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Optimization of Plug Flow Reactor for Thermal Cracking of Ethane to Ethylene

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Abstract | **Original Research Article**

This study investigated the optimization of ethylene production in a plug flow reactor (PFR) through mathematical modeling, simulation, sensitivity analysis, and process optimization. A comprehensive reactor model was developed based on material and energy conservation principles under steady-state operating conditions. The model incorporated the kinetics of ethane steam cracking and accounted for the effects of reactor temperature and reactant concentration on ethylene production. The resulting system of coupled ordinary differential equations was solved numerically using the Runge–Kutta ODE45 algorithm in MATLAB R2023b. Simulation results were used to evaluate key reactor performance parameters, including reactor diameter, reactor length, reactor volume, volumetric flow rate, residence time, and space velocity, which were found to be 1.6 m, 20 m, 40.21 m^3, 0.40 m^3/s, 10 s, and 0.0995 s^{-1}, respectively. A sensitivity analysis was conducted to investigate the effects of catalyst effectiveness factor, volumetric flow rate, reactor temperature, residence time, and inlet ethane concentration on ethylene production and reactor performance. The analysis revealed that variations in these parameters significantly influenced ethylene concentration, fractional conversion, and reactor temperature profiles. To identify optimum operating conditions, the sensitivity analysis results were subjected to curve fitting using Microsoft Excel to generate predictive regression models. The fitted models exhibited excellent predictive capability with coefficients of determination ((R^2)) ranging from 0.9829 to 0.9987. Optimization of the predictive models using differential calculus and MATLAB optimization tools showed that the maximum predicted ethylene concentration of 15.73 mol/m^3 was achieved at a catalyst effectiveness factor of 0.2467. The volumetric flow rate model indicated a minimum ethylene concentration of 7.78 mol/m^3 at a flow rate of 14.224 mol/m^3, while the reactor temperature model predicted a minimum outlet temperature of 1007.43 K at an initial ethane concentration of 55.38 mol/m^3.

Keywords: Packed Bed Reactor, Steady State Model, Simulation, Optimization, MatLab Software.

1.0 INTRODUCTION

Several researches have been carried out on ethylene plant by considering the modeling of an ethylene splitter from an industrial plant. The process presently operates with composition controllers that does not work well during process transition (Mahir *et al*., 2021). Kemal *et al*., 2013 considered the identification process of an ethane-ethylene distillation column system and introduces a procedure for multiple input multiple output (MIMO) system identification using MATLAB's identification toolbox. Jeiveison *et al*., 2018 stated that catalytic dehydration of ethanol is a key step in the production of ethylene from renewable raw materials. Obtaining mathematical model to optimize the ethanol-to-ethylene reactor setup is of great interest to the industry, allowing the optimized design of larger plants and improvements to existing plants. Muhammad *et al.*, 2021focused on the modelling and simulation of ethylene production process in Aspen plus software and energy optimization of the whole process using pinch analysis. Ghaffari & Shahrokh, 2014 considered the dynamic behaviour and control of an industrial fixed bed ethylene reactor was carried out for the purpose of simulation of a pseudo homogeneous one-dimensional model. Soledar *et al*., 2014 stated that in petrochemical industries, steam cracking furnaces are used to process light hydrocarbons like naphtha, ethane, propane, and LPG in order to obtain olefins, like ethylene and propylene. Shruti (2013) clearly posited that ethylene is the largest volume petrochemical produced in the world. It is an important building block for many chemicals like polyethylene, ethylene dichloride, ethylene oxide and

ethyl benzene. Sarbjit & Chauhan, 2016 stated that environmental degradation due to release of pollution from industrial and transport sector is a major concern presently. Meisong (2000) focused on the development of a simplified ethylene plant model, which includes a thermal cracking section, a separation system and an integrated refrigeration system, and then used it to study plant wide time domain optimization. Ping *et al*., 2015 stated that ethylene production plant is one of the most important units in the petrochemical industry, and the decane cracking furnace is the core of the plant.

