Article History: *Received: 3rd May, 2024 Revised: 4th July, 2024 Accepted: 17th July, 2024*

CARITAS UNIVERSITY AMORJI-NIKE, EMENE, ENUGU STATE
Caritas Journal of Chemical Engineering and Industrial Biotechnology
CJCEIB, Volume 1, Issue 1 (2024)

Development of the Kinetic Parameters for Enhanced Production of Ethylene Glycol in a Continuous Stirred Tank Reactor

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ABSTRACT

This research aims to optimize the kinetic parameters of the ethylene glycol production process in a Continuous Stirred Tank Reactor (CSTR) using Matrix Laboratory (MATLAB) simulations to enhance the efficiency of the process. Ethylene glycol is a petrochemical product that plays an essential role in various industries due to its applications in the production of paint, polyesters, synthetic waxes, plastics, coolants, and automotive radiators. As such, process industries have been making significant efforts to produce ethylene glycol more effectively. The proposed method involved the simulation of the CSTR process using MATLAB based on the principles of mass and energy conservation. The initial and final reaction kinetic parameters for the process were obtained from literature data and were optimized using an Excel spreadsheet and the simulation tool. The optimized kinetic parameters resulted in better performance characteristics as indicated by the profiles of temperature and concentration of ethylene glycol, which indicated a significant increase in the yield of ethylene glycol using the optimized parameters. The optimized kinetic parameters were found to be (21793kJ/mol and 88.9781g/mol) for activation energy, (0.044185-1 and 0.07035-1) for the pre-exponential factor, and (0.70% and 0.10%), (0.01% and 0.18%), and (0.87% and 34.10%) for the rate constant, temperature, and catalyst loading, respectively. These optimized parameters led to higher yields and purities of the target product, ethylene glycol, indicating that the optimization of kinetic parameters was an effective strategy for enhancing the efficiency of the ethylene glycol production process. The simulation of the CSTR process using MATLAB and the optimization of kinetic parameters showed promising results in enhancing the efficiency of the ethylene glycol production process. The model proposed in this research can be used as a basis for designing more efficient and cost-effective processes for ethylene glycol production and other chemical reactions in CSTRs.

Keywords: ***CSTR, Ethylene Glycol, Models, Optimization, Petrochemicals***.

1. INTRODUCTION

Ethylene glycol is an important petrochemical product used in numerous industrial applications, including the production of paints, plastics, and synthetic waxes [1]. It is also widely used in the automotive industry as a coolant. Consequently, there is a high demand for ethylene glycol worldwide, and production processes need to be optimized to ensure maximum efficiency. The most common method for producing ethylene glycol is by reacting ethylene oxide with water in a Continuous Stirred Tank Reactor (CSTR). The reaction kinetics of this process are complex and require accurate optimization to improve the yield and quality of the final product [2,3].

In recent years, mathematical modelling and simulation have become a popular approach to optimizing chemical processes [4]. The unique advantage of this approach is that it allows for a more accurate prediction of the behaviour of the system under different conditions. MATLAB, a widely used numerical computing software, is an excellent tool for simulating complex chemical processes [5,6]. There is still a gap in the literature on the optimization of kinetic parameters for the enhanced production of ethylene glycol in a CSTR using MATLAB simulation. The novelty of this research lies in the development of a comprehensive optimization model using MATLAB simulation. This study presents an approach to optimizing the kinetic parameters of the ethylene glycol production process in a CSTR using MATLAB simulations. The approach leverages the principles of mass and energy conservation to simulate the reactions that occur in the CSTR. The optimized kinetic parameters were obtained by using central composite design (CCD) techniques. The study considered the initial and final kinetic parameters of the reaction process, such as activation energy, pre-exponential factor, and rate constant. Using the optimized kinetic parameters, the yield and purity of the ethylene glycol increased drastically, which suggests that the proposed model could be used to improve the efficiency of the ethylene glycol production process in industrial settings. This study represents an important contribution to the optimization of the ethylene glycol production process. The use of MATLAB simulations, and techniques provides a novel and comprehensive optimization model that can be applied to improve other chemical reactions in CSTRs.

Design models of a continuously stirred tank reactor (CSTR) where propylene oxide hydrolysis occurs for propylene glycol production using the principle of mass and energy balance. The developed models were simulated using MATLAB for the determination of the reactor parameters such as volume, height, diameter, space-time, and space velocity at fractional conversion between 0.1 to 0.9. The relationship between changes in reactor parameters and fractional conversion was presented in profiles [7,8]. Ethylene glycol can be produced from the non-catalytic hydrolysis of ethylene oxide in a continuously stirred tank reactor. They developed the reaction kinetic scheme of the process and applied the principles of mass and energy conservation in the development of mass and energy balance models of the process as well as the process control models for optimum performance of the process[9]. According to the researchers, ethylene glycol also called ethane-1,2-diol is an organic compound that is often used in the production of polyester, fibres, fabrics, solvents for paints and plastics, etc. Ethylene glycol (EG) production in industries can either be via a catalytic process where the reaction is catalyzed by an acid or base on non-catalytic where the reaction is catalyzed by an acid or base or non-catalytic where the reaction occurs at neutral pH and appreciable rise in temperatures noted that the latter is most widely used [9]. The mass, energy, and process control models were simulated using MATLAB and the result shows that the configuration of the process control closed loop system enhances process stability and optimum yield of the target product or product of interest [10,11].

