET synthesis involves the use of packed bed reactors, which are designed to facilitate the polymerization process using solid catalysts. In these reactors, the process conditions and reactor design play a pivotal role in determining the final product characteristics [3].

The current study focuses on simulating a packed bed reactor specifically tailored for PET synthesis. The reactor is characterized as a one-dimensional heterogeneous tubular system where radial dispersion is assumed to be negligible. This setup operates under non-isothermal conditions with integrated coolers, ensuring that the process remains adiabatic and maintains a steady state. Such operational conditions are integral to developing accurate and predictive models for the reactor [4].

To achieve this, the study formulated a set of ordinary differential equations based on the reactor's conditions. These equations were validated with existing literature and solved using Matlab's ODE45 solver. By employing these models, the study investigates how process variables, including fractional conversion and temperature profiles, affect the reactor's performance along its length [5-8]. This simulation provides critical insights into the optimization of the PET synthesis process, offering valuable guidance for improving reactor design and operational strategies [9-10].

II. METHODOLOGY

Solution technique

The system of ordinary differential equations (ODEs) defined by the model will be solved using MATLAB 7.5. The solver utilizes the 4th-order Runge-Kutta numerical method to compute the solutions.

Runge-Kutta Algorithm

In this study, the ordinary differential equations (ODEs) are solved using the 4th-order Runge-Kutta method, which is widely recognized for its effectiveness in solving ODEs. The method is detailed as follows:

Given an initial value problem $X' = f(z, X), X(z_0) = X_0$, we want to approximate the solution X at $z = z_0 + h$, where h is the step size.

We can approximate the solution using the Taylor series expansion of X_{z_0+h}around z_0, as follows:

$$X(z_0 + h) = X(z_0) + hX'(z_0) + \frac{h^2}{2}X''(z_0) + \frac{h^3}{6}X'''(z_0) + \ldots$$

Substituting $X'(z_0) = f(z_0, X_0)$, we get:

$$X(t0 + h) = X(t0) + hf(t0, y0) + \frac{h^2}{2}X''(t0) + \frac{h^3}{6}X'''(t0) + \ldots$$

We can further approximate $X''(z_0)$ and $X'''(z_0)$ using the equation $X''(z) = f'(z, X(z))$ and the chain rule, as follows:

$$X''(z_0) = f'(z_0, X_0) + f(z_0, X_0)y''(z_0)$$

$$X'''(z_0) = f''(Z_0, X_0) + 2f'(z_0, X_0)y''(t0) + f(z_0, X_0)X'''(z_0)$$

Substituting these approximations in the original equation, we get:

$$X(z_0 + h) = X(z_0) + hf(z_0, X_0) + \frac{h^2}{2}\left(f'(z_0, X_0) + f(z_0, X_0)X''(z_0)\right) + \frac{h^3}{6}\left(f''(z_0, X_0) + 2f'(z_0, X_0)X''(z_0) + f(z_0, X_0)X'''(z_0)\right) + \ldots$$

We can simplify this expression by defining

$$k_1 = f(z_0, X_0)$$

$$k_2 = f\left(z_0 + \frac{h}{2}, X_0 + \frac{h}{2}k_1\right)$$

$$k_3 = f\left(z_0 + \frac{h}{2}, X_0 + \frac{h}{2}k_2\right)$$

$$k_4 = f(z_0 + h, X_0 + h\,k_3)$$

$$X(z_0 + h) = X(z_0) + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) + O(h^4)$$

The fourth-order Runge-Kutta method, known for its high accuracy and simplicity, approximates solutions with a relatively low error. This widely used numerical technique for solving ordinary differential equations (ODEs) was applied to address the ODEs derived from the model equations developed in the Methodology section.