In addition, Francisco (2013) considered the detailed modeling and optimization of an ethylene plant processing fresh propane and recycle streams of ethane and propane. Propane was converted in a steam reactor operating at low pressure but high temperature. Sritharan & Saharudin, 2017 stated that a petrochemical plant training new operators to operate plant safely and consistently is a need. Yan, 2000 in his research focused on the development of a simplified ethylene plant model, which includes a thermal cracking section, a separation system and an integrated refrigeration system, and use it to study plant-wide time-domain optimization. Orantos - Borralho, 2013 detailed modelling and optimization of an ethylene plant processing fresh propane and recycle streams of ethane and propane. while Tristan *et al*., 2023 investigated if simple reactor blocks could be combined to adequately represent complex reactor configurations with the objectives of selecting an appropriate reaction scheme, creating a working simulation and validating the results obtained from the simulation. Therefore, ethylene production process plant faces several challenges ranging from the method of production, the optimum operating conditions that will achieve maximum product yield, the optimization method that should be applied and the type of control configuration. In all the investigations as reviewed in the literatures, it was noted that the process was not optimized for maximum conversion of the reactants as the conversion in Tristan *et al*., 2023 was 4.199% in the convection section of reactor while the conversion at the radiation section of the reactor was 76.45% and overall conversion of ethane was 77.73%. Ethylene production process plant faces several challenges ranging from the method of production, the optimum operating conditions that will achieve maximum product yield, the optimization method that should be applied and the type of control configuration that should be used. In previous researches, it was noted that the process was not optimized for maximum conversion of the reactants as the conversion was 4.199% in the convection section of reactor while the conversion at the radiation section of the reactor was 76.45% and overall conversion of ethane was 77.73% (Tristan *et al*., 2023). Also, the maximum conversion of reactants was 62% in the study of Seyed & Younes, 2014. Therefore, there is need for process optimization to meet the high global demand of ethylene. Thus, this research is focused on optimization of a plug flow reactor for the thermal cracking of ethane to ethylene through the development of mathematical model of a plug flow reactor based on the material and energy balance equations from the application of the principle of conservation of mass and energy balance, solution of the developed model equations using MatLab R2020 software via the application of Runge-Kutta ODE45 algorithm, sensitivity analysis performance and process optimization for improved ethylene yield.

2.0 METHODS

2.1 Model Assumptions

To describe the operation of the plug flow packed bed reactor, a mathematical model of the reactor was developed from first principles by applying the principles of conservation of mass and energy. The following assumptions were made in the development of the model equations.

i. The packed bed plug flow reactor operates under steady state condition, that is the accumulation term is zero
ii. Constant density fluid flow system
iii. Components in the reactor moves in a plug flow manner, that is concentration varies along the length of the reactor bed
iv. The reactions are in the same phase (homogenous reactions)

2.2 Mass Balance Model Development

Considering the schematic diagram shown in Figure 1 for a packed bed plug flow reactor

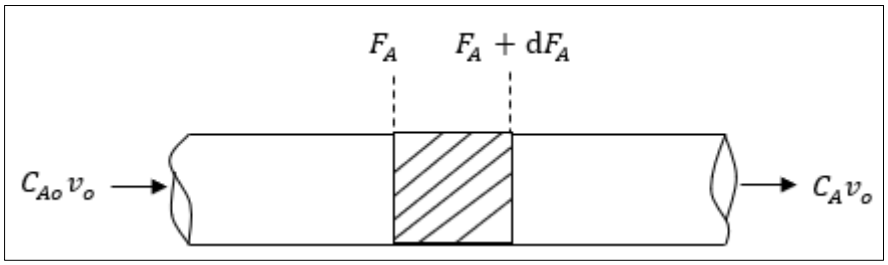

Figure 1: Packed Bed Plug Flow Reactor

The mass balance model can be developed by applying the conservation law of energy thus;

$$\begin{bmatrix}\text{Rate of accumulation of mass within the reactor}\end{bmatrix} = \begin{bmatrix}\text{Rate of mass input into the reactor } system\end{bmatrix} - \begin{bmatrix}\text{Rate of mass output from the reactor } system\end{bmatrix} - \begin{bmatrix}\text{Rate of depletion of mass due to chemical reaction}\end{bmatrix} \quad (1)$$

Defining the terms at steady state and upon variable separation yields

$$V_R = \frac{F_{Ao}}{kC_{AO}} \int_0^x \frac{1}{1-X_A} dx_A \quad (2)$$

Equation (2) is the required mathematical model for the volume of a packed bed plug flow reactor

2.3 Energy Balance Model Development

The energy balance model can be developed by applying the principle of conservation of energy thus;