One of the most used techniques of organic synthesis is the production of mono-ethylene glycol (MEG) also known as ethylene glycol (EG) and its analogue; di-, tri-, tetra-, and poly-ethylene glycols and developed unsteady state models of the non-catalytic process of ethylene oxide hydrolysis. The researcher noted that ethylene glycol is most widely used in the production of polyethene terephthalate and antifreeze while production of polyethylene glycols is used in the production of resin for the gas drying process [12,13]. The research focused on the application of energy and material balance in the development of mathematical models of stirred mixing tanks, lest exchangers, and tubular reactors [14,15]. Linearization of the developed models using the standard method and investigation of the performance of the hydrolysis process using an optimal control system concluded that commercial production of ethylene glycol is via hydrolysis of ethylene oxide [16].

kinetic investigation of consecutive-parallel reactions is a suitable technology for the organic synthesis of ethylene glycol. It considered the development of elementary steps of the scheme (rate laws) and the application of the conservation of mass and energy for the process model development which was simulated using MATLAB as the simulation tool [17,18]. Ethylene oxide can be produced from the reaction of ethylene and oxygen in the presence of a silver catalyst on an alumina oxide carrier at a pressure of approximately 20 bar and temperature of 250^0C. This reaction occurs in flow reactors (plug flow reactors or continuous stirred tank reactors [19,20]. However, the researcher concentrated on the development of a plug flow reactor design model from the principle of mass and energy balance which was simulated using HYSYS and Aspen Plus [21,22].

The use of an In Vitro Enzymatic Cascade Technology in the production of ethylene glycol from glycerol has been studied by researchers. According to the researchers, the use of glycerol for ethylene glycol production is locally content-driven and economically viable since glycerol is readily available and cheap from the production of biofuel. Several researches have shown that biofuel can be produced from plant and animal sources and during the process, glycerols are produced or released as waste (by-product) [23,24]. The In Vitro Enzymatic Technology can be employed in the conversion of this waste to more value-added products like propylene glycol in process industries thereby making this research method/approach a waste-to-wealth program. The research, however, did not consider the reacting media or equipment sizing or design as well as process control strategies for optimum production. Ethylene glycol (EG) also called mono-ethylene glycol (MEG) is the simplest glycol, the first of a homologous series of three dihydroxy alcohols, namely mono, di, and triethylene glycol (MEG, DEG, and TEG). Industrially, ethylene glycol is produced from the hydrolysis of ethylene oxide. The researcher also focused on the health, safety, and environmental factors considerations in ethylene glycol production and considered toxicology, safety, and environmental considerations involved in the process [25]. Laboratory studies have shown is not highly irritating to human skin because of its low penetrating power and absorption through human skin. This low rate of absorption prevents high concentrations of ethylene glycol and its toxic breakdown products from accumulating in the bloodstream. A splash of glycol liquids in the eyes may cause temporary discomfort or irritation but permanent damage is not likely to occur [26].

Ethylene glycol has a high flash point of 240^0F (115^0C) and cannot readily ignite but can burn when exposed to heat and flames. In the case of an accidental discharge, the following protective measures should be taken. Eliminate potential sources of ignition like smoking, flares spark, or flames in the immediate area, Body contact with all spilled materials should be prevented, and wear appropriate personal protective equipment (PPE) when responding to spills [27]. Ethylene glycol is readily biodegradable and thus will not remain in the environment. Its theoretical oxygen demand (THOD) is 1.29P/P (parts per part) while its biological oxygen demand (BOD) is 1.15P/P parts per part [28]. Under both aerobic and anaerobic conditions, biodegradation is expected to be highly moderate, Commercial production of ethylene glycol is via non-catalytic thermal hydrolysis of ethylene oxide in water which is capable of producing chiefly mono-di, and triethylene glycol and a small amount of tetraethylene and heavier glycols [29,30].

Previous studies on the production of ethylene glycol in a Continuous Stirred Tank Reactor (CSTR) have mainly focused on various optimization methods to improve the yield and quality of the final product. However, there are knowledge gaps and inconsistencies in the existing literature regarding the optimization of kinetic parameters for the enhanced production of ethylene glycol. Most studies have relied on empirical methods for optimization, which do not provide a comprehensive understanding of the underlying chemical reactions. This limits the accuracy and reliability of the results. Few studies have explored the use of mathematical models to simulate the complex reaction kinetics of the CSTR [31,32]. The current approaches to optimizing the kinetic parameters of the ethylene glycol production process in CSTRs have not fully explored the effect of variations in the temperature, pressure, and reactant concentrations. Such variations are widely used in industrial processes, yet their impact on the kinetics of the CSTR reaction has not been adequately investigated. There is a lack of studies that have attempted to optimize the kinetic parameters of the ethylene glycol production process using MATLAB simulations. While MATLAB is a powerful tool for simulating complex chemical reactions, its potential in the optimization of CSTR reaction kinetics has not been fully explored in the literature. These inconsistencies in the existing literature highlight the need for further research into the optimization of the

kinetic parameters for the enhanced production of ethylene glycol in a CSTR using MATLAB simulations [33,34]. This research aims to address these issues and contribute to the development of more accurate and reliable optimization methods for the production of ethylene glycol.

