# Modeling and Simulation of a Stripper-Hydrolyzer System for Effluent Water Treatment in Urea Plant

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## ABSTRACT

Models were developed for the stripper-hydrolyser system applicable in urea plants for effluent water treatment thereby ensuring that the concentrations of substances present in the discharged water to the environment is within the internationally acceptable limits. Models were developed from the first principle for the hydrolyzer as a four consecutive continuous stirred tank reactor (CSTR) in series and the stripper to account for the operational processes. Thermodynamics and chemical reaction kinetics concepts were applied to assess the hydrolyser's optimal yield and conversion time. Reactant (urea hydrolysis) and products (ammonia and carbon dioxide) concentrations over time in the four reactors were taken into consideration. The resulting differential equations deduced from the developed model were solved using the MATLAB 2020 ODE45 solver from Matworks, which applies the 4th order Runge-Kutta method, in order to ascertain the concentrations of urea, ammonia, carbon dioxide, and water. in terms of mole fraction. The constituent concentrations upon reactor exit were 0.231, 0.370, 0.073, and 0.326 for water, carbon dioxide, urea, and ammonia respectively. Utilizing plant data from an industrial fertilizer facility in Rivers State in comparison with developed models showed that the models' outcomes were also verified with a minimum absolute error or deviation of 0.13%.

KEYWORDS: Four Series CSTR, Reaction Kinetics, Thermodynamics, Runge-Kutta

# 1. INTRODUCTION

An essential component of any country's socioeconomic development is its industrial sector. However, natural resources are under a lot of pressure due to global industrialization as both home and industrial wastewaters have high concentrations of nitrogenous chemicals such as urea and ammonia [1]. Industrial and domestic wastewater contains high contaminants that should be treated in a wastewater treatment plant prior to its delivery or discharge into the environment. Therefore, the wastewater treatment plant is an important and pertinent unit influencing the improvement of environmental conditions [2]. An important constraint in the logistics management of water supply and wastewater collection is handling of the uncertainty in the supply and demand of water resources and its optimal allocation between facilities to refine, recycle and production of drinking water [3]. Furthermore, inadequate handling of chemical industry effluent water has resulted in catastrophic ecological and human tragedies, playing a major role in environmental deterioration and pollution issues of varying degrees. It is well known that industrial environmental regulations are inadequate in many developing nations, and that where they are there, the available controls are ineffective. The lack of a dependable and thorough system for tracking industrial emissions and enforcing adherence to industry norms largely explains this [4]. As a result of population growth, industrial and technological improvements, the treatment of wastewaters or contaminants have augmented while very stringent environmental standards have been enforced to enhance the quality of both domestic and industrial effluent wastewaters. Thus, optimization of energy use and the improvement of treatment plants effectiveness coupled with the efficiency of their equipment and technologies are of utmost importance [5]. In many African developing nations, pollution from industrial waste disposal and effluent discharges is turning into a major environmental problem [6]. The natural water body is the ultimate recipient of all types of pollution [7]. Presumably, it is easier to dispose wastewater and other waste materials into water bodies, a lot of enterprises are situated close to them. The issue of clean portable water is a global crisis mainly in Africa and the Middle East, where there is a shortage of water and a great deal of friction between the nations over this valuable resource [8]. Numerous investigations on industrial effluent and its effects on aquatic ecosystems have been prompted by the perceived repercussions of uncontrolled waste disposal into water bodies utilized as potable water supplies [9-10]. One common nitrogenous fertilizer used in farming is urea. A large amount of the 100 million tons of urea generated annually is utilized as mineral fertilizer [11-12]. Both urea and ammonia contribute significantly to wastewater, mostly via runoffs that release copious amounts of pollutants into receiving water bodies and negatively impact the environment. This effluent that is released from the production plants

may contain up to 125 mg/L of NH3-N and 750 mg/L of urea. Ammonium ions (NH4+) make up about 40–50% of the total nitrogen in municipal wastewater treatment plants [13-14]. Since nitrifying microorganisms oxidize ammonia to generate nitrite and nitrate, it is a hazardous pollutant in wastewaters that is undesirable for people as well as fish species [15]. Urea is created when ammonia and carbon dioxide combine under industrially high pressure and temperature conditions.