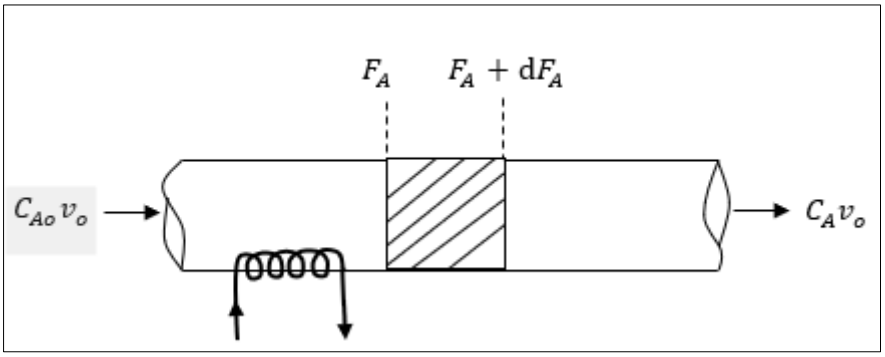

Figure 2: Packed Bed Plug Flow Reactor with Energy Effect

$$\begin{bmatrix}\text{Rate of accumulation of energy within the reactor}\end{bmatrix} = \begin{bmatrix}\text{Rate of Input of energy into the reactor}\end{bmatrix} - \begin{bmatrix}\text{Rate of Output of energy from the reactor}\end{bmatrix} - \begin{bmatrix}\text{Rate of depletion of energy due to chemical reaction}\end{bmatrix} - \begin{bmatrix}\text{Rate of energy removed from the reactor}\end{bmatrix} \quad (3)$$

Defining the energy balance terms at steady state and upon variable separation yields

$$\frac{dT}{dZ} = \frac{\Delta H_R(-r_i)}{U} - \frac{1}{\tau}(T_o - T).\frac{\rho C_p}{U} + \frac{(T_c)}{Z} \quad (4)$$

Equation (4) is the steady state energy balance equation of the packed bed plug flow reactor

2.4 Solution Technique

MatLab software was applied in simulating the developed mass and energy balance differential equations using fourth order Runge-Kutta method, which is also referred as classical fourth order Runge-Kutta. The fourth order Runge-Kutta algorithm are stated thus

$$y_{i+1} = y_i + {}^1\!/_6 (K_1 + 2K_2 + 2K_3 + K_4)h$$

Where:

$K_1 = f(x_i, y_i)$

$K_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}K_1 h\right)$

$K_3 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}K_2 h\right)$

$K_4 = f(x_i + h, y_i + K_3 h)$

2.5 Optimization Technique

Optimization can best be defined as the process of maximizing or minimizing a desired objective function while satisfying the prevailing constraints. Application of optimization principles require good understanding of both the theory and the algorithm as well as the techniques to be used as solution method to the optimization problem. This research applies the technique of second order derivative test to determine the best fractional conversion that gives maximum product yield that can be referred as the optimum product yield. Microsoft excel shall be used to fit the polynomial plots obtained from sensitivity analysis for a polynomial equation generated as a function of fractional conversion versus concentration or as a function of concentration versus fractional conversion. The result generated by MatLab will be differentiated to obtain stationary points, and differentiated a second time to determine if or not a maximum occurs at the stationary point values and if it exists at all the value will be substituted to deduce optimized product yield. The calculus optimization technique applied in this research to optimize product yield from the packed bed plug flow reactor and its flow chart algorithm is shown in Figure 3

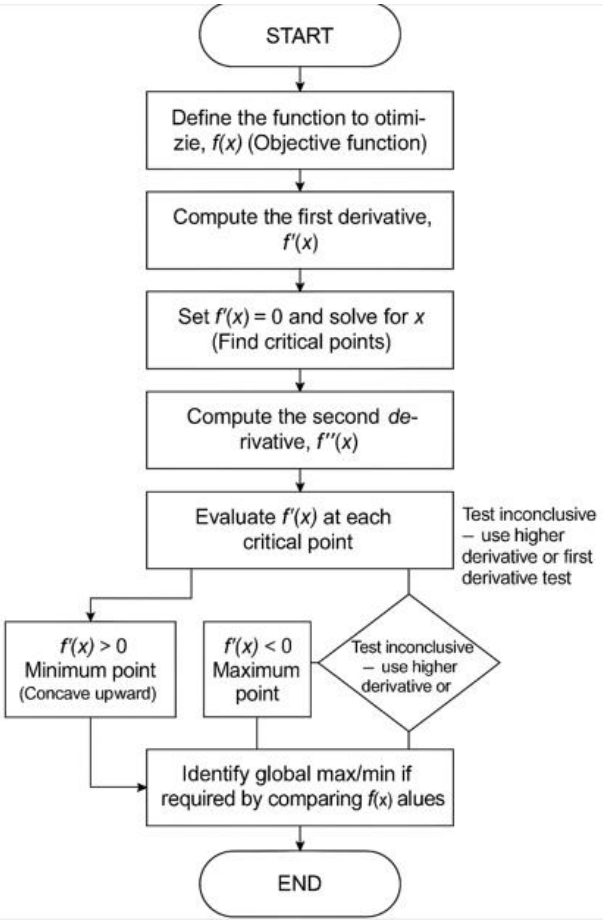

Figure 3: Flowchart of Calculus Optimization Technique

3.0 RESULTS AND DISCUSSION

3.1 Validation of Reactor Simulation Result

The result obtained for the simulation of the packed bed plug flow reactor after solving the developed steady state model equations using Runge-Kutta ODE45 algorithm method were compared with similar study of Seyed & Younes, 2024. This yields 80% ethane conversion in packed bed plug flow reactor as compared to 63% ethane conversion in batch reactor as posited by Seyed & Younes, 2024

