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Performance Evaluation of Fuzzy Logic Controller Application for Temperature Control of Urea Reactors Functions

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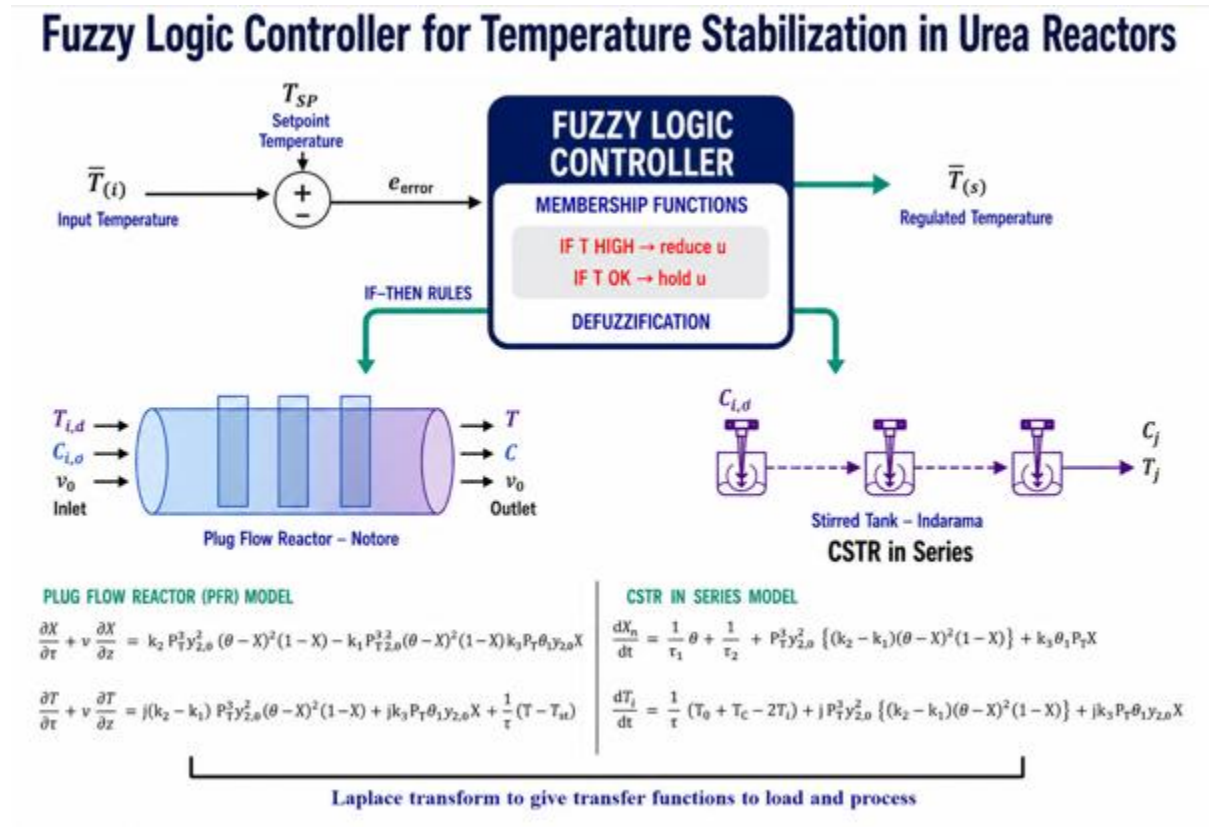
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ABSTRACT