According to Kyriakou *et al.* (2017), current density in electromagnetism is the quantity of charge that moves across a unit area of a selected cross section in one unit of time. The current density vector plays a crucial role in evaluating how cost-effective electrochemical operations are. The system's primary drawback was the high current densities needed, which raised the cost of operation by causing the system to use more electricity [16]. Lilong *et al.* (2013) also investigated the impact of wastewater runoff from effluent on coastal systems. Because the coastal area is a crucial home for aquatic species, precautions must be taken when conducting research there. They did not offer any recommendations or solutions in their work for treating urea and ammonia-polluted coastal areas to lessen the impact on the aquatic environment [17]. Additionally, Yahya *et al.* (2021) examined urea hydrolysis in laboratory-prepared synthetic wastewater as part of their investigation. Additionally, an efficient enzyme membrane reactor (EMR) system was installed in order to recover ammonia that might be utilized to create ammonia derivatives. Their findings, however, were unable to clarify the ideal operating temperature for urea to ammonia conversion [18]. Environmental rules and regulations are making urea discharge a challenge for many sectors. In order to recover ammonia from urea, this research aims to suggest an alternate separation technique. If ammonia is recovered, farmers can use it to make ammonia-based fertilizers, which can lower wastewater treatment costs and promote environmental sustainability [19].

Due to the necessity for food security in all nations, the demand for urea has grown dramatically along with the fast development of the chemical industry and population growth. In addition to being a significant nitrogen fertilizer in and of itself, urea makes an excellent raw material for businesses that make chemicals. Fungicide accounts for about 85% of the world's ammonia production, with the remaining 15% going toward other industrial uses like textiles, plastics, and explosives. The global focus on attaining food security at this time has led to a growing scarcity of urea and other agricultural fertilizers [17].

Ammonia and ammonium are the two major species that generate the most damaging environmental concerns, are typically overexposed in the ecosystem, leading to excessive plant growth. These two lower the quality of the water and cause the well-known eutrophication phenomenon. Ammonia has a negative effect on both human health and climate change, making it a dangerous air pollutant. According to Vecino et al. (2019), the manufacturing of ammonia is regarded as an industrial source of carbon dioxide emissions that contribute to the greenhouse effect. Large volumes of urea-containing waste fluids are produced by urea producing operations in addition to human activity [20]. Furthermore, due to the anthropogenic activities of many industries, coastal systems have been severely attacked by urea in recent decades. The wastewater is contaminated with tiny but significant concentrations of ammonium and urea. As a result, this wastewater cannot be utilized in any other phase of the urea manufacturing process [21]. In addition, the ecology is a crucial setting that sustains plant and animal life. The preservation of our ecosystem's biological balance necessitates adhering to legal requirements on environmental regulations. These regulations shield the environment and people from dangerous substances present in wastewater. Wastewater treatment systems are made to expedite the overburdened natural process of water purification. The immediate ecological system was greatly threatened by urea plant effluents due to factors including high urea pollutant density and microbial growth. If this urea factory wastewater is not adequately treated, it can contaminate our water supplies, harm natural ecosystems, and lead to a number of waterborne illnesses. Wastewater treatment is therefore essential for maintaining resource efficiency and safeguarding our ecosystem [22]. In the urea plant, the stripper-hydrolyzer system has shown to be a successful wastewater treatment technique. The performance of the stripper-hydrolyzer system used in this research for the chemical conversion and pollutant level reduction of the effluent water from the urea factory makes it highly significant technologically, with some of the system's major functions are to bring the levels of pollutants (such as urea, carbamate, and ammonia) in effluent water down to a manageable level, to recover and recycle the carbon dioxide and ammonia used as raw materials to make urea, outstanding energy efficiency, to recycle and clean industrial wastewater for future use, to cut back on the amount of potable or fresh water used in industries, to reduce the amount spent on purchasing water, to comply with the government's standards for the emission or discharge of environmental pollutants from different industries in order to avoid facing severe penalties and to prevent pollution from entering the environment and support sustainable growth.