3.2 Variation of Ethane and Ethylene Concentration Along Reactor Length

As the reaction proceeded the concentration of ethane decreased from is initial concentration of 100 mol/m^3 to 4.8 mol/m^3 while the concentration of ethylene which is the desired product increased from 0 mol/m^3 to a maximum of 95.2 mol/m^3 along the 20m length of the packed bed plug flow reactor. These variations in ethane depletion and ethylene production are sown in Figure 1 and it is in accordance with the principle and trend of chemical reaction engineering.

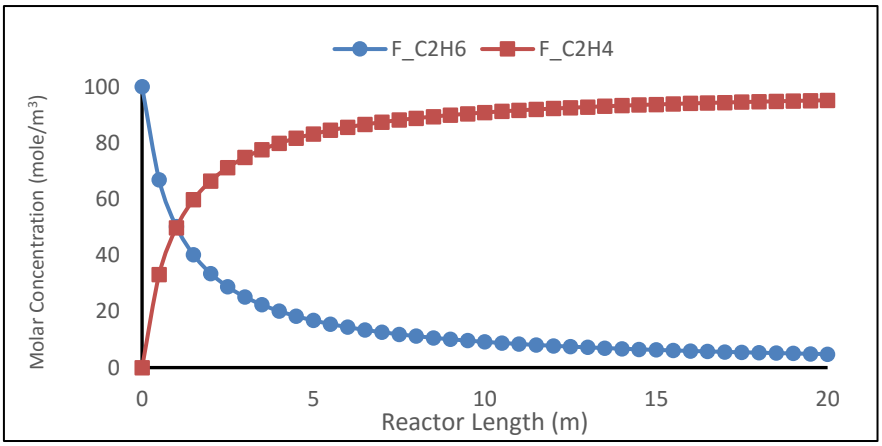

Figure 1: Variation of Concentration Against Reactor Length

Also, the variation of ethane fractional conversion along the reactor length is highlighted in Figure 2, which showed that the fractional conversion of ethane increased from 0 to 0.80, hence the conversion of ethane is 80% while a fractional conversion of 100% may not be feasible in real sense due to unconverted ethane in the process

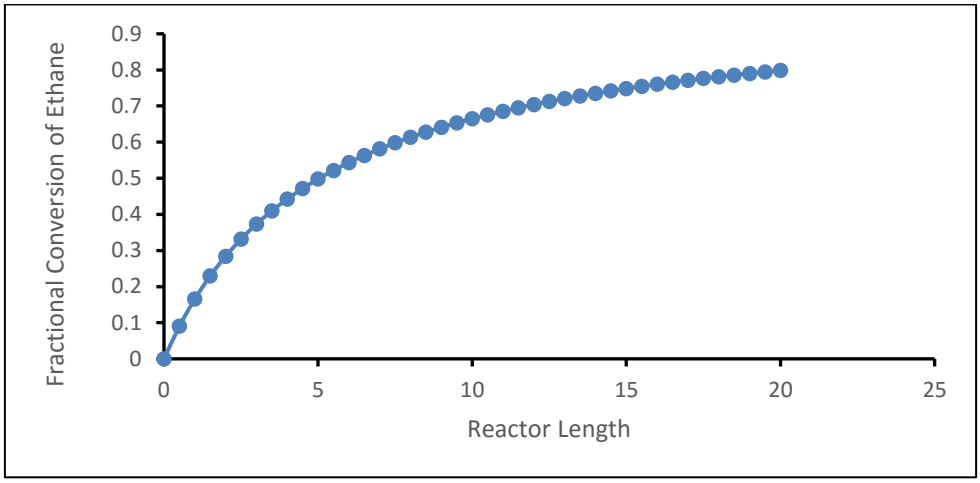

Figure 2: Ethane Fractional Conversion Against Reactor Length

3.3 Temperature Effect Variation Along Reactor Length

The developed steady state energy balance model equation depicts temperature variation along the packed bed plug flow reactor length. Also, chemical reaction engineering principle shows that exothermic reaction process releases heat as the reaction operations proceed. Thus, there is temperature increase (heat liberation) as the conversion of ethane to ethylene occurs in the packed bed plug flow reactor from initial temperature of 950K to exit temperature of 1082.132K as shown in Figure 3. Therefore, a cooling jacket is required for the packed bed plug flow reactor since the operational process is exothermic.