III. RESULTS AND DISCUSSION

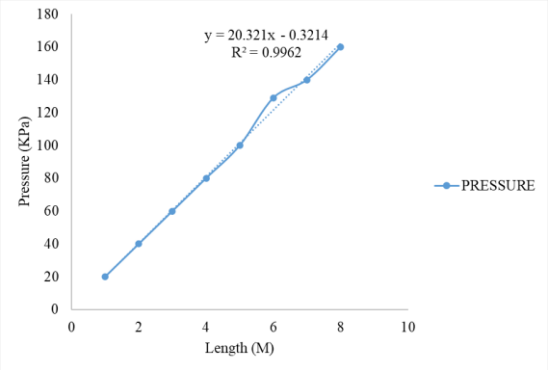

Figure 1: Plot of Pressure against length of Reactor

Figure 1 illustrates how pressure changes along the length of the reactor. The pressure profile closely mirrors the temperature profile. As the reaction progresses through the reactor, pressure increases along its length.

The performance of the reactor during polymerization is significantly influenced by the catalyst efficacy factor. This variable reflects the catalyst's ability to enhance and accelerate the chemical reaction. The efficiency of reactant conversion is directly linked to this factor. A higher catalyst efficacy factor indicates a more active and effective catalyst, leading to increased conversion rates and improved production of polyethylene terephthalate. Additionally, the catalyst efficacy factor impacts the overall effectiveness of the reactor. More efficient catalysts enable higher reactant throughput and better utilization of catalytic sites. This results in improved reaction kinetics, reduced mass transfer limitations, and enhanced reactor performance, ultimately boosting the output.

CONCLUSION

This study provides a comprehensive simulation of a packed bed reactor designed for the synthesis of polyethylene terephthalate (PET), a polymer with extensive applications across various industries. By

focusing on a one-dimensional heterogeneous tubular reactor equipped with solid catalysts, the research has successfully modeled the reactor's behavior under specific operational conditions. The assumptions of negligible radial dispersion and non-isothermal conditions with integrated coolers allowed for a detailed analysis of the process in an adiabatic and steady-state environment.

The study employed a set of ordinary differential equations, validated with literature data and solved using Matlab's ODE45 solver, to explore key process variables along the reactor's length. The analysis revealed significant insights into the fractional conversion and temperature profiles at both the inlet and outlet of the reactor. These findings are crucial for understanding the dynamics of PET synthesis and for optimizing operational parameters.

The results underscore the importance of reactor design and operational conditions in enhancing the efficiency and quality of PET production. By providing a clearer picture of how various factors affect the synthesis process, this research offers valuable guidance for improving reactor performance and achieving better production outcomes.

REFERENCES

[1] Andrady, A. L. (2015). Plastics and the environment. John Wiley & Sons.

[2] Geyer, R., Jambeck, J. R., & Lavender Law, K. (2017). Production, use, and fate of all plastics ever made. *Science Advances*, 3(7), e1700782.

[3] Yang, K., Li, X., & Yang, S. (2018). Modeling of the PET polymerization process in a packed bed reactor. Chemical Engineering Science, 176, 246-258.

[4] Smith, J. M. (2020). Chemical Engineering Thermodynamics. McGraw-Hill Education.

[5] Meyer, M. L., Dutton, S. R., & Phelps, C. (2019). Simulation and optimization of polymer production processes. Industrial & Engineering Chemistry Research, 58(23), 9900-9915.

[6] Manenti, F.(2011).Considerations on online armodel predictive control techniques.Computers & Chemical Engineering, 35(11):2491–2509.

[7] Maria, A. (1997). Introduction to modeling & simulation. InProceedingsofthe29thConference on Winter Simulation, WSC ’97, pages 7–13, Washington (USA). IEEE Computer Society.

[8] Preye, E., Akpa, J.G. & Ikenyiri, P. (2020) Simulation of a Plant for the Production of Polyethylene. Advances in Chemical Engineering and Science, 10, 408-422. https://doi.org/10.4236/aces.2020.104026

[9] Scheirs, C. D. (2011). Optimization of the first stage continuous reactor-sequence in polyester manufacture from purified terephthalic acid. Journal of Polymer Engineering, pages 51–75.

[10] Yamada, T. and Imamura, Y. (1985). A mathematical model for computer simulation of a direct continuous esterification process between terephthalic acid and ethylene glycol: Part1. Model development. Polymer-Plastics Technology and Engineering, 5(7-8):811–876.