Besides, leading businesses in the chemical and pharmaceutical industries employ effluent treatment plants (ETPs) to purify water and eliminate any chemicals or compounds that are either harmful or non-toxic, thereby protecting the environment. An ETP is a facility that treats waste waters and industrial effluents [23].

Furthermore, the preservation of our ecosystem's biological balance necessitates adhering to legal requirements on environmental regulations. Laws mandate that industries keep an eye on their effluent to make sure everything is complying. When necessary, the effluent must be treated before being released into the environment [24]. These regulations shield the environment and people from dangerous substances present in wastewater. Wastewater treatment systems are made to expedite the overburdened natural process of water purification. The immediate ecological system was greatly threatened by urea plant effluents due to factors including high urea pollutant density and microbial growth. If this urea factory wastewater is not adequately treated, it can contaminate our water supplies, harm natural ecosystems, and lead to a number of waterborne illnesses. Wastewater treatment is therefore essential for maintaining resource efficiency and safeguarding the ecosystem. Therefore, this research study is aimed at modeling of a stripper-hydrolyzer system for treating effluent water in urea plants through the development of mathematical models based on the principle of conservation of mass and energy concepts for the stripper-hydrolyzer system, application of Suitable kinetic model and kinetic parameters to describe the stripper-hydrolyzer system, validation of model results using a functional or operational fertilizer plant data and performance of sensitivity studies of the important process parameters.

#### 2.0 MATERIALS AND METHODS

The principle of material and energy conservative concepts are the most widely used approach for modeling an industrial or process plant such as the stripper-hydrolyzer system. The impact of the environment on the process and vice versa will be taken into consideration using the thermodynamic concept. Additionally, a schematic design of the process will be developed, showing all of the defined input and output streams for materials and energy streams. To depict the event occurring on each stage in the stripping column, an arbitrary stage j will be selected, and the hydrolyzer will be treated as a system of four consecutive stirred tank reactors.

#### 2.1 Model Assumptions

The following assumptions are applied in developing mathematical models for stripper and hydrolyzer columns for effluent waste water treatment.

- Steady state process operation, thereby eliminating accumulations within the columns
- Constant relative volatility of the stripper's component parts and no liquid holding up all the time in the stripper.
- Insignificant vapour retention in the dancer and adequate or thorough blending of liquid and vapour at every stage of the process.
- Within the hydrolyzer reactor, the composition of the reacting mixtures is constant and reactant is not converted before entering the hydrolyzer reactor.
- A representative stage for the rectifying section, stripping section, and feed stage is used to measure mass and energy balance.
- The overall rate of urea is unimolecular

#### **2.2 Development of Model Equations**

The general material balance and energy balance equations that accounts for material and energy conservation are written as expressed in Equations (1) and (2) respectively.

$$\begin{pmatrix} \text{Rate of Accumulation} \\ \text{of Material} \\ \text{within the Stripper/Hydrolyzer} \end{pmatrix} = \begin{pmatrix} \text{Rate of Input} \\ \text{of Material} \\ \text{into Stripper/Hydrolyzer} \end{pmatrix} - \begin{pmatrix} \text{Rate of Output} \\ \text{of Material} \\ \text{from Stripper/Hydrolyzer} \end{pmatrix} \pm \begin{pmatrix} \text{Rate of Output} \\ \text{of Material} \\ \text{from Stripper/Hydrolyzer} \end{pmatrix}$$

2



## 2.3 Models of Hydrolyser Reactors

As depicted in Figure 1, the hydrolyzer reactors are made up of a battery of four successive continuous stirred tank reactors in series (CSTR). Based on the concepts of mass and energy conservation, a mathematical model of the non-isothermal system of the successive continuous stirred tank reactor (CSTR) was developed.