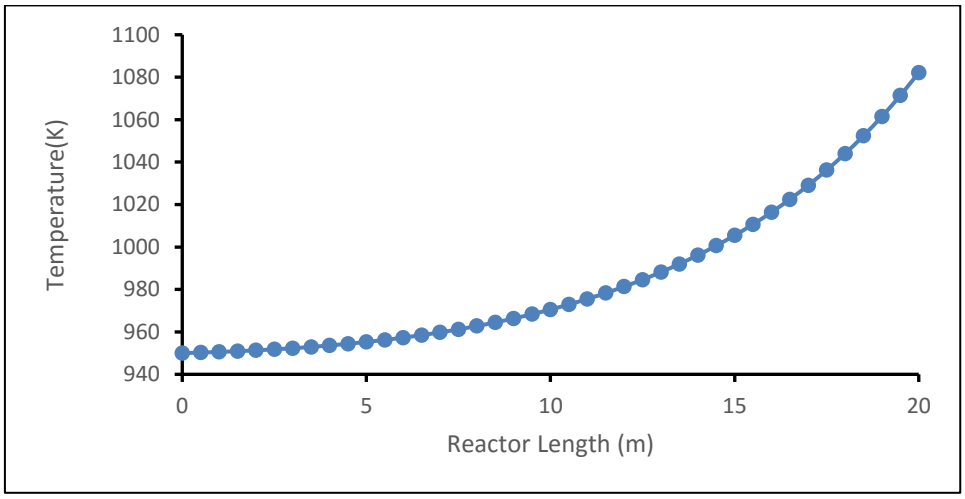

Figure 3: Temperature Profile Along Reactor Length

3.4 Effect of Catalyst Effectiveness Factor

The effect of catalyst effectiveness factor on concentration of ethylene product yield is shown in Figure 4. Catalyst effectiveness factor is the ratio between the observed reaction rate in a pellet and the reaction rate in the absence of intraparticle mass transfer resistances, and it plays an important role in chemical reaction engineering. It is governed by the solution to the reaction-diffusion equation within the catalyst. It can be deduced from Figure 4 that as the value of catalyst effectiveness factor increases from 0.1 to 1, there is improved yield in ethylene product concentration from 15.97mol/m^3 to 19.50mol/m^3. This shows efficient or high activity catalyst favours improved yield of ethylene product.

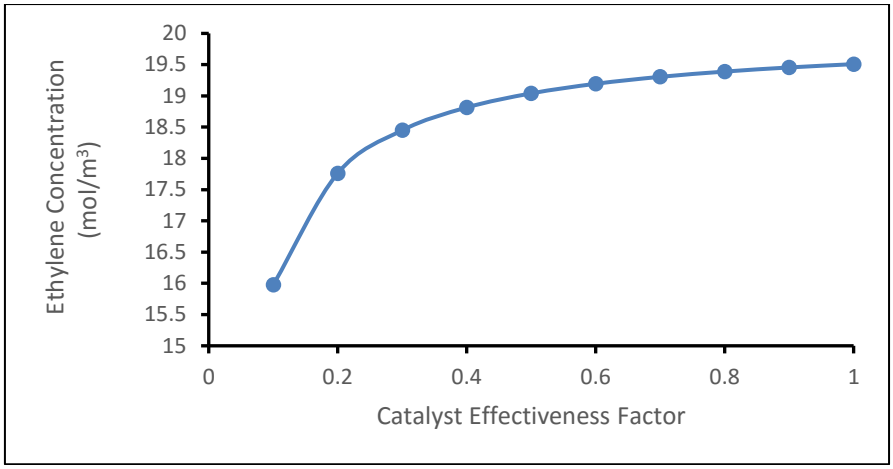

Figure 4: Ethylene Product Concentration Against Catalyst Effectiveness Factor

3.5 Process Optimization Result

Process optimization involves maximizing or minimizing certain objectives while satisfying constraints, thereby leading to improve performance, efficiency, or cost-effectiveness of a chemical process. Sensitivity analysis results of this research were curve fitted to generate a predictive model equation via Microsoft excel. The equation obtained from the curve fitting were then optimized to find the optimum values through the application of MatLab calculus toolbox optimization. The technique involves differentiating the function or model to obtain the second derivative and if the second derivative gives a negative value, then a maximum point is achieved but if it gives a positive value, it is a minimum point.