Performance evaluation of fuzzy logic (FL) controller on urea reactors functions was studied. FL controller could be an efficient and reliable controller in the process industries to control process variables and conditions to a desirable set point value, suitable for optimum performance of the industrial reactors if introduced to the production process plant. Two industrial reactors; the plug flow reactor (PFR) and continuous stirred tank reactor (CSTR) typically used in Notore and Indorama plants respectively were considered in the study. The urea synthesis from the feed reactants of NH_3 and CO_2 is an equilibrium reaction process that obeys Le Chatelier's principle, must be controlled to maintain the conditions and variables of the process. The rate expression model, the ordinary and partial differential fractional conversions and temperatures models for the CSTR and PFR respectively describing the processes were developed. The kinetic parameters optimization models were derived using the statistical nonlinear regression and FL controller mode for the reactors were constructed based on the imputation of membership functions, the fuzzy rules, and the linearized reactors' models. Simulations of these models were carried out in Simulink/MATLAB version 8.0 using plant and literature data with input conditions of flowrate (63.5 kgs^{-1}), temperature (184°C), and pressure ($160 \text{ kgcm}^{-2}\text{G}$). The results showed that, the urea reactors were unstable, producing sinusoidal signals, indicating that a suitable controller was needed to control the urea reactors. The validated models and kinetics with plant and literature values, gave negligible root mean square errors of ranged $7.0\text{e-}4$ to $8.5\text{e-}4$ and $7.0\text{e-}3^\circ \text{C}$ to $2.1\text{e-}1^\circ \text{C}$ for conversion and temperatures, and $2.0\text{e-}4$ to $7.5\text{e-}4 \text{ [kJ/mol]}$ and $1.4\text{e-}4$ to $8.2\text{e-}4 \text{ [m}^6\text{mol}^{-1}\text{s}^{-1}\text{]}$ for the activation energies, and pre-exponential and rate constants respectively, evidenced that the reactors models are better describe the urea processes. FL controller for PFR outperformed the CSTR as it gave lower settling time and minimum errors of 1.05 [s] and 0.138°C compared to 3.32 [s] and 0.147°C . The turbulent nature of the PFR when conditions are changed (below or above the setpoint values), showed better response of CSTR urea reactor to control due to minimum errors and settling time. The results of the work proved that the controller enhanced performance and deal with imprecision, irregularities and nonlinearity in complex control situations for both reactors, and should be recommended.

Keyword: Fuzzy logic controller, temperature, CSTR, PFR, kinetic parameters, optimization, and urea process.

GRAPHICAL ABSTRACT



1. Introduction

Urea, as an organic fertilizer, provides 46 % of N_2 in the soil for nitrification to generate nitrates, which is an essential manure for improving soil fertility or nutrients to enhance crop productivity for subsistence and commercial purposes [1]. The global demand for urea outnumbers the quantity of urea produced worldwide, especially in Africa, as outlined vividly and clearly in the research conducted by Ojong et al. [2]. Urea synthesis from ammonia and carbon (IV) oxide, as secondary raw materials for the commercial production of the organic fertilizer, takes place in either tubular or continuous stirred tank reactors with a complex equilibrium reaction [2] that must be properly controlled to maintain the optimal yield of the product. Process variables such as temperature, pressure, flow rate, and ammonia-carbon dioxide ratio are to be controlled at setpoint values to avoid downtime performance of the reactors and to obtain maximum yield.

Ensuring that processes operate as intended in a safe and cost-effective manner is the goal of process control, which is challenging because most processes are prone to numerous disturbances that continuously cause the controlled variables to deviate from their intended values (or setpoints). This can be avoided by adjusting other process inputs (or manipulated variables) to return the process to the intended state [3, 4]. One class of technique well suited to handling such disturbances is fuzzy logic. Fuzzy logic or models are soft computing techniques that use inexact information to make exact predictions or inferences, taking into account the uncertainty in human decision-making to make certain predictions with a remarkable ability of the human mind to reason and learn in an environment of uncertainty and imprecision [5, 6]. Fuzzy logic control offers a flexible and robust approach to temperature regulation in industrial plants, allowing for effective control even in the presence of uncertainty and complex nonlinear

reactors' dynamics [7]. The key to success is a thorough understanding of the plant's characteristics and a well-designed fuzzy logic control system [8, 9].

This suitability warrants a closer look at the underlying framework. Fuzzy logic is a mathematical framework useful in control systems and decision-making processes. The fuzzy logic algorithm consists of several steps to process fuzzy inputs and produce fuzzy outputs [10], particularly useful when dealing with systems or problems that involve ambiguity, imprecision, or subjectivity [5]. Fuzzy logic controllers have been applied in various fields, including control systems, expert systems, decision support systems, pattern recognition, and artificial intelligence. They are known for their ability to handle real-world situations characterized by ambiguity and imprecision, where traditional binary logic may be insufficient [11]. Fuzzy logic controllers are useful in situations where precise mathematical models are challenging to develop or where human reasoning and expertise are essential [11, 12].

This ability rests on a specific conceptual foundation. Fuzzy logic conceptualizes the human mind's ability to reason uncertainty and inexactness in a manner that reasoning cannot be expressed precisely, not even with statistical or probability methods [13]. Fuzzy logic is defined as a many-valued logic form, in which variables can take any real number truth values between 0 and 1. Fuzzy logic (FL) algorithms help solve problems by considering all available data and making the best possible decisions for the given inputs. Though PID controllers are popular in the industry [14, 15], fuzzy logic controllers (FLC) are widely used in practice as evidenced by the cited literature [15, 16].