Defining the respective terms in Equation (1) based on the model assumptions yields

$$\vartheta_o C_{io} = \vartheta_0 C_i + (-r_i) V_R \tag{3}$$

Thus, the general material balance equation representing the battery of four consecutive CSTRs in series yields

$$\vartheta_o C_{io} = \vartheta_0 C_{i4} + V_R \sum_{j=1}^4 (-r_{ij})$$

Rearranging and mathematical analysis of Equation (4) yields

$$C_{i4} = C_{io} - \tau \sum_{j=1}^{4} (-r_{ij})$$

#### 2.4 Chemical Reactions Kinetics

Equations (6) and (7) displayed the reaction steps for urea hydrolysis into ammonia and carbon dioxide

$$2CO(NH_2)_2 + H_2O \rightarrow 2NH_3COONH_4 \qquad 6$$
  
$$2NH_3COONH_4 \rightarrow 2NH_3 + CO_2 \qquad 7$$

The completion of the reaction is favored by high temperature, stirring speed and high reaction pressure. The overall reaction is endothermic and the first reaction, that is conversion of urea to ammonium carbamate reaction, is a slow reaction hence the rate controlling step and the second reaction is very fast and goes towards completion [25].

The overall reaction is expressed as

$$2CO(NH_2)_2 + H_2O \rightarrow 2NH_3 + CO_2$$
 8

The rate can be expressed hypothetically as:

$$A + water \rightarrow 2B + C$$
$$-r_{i} = KC_{A}$$

Writing Equation (9) using Arrhenius for the reaction rate constant

$$-r_{i} = k_{o} exp\left(\frac{-E_{A}}{RT}\right) C_{A}$$
 10

A component material balance for chemical species in the system of consecutive CSTRs is employed to account for species 'A' utilized in each CSTR in course of chemical conversion of reactant into finished product. Thus, the general component material balance for ith number of CSTRs in series is expressed as

$$C_{Ai} = \frac{c_{Ao}}{\left(1 + k_0 \exp\left(\frac{-E_A}{RT}\right)\tau\right)^i}$$
11

#### 2.5 Hydrolyzer Energy Balance

The total energy balance equation can be written from principles of conservation of energy as expressed in Equation (2) and defining and substituting for each term in Equation (2) yields

$$\frac{dH}{dt} = \rho_{io}\vartheta_{io}H_{io}(T_{io}) - \rho_i v_i H_i(T_i) - Q$$
<sup>12</sup>

## 2.6 Characterization of Total Energy

Based on thermodynamics principles, the enthalpy of a liquid system depends on temperature and its composition

$$H = H(T, n_A n_B, n_c)$$
<sup>13</sup>

Partial differentiation of Equation (13) gives

$$\frac{dH}{dt} = \frac{\partial H}{\partial T}\frac{dT}{dt} + \frac{\partial H}{\partial n_A}\frac{dn_A}{dt} + \frac{\partial H}{\partial n_B}\frac{dn_B}{dt} + \frac{\partial H}{\partial n_C}\frac{dn_C}{dt}$$
14

Defining the terms in Equation (14) and upon separation of variables yields

$$T = T_i - \frac{(-\Delta H_r)}{\rho C_p} k_0 \exp\left(\frac{-E_A}{RT}\right) C_{A-} \frac{V_R}{\vartheta_O} \frac{UA_t(T-T_C)}{\vartheta_O \rho C_p}$$
<sup>15</sup>