3.5.1 Optimum Catalyst Effectiveness Factor

The result for the optimum values of catalyst effectiveness factor and ethylene product concentration is presented in Figure 7.

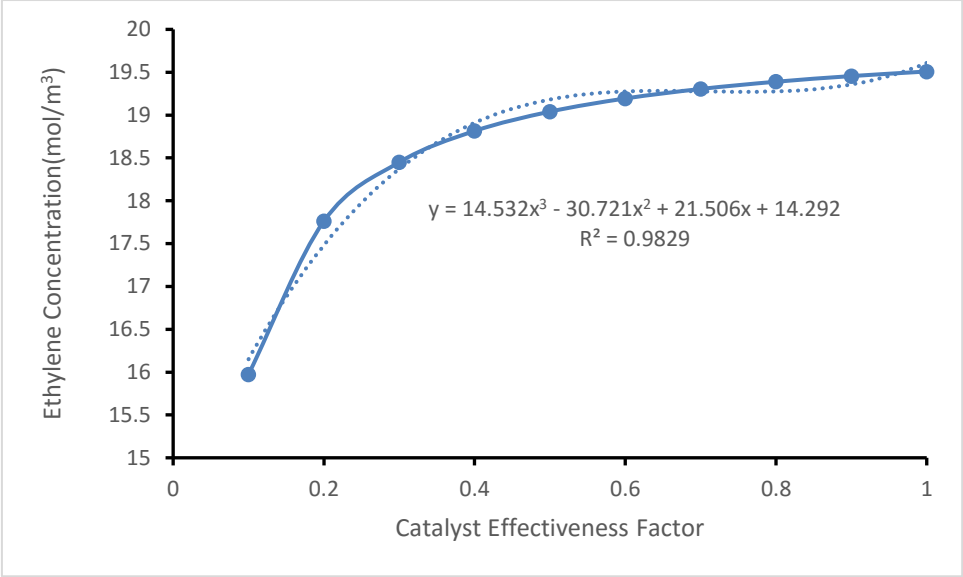

Figure 7: Outlet Temperature Versus Catalyst Effectiveness Factor

The coefficient of determination (R^2) was 0.9829, indicating that the model explains approximately 98.29% of the variation in the experimental data. Differentiation of the fitted polynomial and application of the second derivative test revealed a stationary point at a catalyst effectiveness factor of 0.2467, corresponding to a maximum predicted ethylene concentration of 15.726. Although a minimum point was mathematically identified at a catalyst effectiveness factor of 1.1626, this value lies outside the practical catalyst effectiveness factor range of 0–1 and is therefore not physically meaningful. Considering the feasible operating range, the lowest predicted ethylene concentration was 10.609 at a catalyst effectiveness factor of 1.0. Thus, the model indicates that the optimum catalyst effectiveness factor for maximizing ethylene production is approximately 0.247.

3.5.2 Optimum Volumetric Flow Rate

The result of curve fitting predictive model for volumetric flow rate and ethylene product concentration is depicted in Figure 8. The coefficient of determination

(R^2) was 0.9987 showing that the model explains approximately 99.87% of the variation in the data. Optimization of the fitted model by differentiation revealed a stationary point at a volumetric flow rate of 14.224 mol/m³. The positive second derivative ($d^2y/dx^2 = 0.1084$) confirms that this point corresponds to a minimum ethylene product concentration. The minimum predicted ethylene concentration at this flow rate was approximately 7.78 mol/m³. Thus, the fitted model indicates that a volumetric flow rate of 14.224 mol/m³ represents the condition at which the ethylene concentration reaches its lowest value within the modeled range.