2.0 Methodology

2.1 Development of the Reaction Kinetic Scheme of the Process

The reaction kinetic scheme of ethylene oxidation to form ethylene oxide and the hydrolysis of ethylene oxide to produce ethylene glycol is presented below [35].

$$\text{Ethylene + oxygen} \xrightarrow{K_1} \text{ethylene oxide + water} \xrightarrow{K_2} \text{ethylene glycol} \quad (1)$$

Equation (1) can be expressed molecularly as

$$C_2H_4 + O_2 \xrightarrow{K_1} C_2H_4O + H_2O \xrightarrow{K_2} C_2H_6O_2 \quad (2)$$

Equation (2) can be expressed symbolically in terms of reactant and product of interest as;

$$A \xrightarrow{K_1} B \xrightarrow{K_2} C \quad (3)$$

Where A represents ethylene, B is ethylene oxide and C represents ethylene glycol, K_1 and K_2 represents the kinetic rate constants which is an indication that the reaction process is temperature-dependent and the process condition is non-isothermal. The rate constants are a function of temperature and activation energy as shown in equations (4) and (5) respectively.

$$K_1 = K_{10}\, e^{\left(-E_1/RT\right)} \quad (4)$$

$$K_2 = K_{20}\, e^{\left(-E_2/RT\right)} \quad (5)$$

Where K_{10} is the Arrhenius constant also called the pre-exponential constant of the first reaction process for the production of ethylene oxide from ethylene, K_{20} is also the Arrhenius or pre-exponential constant of the second reaction process for the production of ethylene glycol from the hydrolysis of ethylene oxide, E_1 and E_2 are the activation energies in kJ/kmol of ethylene oxide and ethylene glycol respectively. T_1 and T_2 are the respective temperatures of the processes in Kelvin and R is the gas constant in J/molk.

The rate expression of the series of reactions occurring consecutively can be expressed as a function of feed rate depletion as follows [36]:

For the depletion of ethylene to produce ethylene oxide, the rate law is expressed mathematically as:

$$-r_A = \frac{-dC_A}{dt} = K_1 C_A \quad (6)$$

Where $-r_A$ is the rate of depletion of ethylene, C_A is the concentration of ethylene after the reaction in mol/m^3 and t is the reaction time in seconds.

For the formation of ethylene oxide and its depleting rate for ethylene glycol production, the rate law can be expressed mathematically as [37]:

$$-r_B = \frac{-dC_B}{dt} = -K_1 C_A + K_2 C_B \quad (7)$$

Finally, the rate law for the production of ethylene glycol from the depletion of ethylene oxide is mathematically expressed as:

$$-r_C = \frac{-dC_C}{dt} = -K_2 C_B \quad (8)$$

Where $-r_B$ is the rate of reaction for ethylene oxide formation and its depleting rate, $-r_C$ is the ethylene glycol formation rate and C_B is the concentration of ethylene oxide in mol/m^3.

Substituting equations (4) and (5) into equations (6), (7), and (8) respectively yields

$$\frac{-dC_A}{dt} = K_{10}\, e^{\left(-E_1/RT_1\right)} C_A \quad (9)$$

$$\frac{-dC_B}{dt} = K_{20}\, e^{\left(-E_2/RT_2\right)} C_B - K_{10}\, e^{\left(-E_1/RT_1\right)} C_A \quad (10)$$

$$\frac{-dC_C}{dt} = K_{20}\, e^{\left(-E_2/RT_2\right)} C_B \quad (11)$$

Equation (11) is the rate expression or model for ethylene glycol production and can be expressed in terms of fractional conversion as follows [38]:

$$-r_C = -K_{20}\, e^{-E_2/RT_2} C_{B0}(1 - X_B) \quad (12)$$

2.2 Development of CSTR Optimization Models

Consider the schematic representation of CSTR in series for oxidation of ethylene and hydrolysis of ethylene oxide for ethylene glycol production as shown below:

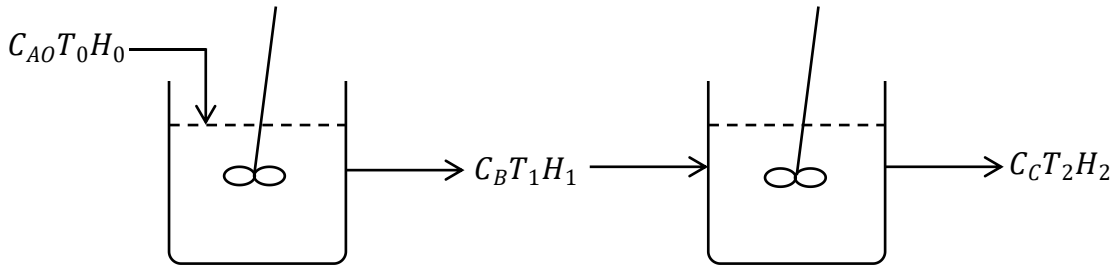


Figure 1: CSTR in Series for Ethylene Glycol Production

The feed stream consists of Ethylene oxide and Water, While the product stream is Ethylene glycol Optimization Assumptions are: The feed assumes a uniform composition throughout the reactor, The reacting mixture is well stirred, the composition of the exit stream is the same as that within the reactor, Shaft work by the impeller or the stirrer is negligible, and that the temperature within the reactor is kept at a constant value by the heat exchange medium [39].