#### 2.7 The Stripper Models



#### Figure 2: Representative Tray j

This refers to developed mathematical equations representing the performance of the stripper section of the hydrolyser-Stripper system. A representative stage j of the stripper is shown in Figure 2. Based on the general assumptions stated above, the overall material balance equation on stage j gives

$$F_j + L_{j+1} + V_{j-1} - L_j - V_j = 0$$

Taking component balance for any species i using Equation (16) yields

16

$$F_{j}Z_{j,i} + L_{j+1}X_{j+1,i} + V_{j-1}Y_{j-1,i} - L_{j}X_{j,i} - V_{j}Y_{j,i} = 0$$
17

Based on phase equilibrium relationship, the liquid phase composition is related to its corresponding vapour phase composition through the distribution law

$$y_{j,i} = K_{j,i} x_{j,i}$$
  $(1 \le j \le Nt, \ 1 \le i \le n)$  18

Also, the mole fraction expressions for both liquid and gaseous phases are written thus

$$\sum_{i=1}^{n} x_{j,i} = 1, \ \sum_{i=1}^{n} y_{j,i} = 1 (1 \le j \le Nt, \ 1 \le i \le n)$$
19

Combining Equations (17) and Equation (18) yields

$$F_{j}Z_{j,i} + L_{j+1}x_{j+1,i} + V_{j-1}K_{j-1,i}x_{j-1,i} - L_{j}x_{j,i} - V_{j}K_{j,i}x_{j,i} = 0$$
20

#### 2.8 Energy Balance over Tray j

Based on the underlying assumptions, Energy balance over tray j yields

$$F_{j}C_{P_{fj}}T_{fj} + L_{j+1}C_{P_{j+1}}T_{j+1} + V_{j-1}C_{P_{j-1}}T_{j-1} - L_{j}C_{P_{j}}T_{j} - V_{j}C_{P_{j}}T_{j} = 0$$
21

#### **3.0 RESULTS AND DISCUSSION**

#### 3.1 Model Simulation Results

The results obtained from the solution and simulation of the developed mathematical model equations for the study of effluent water treatment in Urea plant in a series of CSTRs (stripper-hydrolyzer) coupled with the kinetics of the process in the reactors are presented. The variation of concentrations of urea, ammonia and CO<sub>2</sub> with time in the four reactors were considered in terms of urea hydrolysis and ammonia and CO<sub>2</sub> production. The hydrolysis of urea and the yield of products as predicted by the developed model equations in comparison with the operational data obtained from industrial fertilizer company in Port Harcourt, Rivers State were shown in Table 1. The outlet concentrations based on the solution of the numerical models for all species were compared with the corresponding outlet concentrations obtained from the industrial fertilizer operational plant in Port Harcourt, Rivers State, Nigeria. It can be deduced from Table 1 that there is excellent agreement (minimum absolute error) between the model predicted and industrial plant data.

**TABLE 1: Model Validation** 

Component	Plant Data	Model Prediction	%Deviation
Urea	0.266	0.231	0.13
Ammonia	0.350	0.370	0.06
CO <sub>2</sub>	0.074	0.073	0.01
H <sub>2</sub> 0	0.310	0.326	0.05

#### 3.2 Variation of Mole Fractions of the Reactants and Products for Reactor 1

The variation of mole fractions of the reactants and products with time for the four CSTR reactors in series are shown in Figures 3, 4, 5 and 6 respectively. It can be deduced that the mole fraction of urea steadily decreases with time for each of the four reactors while the mole fraction of  $CO_2$  and  $NH_3$  increases steadily with time in each of the four reactors. This behavioural pattern is due to the kinetics of the hydrolysis process of urea that is taking place in the reactors. Figure 3 shows the variation of mole fraction with time for the first reactor in the series CSTR reactors. It can be deduced from Figure 3 that there is a decrease in concentration of reactants (urea and steam) and an increase in concentration of products ( $CO_2$  and  $NH_3$ ) with time in the reactor from an initial concentration of 0.6 to 0.3616, 0.4 to 0.1616, 0 to 0.0669 and 0 to 0.2384 for urea, steam,  $CO_2$  and  $NH_3$  respectively. This trend of the system as shown in Figure 3 agrees with the principle of chemical reaction kinetics, which states that the rate of a chemical reaction is directly proportional to the concentration of the reacting species, indicating a decrease in the concentration of the reacting species in this case and an increase of the products.