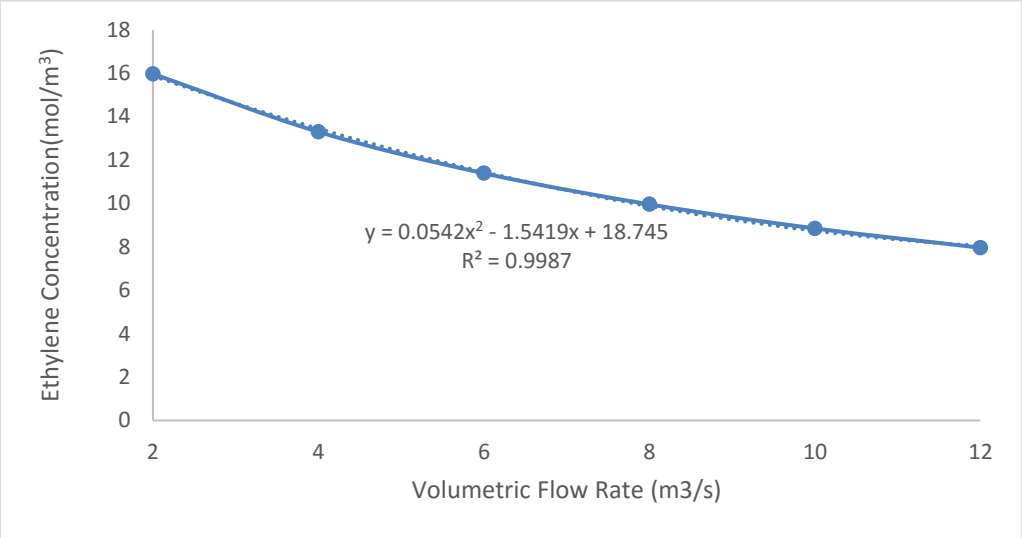

Figure 8: Ethylene Concentration Against Volumetric Flow Rate

3.5.3 Optimum Reactor Temperature

The result for the optimum values of outlet reactor temperature and initial concentration of ethane is presented in Figure 9. The coefficient of determination (R^2) was 0.9894 highlighting that the model explains approximately 98.94% of the variation in the process data. Optimization of the fitted model using the first and second derivative tests revealed a stationary point at an ethane concentration of 55.38 mol/m³. The positive value of the second derivative at this point confirms that it corresponds to a minimum reactor outlet temperature of 1007.43 K. A second stationary point was predicted at an ethane concentration of 115.96 mol/m³, corresponding to a maximum reactor outlet temperature of 1040.46 K. However, this concentration lies outside the investigated operating range of 38.3–100 mol/m³ and is therefore not physically attainable within the scope of the study. Consequently, only the minimum temperature point at 55.38 mol/m³ represents a valid optimum within the curve fit domain.