To situate the present study within this body of work, several related studies on the use of fuzzy logic and other controllers to control reactors or systems were reviewed, and the key findings are as follows: Mahmoud et al. [17] applied adaptive model predictive, adaptive neural network model predictive, and adaptive neuro-fuzzy sliding mode controllers to control ammonia and urea production processes aimed at achieving stability of the outlet concentrations of ammonia and urea, stable reaction rates, increased conversion of CO_2 , increased ammonia and urea production, maintenance of the NH_3/CO_2 ratio of 3:1, and reactor temperatures within suitable operating ranges in response to external disturbances or variations in reactor parameters. The simulation on the developed models for the processes in terms of concentrations and temperatures showed that the adaptive neuro-fuzzy sliding mode controller was more effective than the others in handling external disturbances and parameter changes.

In a related effort, Manozca et al. [18] used model predictive control techniques to control the synthesis section of a urea plant. Key variables, including the NH_3/CO_2 ratio, reactor level, reactor pressure, and reactor temperature, were stabilized to their design values or within the operating range, thereby maximizing the load of the synthesis section via feed flows.

Beyond the synthesis reactor itself, fuzzy-logic-based control has also been extended to downstream emission-control units associated with urea use. You et al. [19] investigated the urea dosage controller design for two-cell selective catalytic reduction (SCR) systems. Models for the SCR of two cells were developed, and the fuzzy logic urea dosage controller design procedure was carried out. Simulations and comparisons for the fuzzy logic urea dosage controller and experimental results indicated that high concentrations of NO_x were reduced to the barest minimum.

Closer to the focus of this study, Nilesh et al. [20] developed a nonlinear CSTR model and type-2 FLC built in MATLAB/Simulink to control the concentration instabilities within the reactor based on flow rate adjustments within the plant. The analysis showed that type-2 FLCs are generally more robust than their type-1 counterparts, as they successfully controlled disturbances and uncertainties by eliminating oscillations.

Building on this CSTR-specific line of work, more recent studies have further advanced the stability and control of the CSTR. Shi et al. [21] developed a nonlinear PID controller for a continuous stirred tank reactor whose parameters were optimized using a radial basis function (RBF) neural network and reported improved tracking accuracy and stronger robustness to parameter uncertainty than conventional PID

tuning. In a similar PID-based framework, Achu Govind et al. [22] designed a robust decentralized PID controller for a benchmark CSTR system by combining nonlinear constraint optimization with Kharitonov-Hurwitz stability analysis, achieving wider closed-loop stability margins under loop interactions than classical decentralized designs.

Cui et al. [23] proposed an adaptive robust controller for a nonlinear constrained stirred-tank reactor using a self-organizing fuzzy neural network together with time-varying integral barrier Lyapunov functions, which kept the reactant concentration and mixture temperature within safe operating bounds while guaranteeing closed-loop stability under strong nonlinearities and uncertainties.

While the CSTR has received considerable attention, the plug flow reactor (PFR) – the second reactor type modelled in this study – has also been the subject of recent stability and control research. Liavoli et al. [25] developed an Extended State-Dependent Differential Riccati Equation (ESDDRE) controller for a non-isothermal plug-flow reactor governed by a time-delay partial differential equation, achieving sub-optimal nonlinear stabilization despite the reactor's inherent time-delay dynamics. Addressing a similar class of delayed hyperbolic PDE systems but through a fuzzy-logic lens, Zhang et al. [26] designed a robust non-fragile H_∞ fuzzy controller for uncertain nonlinear-delayed hyperbolic PDE systems representative of plug-flow reactor dynamics, using a Takagi-Sugeno fuzzy PDE model and spatial linear matrix inequalities to guarantee exponential stability under delay and parameter uncertainty.

Moving away from delay-compensating designs toward optimal control formulations, Yevgenieva et al. [27] addressed the periodic optimal control of a plug flow reactor model under an isoperimetric constraint, deriving bang-bang optimal control strategies for isothermal PFR systems with periodic flow-rate inputs. Taking a data-driven approach to this same optimal control problem, Grancharova et al. [28] proposed a Gaussian-process-based adaptive optimal control approach for a tubular reactor, using a nonlinear autoregressive model with exogenous inputs (NARX) to capture the reactor's distributed-parameter dynamics and achieve robust control despite stochastic feed disturbances. The CSTR and PFR specific studies confirm that both reactor types require robust, adaptive control strategies capable of handling strong nonlinearities and distributed or time-delay dynamics, reinforcing the motivation for this study's application of FLC to both the CSTR and PFR urea reactors.