The optimization models can be developed from the first principle of mass and energy balance below [40]:

$$\begin{bmatrix} Rate\ of \\ Accumulation \\ of\ material \end{bmatrix} = \begin{bmatrix} Rate\ of \\ inflow\ of \\ material \end{bmatrix} - \begin{bmatrix} Rate\ of \\ outflow\ of \\ material \end{bmatrix} - \begin{bmatrix} Rate\ of\ depletion \\ of\ materials\ due\ to \\ chemical\ reaction \end{bmatrix} \quad (13)$$

For ethylene, denoted as specie A, the terms in equation (13) can be defined as follows:

$$\begin{bmatrix} Rate\ of \\ Accumulation \\ of\ material \end{bmatrix} = -\frac{dC_A}{dt} \quad (14)$$

$$\begin{bmatrix} Rate\ of \\ inflow\ of \\ material \end{bmatrix} = v_O C_{AO} \quad (15)$$

$$\begin{bmatrix} Rate\ of \\ outflow\ of \\ material \end{bmatrix} = v_O C_A \quad (16)$$

$$\begin{bmatrix} Rate\ of\ depletion \\ of\ materials\ due\ to \\ chemical\ reaction \end{bmatrix} = K_1 C_A V_R \quad (17)$$

Combining equation (14) to (17) into equation (13) yields

$$-\frac{dC_A}{dt} = v_O C_{AO} - v_O C_A - K_1 C_A V_R \quad (18)$$

At steady state, $-\frac{dC_A}{dt} = 0$ and equation (18) transforms to

$$C_A = \frac{C_{AO}}{1+K_1\tau} \quad (19)$$

where C_{AO} is the initial concentration of ethylene in mol/m^3, and τ is the space-time in seconds.

For ethylene oxide donated as specie B, the terms in equation (13) can be defined as follows [41]:

$$\begin{bmatrix} Rate\ of \\ Accumulation \\ of\ material \end{bmatrix} = -\frac{dC_B}{dt} \quad (20)$$

$$\begin{bmatrix} Rate\ of \\ inflow\ of \\ material \end{bmatrix} = v_O C_{BO} \quad (21)$$

$$\begin{bmatrix} Rate\ of \\ outflow\ of \\ material \end{bmatrix} = v_O C_B \quad (22)$$

$$\begin{bmatrix} Rate\ of\ depletion \\ of\ materials\ due\ to \\ chemical\ reaction \end{bmatrix} = K_1 C_B V_R \quad (23)$$

Assuming a constant volume, $V_O = V_i = V$

Combining equation (20) to (23) into equation (13) yields

$$-\frac{dC_B}{dt} = v_O C_{BO} - v_O C_B - K_2 C_B V + K_1 C_A V \quad (24)$$

At a steady state, $\frac{dC_B}{dt} = 0$ and let the initial concentration of ethylene oxide be zero

$$C_B = \frac{K_1 \tau C_A}{1+K_2\tau} \quad (25)$$

Substituting equation (19) into (25) yields

$$C_B = \frac{K_1\tau C_A}{1+K_2\tau}\left(\frac{C_{AO}}{1+K_1\tau}\right)$$

$$C_B = \frac{K_1\tau}{(1+K_2\tau)(1+K_1\tau)}C_{AO} \quad (26)$$

For ethylene glycol, denoted by specie C, the terms in equation (19) can be defined as follows;

$$\begin{bmatrix} Rate\ of \\ Accumulation \\ of\ material \end{bmatrix} = \frac{dC_C}{dt} \quad (27)$$

$$\begin{bmatrix} Rate\ of \\ inflow\ of \\ material \end{bmatrix} = v_O C_{BO} \quad (28)$$

$$\begin{bmatrix} Rate\ of \\ outflow\ of \\ material \end{bmatrix} = v_O C_B \quad (29)$$

$$\begin{bmatrix} Rate\ of\ depletion \\ of\ materials\ due\ to \\ chemical\ reaction \end{bmatrix} = K_2 C_B V_R \quad (30)$$

Assuming a constant volume, $v_O = v_i = v$

Combining equation (27) to (30) into equation (13) yields

$$\frac{dC_C}{dt} = v_O C_{BO} - v_O C_C + K_2 C_B V \quad (31)$$

At a steady state, $\frac{dC_C}{dt} = 0$, equation (31) transforms to:

$$C_C = K_2\tau C_B \quad (32)$$

Substituting equation (26) into equation (32) yields

$$C_C = \frac{K_1K_2\tau^2}{(1+K_2\tau)(1+K_1\tau)}C_{AO} \quad (33)$$

The yield of ethylene glycol Y_C can be obtained from equation (33) as follows;

$$\frac{C_C}{C_{AO}} = Y_C = \frac{K_1K_2\tau^2}{(1+K_2\tau)(1+K_1\tau)} \quad (34)$$

Where Y_C is the yield of ethylene glycol in percentage (%)

2.3 Determination of Optimum Time (τ) and Yield of Ethylene Glycol

This can be obtained by considering equation (34) as follows;

$$Y_C = \frac{K_1K_2\tau^2}{(1+K_2\tau)(1+K_1\tau)} \quad (35)$$

At an optimum point, $\frac{dY_C}{d\tau} = 0$

In equation (35), applying the quotient rule of differentiation is as follows:

$$Y_C = \frac{U}{V}$$

$$\frac{dY_C}{d\tau} = \frac{\frac{VdU}{d\tau} - \frac{UdV}{d\tau}}{V^2} \quad (36)$$

where,

$$U = K_1 K_2 \tau^2 \quad (37)$$

$$\frac{du}{d\tau} = 2K_1 K_2 \tau \quad (38)$$

Also, $V = (1 + K_1\tau)(1 + K_2\tau)$ (39)