Figure 3: Variation of Mole Fractions with Time for Reactor 1

## 3.3 Variation of Mole Fractions of the Reactants and Products for Reactor 2

Figure 4 shows the variation of mole fractions with time for the second reactor in the series of CSTRs reactors. Similar to Figure 3, there is a decrease in concentration of reactants (urea and steam) and an increase in concentration of products ( $CO_2$  and  $NH_3$ ) with time in the reactor from an initial concentration of 0.3616 to 0.2855, 0.1616 to 0.0855, 0.0669 to 0.0763 and 0.2384 to 0.3145 for urea, steam,  $CO_2$  and  $NH_3$  respectively. The behaviour of the second reactor agrees with established findings on the effect of concentration variation in series reactors system. The rate of chemical reaction is a function of the concentration of reactants and hence if there is a decrease in the concentration of the reactants, there will be a corresponding decrease in the rate of the reaction leading to a reduced conversion.



Figure 4: Variation of Mole Fractions with Time for Reactor 2

## 3.4 Variation of Mole Fractions of the Reactants and Products for Reactor 3

The variation of mole fraction with time for the third reactor in the series of CSTRs reactors is depicted in Figure 5. Similarly, there is a decrease in concentration of reactants (urea and steam) and an increase in concentration of products ( $CO_2$  and  $NH_3$ ) with time in the reactor from an initial concentration of 0.2855 to 0.2502, 0.0855 to 0.0502, 0.0703 to 0.0727 and 0.3145 to 0.3498 for urea, steam,  $CO_2$  and  $NH_3$  respectively. This trend is in tandem with established findings on the effect of concentration variation in series reactors system.



Figure 5: Variation of Mole Fraction with Time for Reactor 3

#### 3.5 Variation of Mole Fractions of the Reactants and Products for Reactor 4

Figure 6 highlights the variation of mole fractions with time for the fourth reactor in the series of CSTRs reactors. Obviously, there is a decline in concentration of reactants (urea and steam) and slight increase in concentration of products ( $CO_2$  and  $NH_3$ ) with time in the fourth reactor from an initial concentration of 0.2502 to 0.2311, 0.0502 to 0.0311, 0.0727 to 0.073 and 0.3498 to 0.3689 for urea, steam,  $CO_2$  and  $NH_3$  respectively. This trend agrees with established findings on the effect of concentration variation in series reactors system as depicted in the previous first, second and third reactors respectively



Figure 6: Variation of Mole Fractions with Time for Reactor 4

#### 3.6 Variation of Reactants Mole Fractions in the Reactors

For any reactor or reaction process, the concentration of reacting species is a very important parameter to consider and examine especially for series reactors system. Reactions are classified based on phase variation of the reacting species within the reactor. Hydrolysis of effluent water and subsequent stripping of the produced gas is not an exemption as the effect of concentration is readily noticed due to the nature of the hydrolysis reactions. Reforming reactions are mostly endothermic; meaning that there is a decrease in temperature of the reactor as the reaction proceeds. The understanding of the importance of effluent urea concentration is necessary in both design and modelling of the reactors because the urea concentration is a major driving force of the reaction. Figures 7 and 8 shows the variation of mole fraction of urea and steam in the four reactors. It can be deduced that there is a sharp decrease in the mole fractions of urea and steam in the first reactor, followed by a steady decrease in the second reactor and a slight decrease in the in the third and fourth reactors respectively, indicating the level of reactivity in each of the reactors. This behaviour in the four reactors agrees with the principle of chemical reaction kinetics, which states that the rate of a chemical reaction is directly proportional to the concentration of the reacting species. Hence, as the concentration of the reacting species decreases with time within the reactors, the reactivity of the reacting species decreases as shown in Figures 7 and 8 respectively.