Beyond reactor-specific applications, fuzzy-logic-based approaches have also proven effective in broader process safety and general process control problems, further illustrating the versatility of the technique. Wright and Kravaris [29] applied a two-layer fuzzy inference system to control and implement the root causes of a system hazard. The IF-THEN rules embedded in the inference engine, using real-time measurement data, were used to compute numerical simulations, which demonstrated the feasibility of the proposed approach.

Similarly, Mendel et al. [30] used a self-adaptive fuzzy logic controller for real-time pH normalization. The suggested self-adaptive method used different scaling factors based on error and change in error levels to update control parameters and the normalized universe of discourse of output fuzzy membership functions. The self-adaptive scheme's real-time pH control performance demonstrated promising outcomes. The controller was user-friendly and could be adopted by process engineers.

Despite this broad evidence of FLC's effectiveness across diverse control problems, the urea synthesis process itself imposes strict requirements that few of the studies above address directly. These requirements include ensuring that the reaction between NH_3 and CO_2 occurs with stoichiometric mole ratios of 3:1 in equilibrium, obeying Le Chatelier's principle, and maintaining temperature and reactor pressure within the ranges of 180 °C to 184 °C and 160 atm to 180 atm, respectively. Minimum biuret formation of 1.5 % by weight, an N/C ratio of 5:1, an H/C ratio of 3:1, and a residence time of 2 to 6 mins must also be achieved. These principles and process conditions can only be achieved through the application of a robust controller, as local system control cannot withstand external disturbances.

Over the years, PID and other controllers have been used to control the urea production process [31-33]. However, these controllers are analog and struggle with handling imprecisions and nonlinearity in complex control situations. Additionally, PID controllers wait until thermal irregularities, such as during start-ups or system upsets, occur before executing control, which is not ideal as failure to control can cause damage to the plant, humans, and finances. There is an urgent need for a more reliable, self-tuning, artificial intelligence-based [34], and digital controller to minimize control errors, enhance performance during irregularities, and quickly recover from start-ups or system upsets. Again, the process involves excess of the green-house gas (CO₂) which poses safety risks to the environment and the process; hence, a better and reliable controller is needed to control such release to reduce the hazards and toxicity of the process. Fuzzy logic controller (FLC) has proven to handle these challenges effectively and efficiently by dynamically adjust PID gains in response to changing system conditions [35].

Again, optimized kinetic parameters will improve the performance of the controller since no literature was stated on the optimization of the pre-exponential constants, activation energies, and rate constants of the synthesized equilibrium reaction that gave urea product.

Thus, this study aimed to apply FLC to control temperature fluctuations in the CSTR and PFR urea reactors, thereby reducing the excessiveness of the toxic gas by allowing the required amount needed for the synthesis process. This is achieved after the kinetics of the process have been optimized using non linear statistical regression search tool.

The objectives of the study are to apply the rate expression and the transient temperature models [2] to develop uncontrolled, and optimize kinetic models, generate transfer functions for the two reactors, design and integrate fuzzy inference mechanism, indicating the membership functions, use the fuzzy logic rules in the fuzzy block to control temperature fluctuations to an acceptable range within the reactors, and evaluate the effectiveness of the FLC on reactors' types.

2. Methodology

The study entails the adoption of rate expression models for urea synthesis [2], the development of the uncontrolled urea reactors mole fraction and temperature models [2], the derivation of optimal kinetic models, the generation of the transfer functions for the temperature control, the validation of the uncontrolled models results, and comparative performance of the FLC on temperature control of the urea reactors.

2.1 Rate Expression and Transient Models for the Urea Process

The rate expression model for urea synthesis developed by Ojong et al. [2] is based on first principles derivation from the equilibrium reaction of ammonia and carbon dioxide as indicated in model 1

$$\frac{dy_4}{d\tau} = (k_2 - k_1)P_T^3 y_1^2 y_2 - k_3 P_T y_3 \quad (1)$$

where, y_1, y_2, y_3 , and y_4 are the mole fractions for ammonia, carbon dioxide, ammonium carbamate, and urea respectively, P_T is total pressure of the system, k_1, k_2 , and k_3 are the rate constants for the forward and backward equilibrium reaction of ammonia and carbon dioxide, and the forward rate constant for the dissociation of the carbamate to give urea and water.