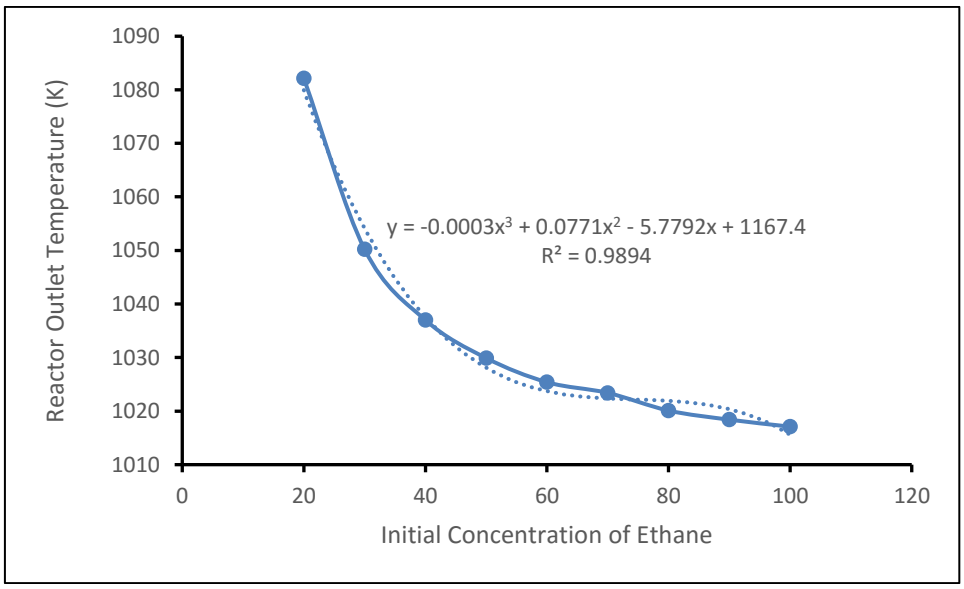

Figure 9: Reactor Outlet Temperature Against Ethane Concentration

4.0 CONCLUSION

The optimization of ethylene production in a plug flow reactor (PFR) was investigated in this research through the application of the fundamental principle of material and energy balance equations. The developed models incorporated reaction kinetics based on the Arrhenius equation and accounted for the endothermic nature of the cracking process, enabling the prediction of concentration and temperature variations along the reactor length. The resulting model equations were solved using MatLab numerical solvers thereby providing accurate predictions of reactor performance under varying operating conditions. The simulation results demonstrated the expected behavior of industrial steam-cracking reactors, where ethylene production is strongly influenced by reactor temperature, feed composition, catalyst effectiveness, and volumetric flow rate. Optimization of the fitted predictive models revealed several important operating conditions that include catalyst effectiveness factor model with R^2 value of 0.9829, predicted a maximum ethylene concentration of approximately 15.73 mol/m³ at a catalyst effectiveness factor of 0.2467 within the feasible operating range. The volumetric flow rate model, which exhibited an excellent fit with R^2 value of 0.9987 indicated that a flow rate of 14.224 mol/m³ corresponded to the minimum predicted ethylene concentration of approximately 7.78 mol/m³. Furthermore, the reactor temperature model with R^2 value of 0.9894, predicted a minimum outlet reactor temperature of 1007.43 K at an initial ethane concentration of 55.38 mol/m³. Although the fitted model mathematically predicted a maximum temperature at an ethane concentration outside the investigated operating range, this optimum was not physically attainable and was therefore excluded from practical consideration. Thus, the deductions from this research showed that mathematical modeling combined with simulation and optimization techniques provides an effective approach for improving ethylene reactor performance. The developed framework can serve as a valuable tool for process design, operational decision-making, and optimization of industrial ethylene production system.

REFERENCES

- Francisco, J. O. (2013). *Detailed modeling and optimization of an ethylene plant* [Master's thesis, University of Lisbon]. University of Lisbon Campus Repository.
- Ghaffari, S., & Shahrokhi, M. (2014). Modeling and control of an ethylene oxide reactor. *Proceedings of the 8th International Chemical Engineering Congress and Exhibition (ICHEC), 8*(1), 24–27.
- Jeiveison, G. S., Rafael, B. D., Argimiro, R. S., Priamo, A. M., Roberto, W. D., & Gabriel, S. G. (2018). Process modeling and simulation of an industrial-scale plant for green ethylene production. *Industrial & Engineering Chemistry Research, 57*(18), 64–76.
- Kemal, L., Nedim, O., & Zeljko, J. (2013). Identification of an ethane–ethylene distillation column system: A procedure for MINO system identification using the IDENT toolbox. *Proceedings of the 21st Telecommunications Forum (TELFOR), 5*(1), 26–38.
- Mahir, J., Yoel, S., Vladimir, M., & Prashant, M. (2021). Adaptive system identification of industrial ethylene splitter: A comparison of subspace identification and artificial neural networks. *Computers & Chemical Engineering, 147*(7), 107–117.
- Meisong, B. E. (2000). *Simulation and optimization of an ethylene plant* (Master's thesis, Texas Tech University, Department of Chemical Engineering).
- Muhammad, M., Muhammad, A., Iftikhar, A., & Muhammad, N. A. (2021). Process modeling and simulation of ethylene oxide production by implementing pinch cost analysis. *Engineering Physics and Mathematics, 21*(1), 1–9.
- Orantos-Borralho, F. J. (2013). *Detailed modelling and optimisation of an ethylene plant* (Master's thesis, Instituto Superior Técnico, Lisbon, Portugal).
- Ping, L., Tian, L., & Jiangtao, C. (2015). Advanced process control on ethylene cracking furnace. *Measurement and Control, 48*(2), 50–53.
- Sarbjit, S., & Chauhan, S. (2016). Modeling and simulation of catalytic converters for oxidation of hydrocarbon pollutant ethylene. *International Journal of Advanced Research in Science and Engineering, 5*(8), 645–654.
- Seyed, H. E., & Younes, A. (2014). *Mathematical modeling for production unit of ethylene by steam cracking process.* Retrieved from https://www.researchgate.net/publication/237047017.
- Shruti, P. (2013). *Simulation and multi-objective optimization of cold-end separation process of an ethylene plant* (Master's thesis, National University of Singapore).
- Soledar, A., Christman, A. R., & Muniz, S. P. (2014). Modeling and simulation of the ring length of an ethane furnace for industrial application. *Journal of Chemical Engineering, 5*(8), 171–182.
- Sritharan, S., & Saharudin, H. (2017). Operator training simulator for ethylene plant. *Chemical Engineering Transactions, 56*(1), 1621–1626.
- Tristan, L. Z., David, L., Swamy, K., & Meikap, B. C. (2023). Modeling and simulation of ethane cracker reactor using Aspen Plus. *South African Journal of Chemical Engineering, 43*(1), 204–214.
- Yan, M. (2000). *Simulation and optimization of an ethylene plant* (Master's thesis, Texas Tech University, Department of Chemical Engineering). Retrieved from https://ttu-ir.tdl.org/handle/2346/etd-01202001-312144.

Nomenclature

$\emptyset$ = average slope used to make the final prediction at the end of the interval
h = step size
x_i = independent variable
y_i = dependent variable
k_1 = slope at the end of the first interval
k_2= slope at the end of the second interval
k_3= slope at the end of the third interval
k_4 = slope at the end of the fourth intervals