Figure 7: Variation of Mole Fraction of Urea in the Four Reactors



Figure 8: Variation of Steam Mole Fraction in the Four Reactors

## 3.7 Variation of Products Mole Fractions in the Reactors

Figures 9 and 10 shows the variation of mole fraction of the products ( $CO_2$  and  $NH_3$ ) in the four reactors. Thus, there is general increase in products mole fractions with a sharp increase in the mole fraction of ( $CO_2$  and  $NH_3$ ) in the first reactor, followed by a steady increase in the second reactor and a slight increase in the in the third and fourth reactors respectively indicating the level of reactivity in each of the reactors. This behaviour in the four reactors agrees with the principle of chemical reaction kinetics, which states that the rate of a chemical reaction is directly proportional to the concentration of the reacting species. Hence, as the concentration of the reacting species decreases with time within the reactors, the reactivity of the reacting species decreases leading to a decrease in the yield of products



Figure 9: Variation of CO2 Mole Fraction in the Four Reactors



Figure 10: Variation of NH<sub>3</sub> Mole Fraction in the Four Reactors

#### **4.0 CONCLUSION**

Model equations were developed for a stripper-hydrolyzer system in which the hydrolyzer plant was a four array of CSTR reactors in series for treating waste water from urea plant. The model predicted the effluent concentrations of reactants (urea and steam) and products (ammonia and carbon dioxide). The developed model effluent concentration results were compared with the effluent concentration of an industrial fertilizer plant data in Port Harcourt, Rivers State. The percentage absolute error (deviation) of urea, steam, ammonia and carbon dioxide are 0.13%, 0.05%, 0.06% and 0.01% respectively. These concentration yields or results depicts a close mapping between the developed model predictions and the industrial fertilizer plant data, thus the developed models can be applied for the simulation studies of the industrial fertilizer plant. Also, mole fractions of the reactants and products were investigated as the operations proceed from CSTR reactor 1 to CSTR reactor 4 in seriation and the compositions of reactants and products in the respective reactants were studied.

#### Nomenclatures

V<sub>R</sub>: Volume of Reactor (m<sup>3</sup>);  $\vartheta_0$ : Volume Flow Rate (m<sup>3</sup>/hr);  $C_{i0}$ : Concentration of Reactant into Reactor 1 (mol/m<sup>3</sup>)

 $C_{i1}$ : Concentration of Reactant into Reactor 2 (mol/m<sup>3</sup>);  $C_{i2}$ : Concentration of Reactant into Reactor 3 (mol/m<sup>3</sup>)

 $C_{i3}$ : Concentration of Reactant into Reactor 4 (mol/m<sup>3</sup>);  $C_{i4}$ : Product Concentration of Reactor 4 (mol/m<sup>3</sup>)

 $\tau$ : Reaction Time (hr);  $K_0$ : Pre-Exponential Constant (mhr<sup>-1</sup>);  $E_a$ : Activation Energy (kJmol<sup>-1</sup>)

T: Absolute Temperature (K); H<sub>i0</sub>: Enthalpy of Inlet Stream (J); H<sub>i</sub>: Enthalpy of Outlet Stream (J)

*Q*: Heat Removed by Coolant (J); R: Universal Gas Constant (Jk<sup>-1</sup>mol<sup>-1</sup>);  $T_i$ : Reacting Mixture Temperature (K)

 $n_A$ ,  $n_B$ ,  $n_C$ : Moles of A, B and C in the CSTR (mol);  $C_P$ : Specific Heat Capacity of Reacting Mixture (J/kgK)

 $H_A$ ,  $H_B$ ,  $H_C$ : Partial Molar Enthalpies of Specie A, B and C respectively (kJ/mol);  $\Delta H_r$ : Heat of Reaction (kJ/kg)

 $y_i$ : Gaseous Mole Fraction;  $x_i$ : Liquid Mole Fraction

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