Expanding equation (39) yields

$$V = 1 + K_2\tau + K_1\tau + K_1 K_2 \tau^2 \quad (40)$$

$$\frac{dv}{d\tau} = K_2 + K_1 + 2K_1 K_2 \tau \quad (41)$$

Combining equation (37) to (41) into equation (36) yields

$$\tau_{opt} = \frac{-2}{K_1 + K_2} \quad (42)$$

Equation (42) is the optimum space-time for ethylene glycol production

At τ_{opt}, equation (35) becomes,

$$Y_{C,opt} = \frac{K_1 K_2 \tau_{opt}^2}{(1+K_1\tau_{opt})(1+K_2\tau_{opt})} \quad (43)$$

Substituting equation (42) into (43) yields

$$Y_{C,opt} = \frac{2}{1 - \frac{K_2}{2K_1} - \frac{K_1}{2K_2}} \quad (44)$$

Equation (44) is the optimum yield for ethylene glycol production

2.4 Kinetic Parameter Optimization

Kinetic parameters such as the Arrhenius constant also called the pre-exponential constant (A_1 and A_2), the activation energies (E_1 and E_2) as well as the rate constants (K_1 and K_2) can be optimized for optimum production of ethylene glycol as follows [42]:

Optimized: $C_C = f(K_i T, t)$ (45)

Subject to: $\frac{dC_A}{dt} = -K_1 C_A$ (46)

$$\frac{dC_B}{dt} = K_1 C_A - K_2 C_B \quad (47)$$

$$K_i = K_{i,O}\, e^{-E_i/RT_i} \quad (48)$$

$$C_{A(O)} \geq 0 \quad (49)$$

$$C_{B(O)} \geq 0 \quad (50)$$

$$T_{i,O} \geq 0 \quad (51)$$

And $C_C, C_B, C_A, K_{i,O}, E_i, K_i, T_i \geq 0$ (52)

This optimization of kinetic parameters models can be resolved using a numerical optimizer or statistical approach. In this research, the statistical approach was used. The objective function(s) for the optimization method is given:

$$S = \sum_{i=1}^{n} \left[\left(y_{i,plant} - y_{i,cal.} \right)^2 + \left(T_{O,plant} - T_{O,cal.} \right)^2 \right] \quad (53)$$

Where $y_{i,plant}$ and $y_{i,cal}$ are the mole fractions of species i in plant and model respectively while $T_{O,plant}$ and $T_{O,cal}$ are temperatures of plant data and model respectively

$$\bar{y}_i = \frac{\Sigma y_i}{n} \quad (54)$$

$$\overline{T}_i = \frac{\Sigma T_i}{n} \quad (55)$$

Where, $\bar{y}_i$ and $\overline{T}_i$ are the mean values of the mole fractions and temperature of species i. The sum of the square mean (SSM) is given as:

$$SSM = \sum_{j=1}^{n} \left[\left(y_{i,cal} - \bar{y}_{o,cal.} \right)^2 + \left(T_{o,plant} - \overline{T}_{o,cal.} \right)^2 \right] \quad (56)$$

The F_{cal} or computed F_{-value} is given as

$$F_{cal} = \frac{SSM/P}{SSE/_{n-p}} = \frac{MSM}{MSE} \quad (57)$$

Where SSE is the sum of the residual errors computed as

$$SSE = \sum_{j=1}^{m} \left[\left(y_{i,plant} - y_{i,cal.} \right)^2 + \left(T_{o,plant} - T_{o,cal.} \right)^2 \right] \quad (58)$$

Where MSM is the mean of the square mean which is mathematically given as

$$MSM = \frac{SSM}{P} \quad (59)$$

The mean of square error is mathematically given as

$$MSE = \frac{SSE}{n-p} \quad (60)$$

Where p is the number of kinetic parameters to be optimized and n is the number of iterations obtained from the simulation of the models or experimental data number.

F_{tab} will be obtained from the statistical table at a 5% confidence level which will be compared with F_{cal}. The value of F_{tab} is a function of the degree of freedom (df) and the corrected degree of freedom at the interval of $(1 - \propto, p-1, n-p)$ where $\propto$ is the confidence interval:

The optimized activation energy is the Arrhenius constant which depends on the convergence of the iterations which is given as [43]:

$$E_i^{j+1} = E_i^j + \propto D \quad (61)$$

$$E_{o,i} = K_{o,i}^j + \propto D \quad (62)$$

Where $\propto$ is a scalar factor or a range $0 < \propto < 1$ and D is the increment given as

$$D = -(J_r J_r^T)^{-1} J_r \quad (63)$$

Where, J_r is matrix of $(n \times p)$, J_r^T is the transpose of matrix J_r that is $(p \times n)$ and $(J^r J_r^T)^{-1}$ is the inverse of the product of the matrix J_r and its transpose J_r^T.

Hence, $D = -[(n \times p)(p \times n)]^{-1}(n \times p)$ (64)

The criterion for termination of iteration of the simulation of equations (61) and (62) depends on if $F_{cal} \geq F_{tab}$ at 5% confidence level, iteration will be terminated. Current values of E_i^{j+1} and $K_{o,i}^{j+1}$ are the optimized value, else, continue iterations until convergence is achieved.

The optimal value of the rate constant will be obtained using

$$K_{i,opt} = K_{o,i}^{j+1} e^{\left(-E_i^{j+1}/RT\right)} \quad (65)$$

Where $K_{i,opt}$ is the optimum kinetic rate constant for species? K_i, R is the ideal gas constant in J/molK and T is the absolute temperature in Kelvin [44].

2.5 Data for Evaluation

The data for evaluation in this research are the properties/thermodynamic data, calculated/derived data, and data obtained from pieces of literature as presented in Tables 1-3 respectively.

Table 1: Properties/Thermodynamic Data

Data/parameter	Values	Description
ρ_A	$882\ kg/m^3$	Density of ethylene oxide
ρ_B	$997\ kg/m^3$	Density of water
ρ_C	$1110\ kg/m^3$	Density of ethylene glycol
P_0	$101325\ N/m^3$	Initial pressure
R	$8314\ Nmmol^{-1}/k^{-1}$	Gas constant

Table 2: Calculated Design Data

Data/Parameter	Values	Description
M_A	$44\ kg/mol$	The molecular weight of ethylene oxide
M_B	$18\ kg/mol$	The molecular weight of water
M_C	$62\ kg/mol$	The molecular weight of ethylene glycol
G_C	$38.58\ kg/S$	The mass flow rate of ethylene glycol
G_A	$26.524\ kg/S$	The mass flow rate of ethylene oxide
G_B	$10.851\ kg/S$	The mass flow rate of water
$\overline{V}_A$	$0.00113\ m^3/kg$	The specific density of ethylene oxide

$\overline{V}_B$	$0.001003\ m^3/kg$	The specific density of water
$\overline{V}_C$	$0.000901\ m^3/kg$	The specific density of ethylene glycol
Q_A	$0.030\ m^3/S$	Volumetric flow rate of ethylene oxide
Q_B	$0.011\ m^3/S$	The volumetric flow rate of water
V_0	$0.041\ m^3/S$	Total volumetric flow rate of reactants
C_{A0}	$0.030\ mol/m^3$	Initial concentration of ethylene oxide
F_{A0}	$0.00123\ mol/m^3$	The initial molar flow rate of ethylene oxide
X_A	0.95 (Dimensionless)	Maximum fractional conversion

Table 3: Data Obtained from Literature

Data	Values	Description	References
T_0	$463k$	The initial temperature of the feed	1
T	$473k$	The operating temperature of the reactor	1
T_C	$468k$	Coolant temperature	1
A_1	$0.0442S^{-1}$	Pre-exponential factor	1
A_2	$0.0698S^{-1}$	Pre-exponential factor	1
E_1	$21193\ kJ/mol$	Activation energy	1
E_2	$88.692\ kJ/mol$	Activation energy	1
K_1	$7.2330S^{-1}$	Rate constant	1
K_2	$0.07143S^{-1}$	Rate constant	1
ΔH_R	$2145.28\ kJ/mol$	Change in enthalpy of reactants	29
ΔC_P	$11664kJ/\ ^0C$	Change in specific heat capacity of reactants	29
UA_C	$1.7\ kg/m^2S^0C$	Heat transfer coefficient	29

2.6 Solution Techniques

The kinetic parameters optimization models were solved using a statistical approach and the relationship between temperature concentration and time taken with acid and without kinetic parameters, optimization was developed and presented in profiles using Excel Spread Sheet and the simulation tool.

3.0 Results and Discussion

3.1 Optimization

The results showing the difference between the literature kinetic parameter data and the optimized kinetic parameter data are presented in Table 4 below and the performance effect of both the literature and optimized kinetic parameter data on the temperature and concentration of feed or reactant material as well as the product during hydrolysis of ethylene oxide for ethylene glycol production are presented in Figures 2 to 5 below:

Table 4: Comparison of Literature and Optimized Kinetic Parameter Data

Kinetic Parameters	Symbols	Literature Data	Optimized Data	Difference (%)
Activation	E_1	21193	21793	0.70
Energy (kJ/mol)	E_2	88.692	88.978	0.10
Pre-Exponential	A_1	0.0442	0.04418	0.01
Factor (S^{-1})	A_2	0.0698	0.0703	0.18
Rate Constant	K_1	7.2330	6.9865	0.87

	K_2	0.07143	0.3779	34.10

Table 4 shows the result of the literature and optimized kinetic parameters (Activation energy, pre-exponential factor or frequency factor, and rate constant) data comparison. From the table, there is a significant difference between the initial and final activation energy of the literature and optimized kinetic value comparison that is 0.70% and 0.10% respectively while a non-significant and significant value difference of the pre-exponential or frequency factor is observed in the initial and final value of both the literature and optimized data, that is 0.01% and 0.18% respectively. Finally, a significant and highly significant percentage difference of the initial and final rate constant values of both the literature and optimized parameters that is; 0.87% and 354.10% respectively. The non-significant, significant, and highly significant values of both the literature and optimized value of kinetic parameters improve process performance as well as profit (yield) maximization.

3.2 Effects of Temperature and Time without Kinetic Parameters Optimization

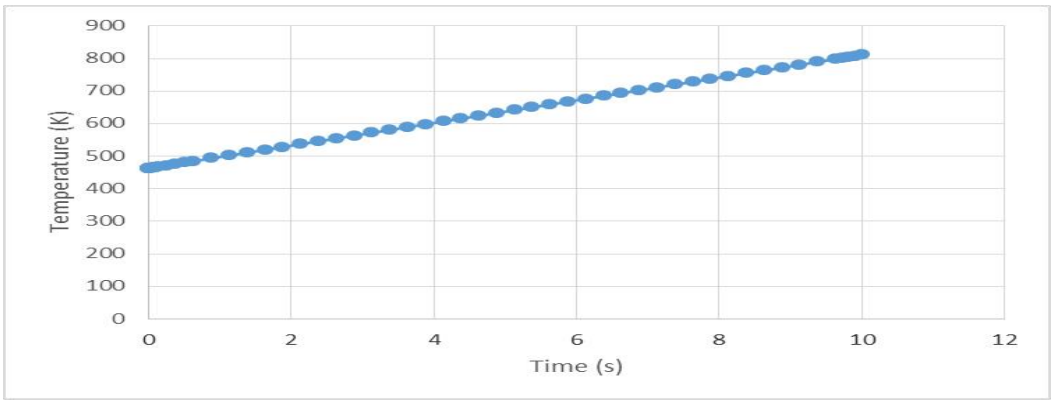
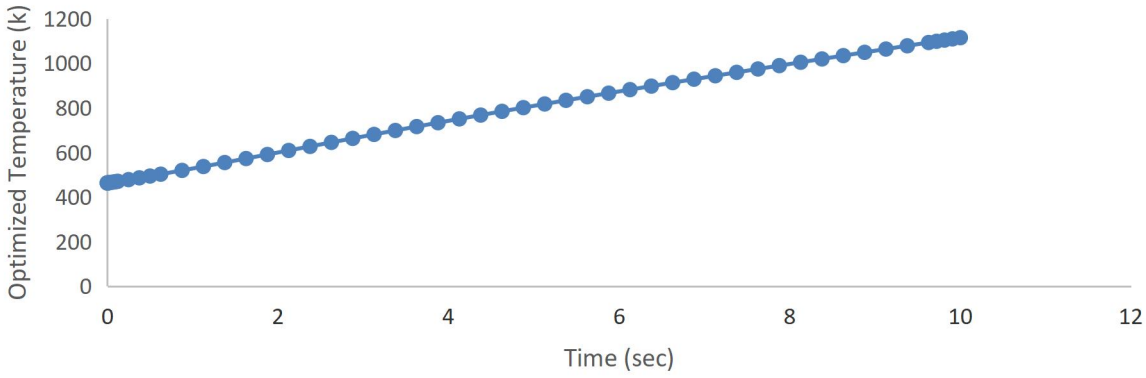


Figure 2: Profile of Temperature and Time without Kinetic Parameters Optimization

Figure 2 shows the behaviour of feed temperature over time during the hydrolysis of ethylene oxide for ethylene glycol production without optimizing kinetic parameters like activation energy, pre-exponential factor, and rate constant. From the profile, the process was initiated at a high temperature of about 475k which is capable of causing loss of feed or reactants as well as product at the end of the process. This high-temperature condition also makes the process economically inefficient because of the high cost of energy consumption hence, there is a need for optimizing the kinetic parameters for the process to be achieved within the least possible or required temperature thereby minimizing feed and product loss at the end of the process.



3.3 Effects of Temperature and Time with Kinetic Parameters Optimization

Figure 3: Profile of Temperature and Time with Kinetic Parameters Optimization

Figure 3 shows the behaviour of feed temperature over time during the hydrolysis of ethylene oxide for ethylene glycol production when the kinetic parameters are optimized. From the profile, the process was initiated with a low temperature of about 450k which is about 25k less than the temperature expended when the kinetic the kinetic parameters were not optimized. This low-temperature prevailing condition which ensures there is no loss of feed or product at the end of the process makes it economically viable as less heat (energy) is expended during the process. This ensures the optimum performance of the process and high recovery of yield or product of interest at the end of the process.

3.4 Effects of Concentration and Time without Kinetic Parameters Optimization

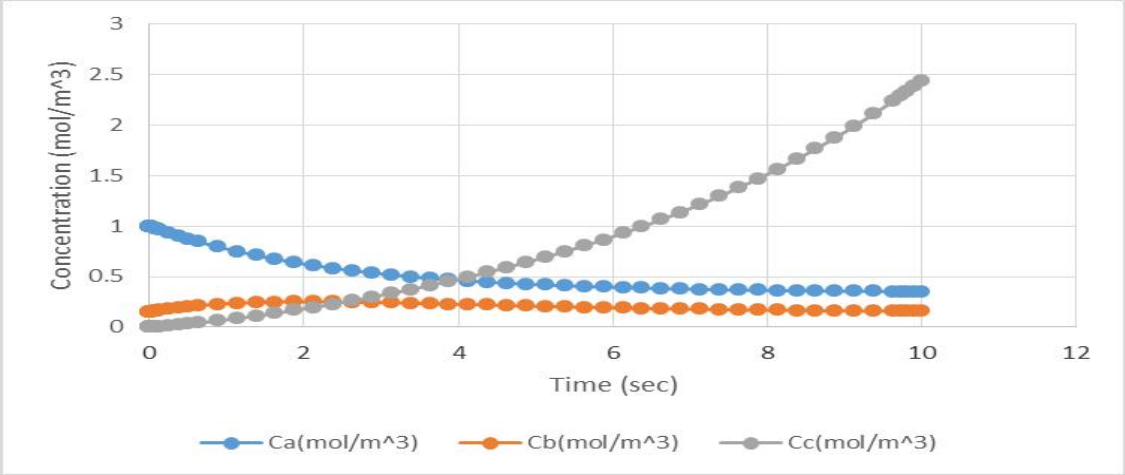


Figure 4: Profile of Concentration and Time without Kinetic Parameters Optimization

Figure 4 shows the concentration of feed materials (ethylene and ethylene oxide) and product formed (ethylene glycol) over time during the oxidation of ethylene to form ethylene oxide and hydrolysis of ethylene oxide to form ethylene glycol. According to the profile behaviour, a low concentration of target product (ethylene glycol) of about 2.5mol/m^3 was recovered at the end of the process when the kinetic parameters (activation energy, pre-exponential factor, and rate constant) were not optimized and hence to make the process more economically viable, kinetic parameters must be optimized to enhance high or optimum recovery of target product (ethylene glycol) concentration at the end of the process.

3.5 Effects of Concentration and Time with Kinetic Parameters Optimization

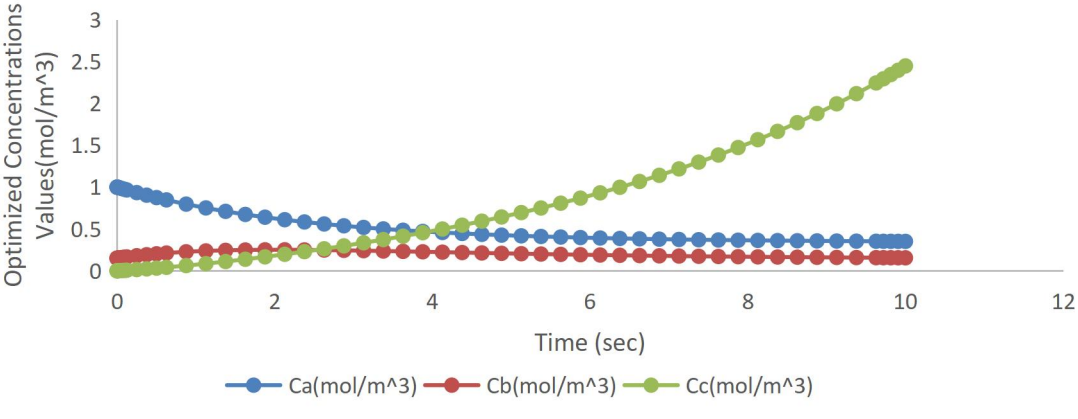


Figure 5: Profile of Concentration and Time with Kinetic Parameters Optimization

Figure 5 shows the concentration of feed materials (ethylene and ethylene oxide) and the product recovered (ethylene glycol) over time during the oxidation of ethylene to form ethylene oxide and hydrolysis of ethylene oxide to form ethylene glycol. According to the profile behaviour, a high concentration of target or product of interest (ethylene glycol) of about 2.7mol/dm^3 was recovered at the end of the process. The result proves better performance characteristics with more recovery ethylene glycol concentration as compared with the recovery rate without optimizing kinetic parameters like activation energy, pre-exponential factor, and rate constant. This is an indication that kinetic parameters optimization results in more yield or recovery of ethylene glycol (target product) at the end of the process

Conclusion

The optimization of the kinetic parameters for the enhanced production of ethylene glycol in a continuously stirred tank reactor is a vital process in maximizing production efficiency and output. It was evident from the results that the optimized parameters played a crucial role in improving the overall performance of the continuously stirred tank reactor. The optimized values resulted in high yield and quality in the production of ethylene glycol. This study highlights the importance of optimizing kinetics parameters to improve the production of ethylene glycol. It presents an effective approach to predict the desired output and demonstrates the efficiency of the continuously stirred tank reactor in ethylene glycol production. Our study on the optimization of the kinetic parameters for the enhanced production of ethylene glycol in a Continuous Stirred Tank Reactor using MATLAB simulation has shown promising results. By combining a mathematical model with a powerful simulation tool like MATLAB, we were able to predict and optimize the reaction kinetics accurately, leading to an increase in the yield and quality of the final product.

This study has also addressed some of the knowledge gaps and inconsistencies in the existing literature and provided solutions to the limitations of previous optimization methods. We have demonstrated that simulating the CSTR reaction kinetics using mathematical models can improve the accuracy and reliability of the optimization process. Also, we have shown the value of exploring the impact of variations in the temperature, pressure, and reactant concentrations on the reaction kinetics to provide a more comprehensive understanding of the CSTR process. Based on these findings, we recommend that future studies focus on applying the optimized kinetic parameters in an industrial setting to assess their commercial viability. We also suggest that further investigations should be done to optimize the other aspects of the ethylene glycol production process, such as energy efficiency, waste reduction, and environmental impact. This research has shown that MATLAB simulation is a powerful tool for optimizing the kinetic parameters of the ethylene glycol production process in a Continuous Stirred Tank Reactor. Our findings provide valuable insights into the challenges and opportunities in the optimization of CSTR reaction kinetics, which can be applied to other chemical processes as well.

Declarations

Ethics approval and consent to participate

Not applicable

Competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper

Authors contributions

W O C, E M E: Conceptualization, Methodology, Original draft preparation, Performed experimental work, and Writing

Funding

The authors received no funding for this study.

Acknowledgement

The authors wish to thank the management and technical staff of the Department of Chemical Engineering at Federal University Otuoke Nigeria for granting the authors access to their laboratories and workshops.

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