Interms of fractional conversion, model1 was transformed to give model 2 as

$$\frac{dX}{dt} = P_T^3 y_{2,0}^2 \{ (k_2 - k_1)(\theta - X)^2 (1 - X) \} - k_3 \theta_1 P_T X \quad (2)$$

where, θ is the ratio of the mole fraction of ammonia to that of carbon dioxide initially present, θ_1 is the ratio of the mole fraction of carbamate to that of carbon dioxide initially present, X is the fractional conversion w.r.t limiting reactant, and $y_{2,0}$ is the initial mole fraction of the limiting reactant, carbon dioxide.

Similarly, the urea reactors for the production of organic fertilizer commercially are mounted at Eleme area of Port Harcourt, Rivers State, Nigeria [36, 37] are known as the Indorama and Notore reactors, which are conventionally identified as continuous stirred tank reactor and tubular reactor as described [2]. The transient fractional conversion and temperature models for these reactors were developed by applying material and energy balance principles on the reactors to give the following equations [2].

The material and energy balance applied to the CSTR in series (see Fig. A in Appendix AA) gave ordinary differential equations (ODEs) describing the production process interms of conversion and temperature as in equations 3a and 3b.

$$\frac{dX_n}{dt} = \frac{1}{\tau_1} \theta + \frac{1}{\tau_2} + P_T^3 y_{2,0}^2 \{ (k_2 - k_1)(\theta - X)^2(1 - X) \} + k_3 \theta_1 P_T X \quad (3a)$$

where, X_n is mole fraction of nth reactor as n is 1, 2 and 3 for specifying the 3 reactors in series, τ_1 is the space time interms of ammonia flow, and τ_2 is the space time interms of carbon dioxide flow, defined mathematically as, $\tau_1 = \frac{V_R}{v_1}$, and $\tau_2 = \frac{V_R}{v_2}$, V_R is the volume or capacity of the reactor [m^3], v_1 and v_2 is the volumetric flow rate of the ammonia and carbon dioxide respectively [m^3/s].

$$\frac{dT_i}{dt} = \frac{1}{\tau} (T_0 + T_C - 2T_i) + j P_T^3 y_{2,0}^2 \{ (k_2 - k_1)(\theta - X)^2(1 - X) \} + j k_3 P_T \theta_1 y_{2,0} X \quad (3b)$$

where, $j = \frac{(-\Delta H_r)}{\rho C_p}$ [$m^3 K$], T_i is system temperature for either product formation (with i indicating CSTR number 1, 2, and 3), $\frac{1}{\tau}$ is space velocity or reciprocal of space time, defined mathematically: $\frac{UA}{\rho C_p V_R} = \frac{v_0}{V_R}$, T_0 is the input temperature, T_C is the coolant temperature, UA is the product of the overall heat transfer coefficient [$kW/m^2.K$] and surface area [m^2] of the coolant system, ρC_p is the product of the density [kg/m^3] and specific heat capacity [$kJ/kg K$] of the mixture stream, and v_0 is the volumetric flow rate of the materials [m^3/s].

Similarly, material and energy flow across the PFR as shown in Fig. B (see Appendix AA) was applied to developed partial differential equations (PDEs) describing the conversion and temperature progression in the reactor as shown in models 4a and 4b respectively.

$$\frac{\partial X}{\partial \tau} + v \frac{\partial X}{\partial z} = k_2 P_T^3 y_{2,0}^2 (\theta - X)^2 (1 - X) - k_1 P_T^3 y_{2,0}^2 (\theta - X)^2 (1 - X) - k_3 P_T \theta_1 y_{2,0} X \quad (4a)$$

where, v is the fluidized velocity of the system.

$$\frac{\partial T}{\partial \tau} + v \frac{\partial T}{\partial z} = j (k_2 - k_1) P_T^3 y_{2,0}^2 (\theta - X)^2 (1 - X) + j k_3 P_T \theta_1 y_{2,0} X + \frac{1}{\tau} (T - T_{st}) \quad (4b)$$

2.2 Kinetic Optimization

Statistical non-linear regression analysis is applied to obtain the most suitable kinetics to control the process. The rate constants, the energies of activation, and pre-exponential constants are optimized for proper control and design [38]

The kinetics k_i to be optimized, is defined mathematically for temperature process as,

$$k_i = k_{i,0} \exp (E_i/RT), \quad (5)$$

where, $k_{i,0}$ is the pre-exponential constants for reversible and irreversible reactions, E_i is the energies of activation for the reacting species i , ($i = 1, 2, 3$) in the equilibrium urea reaction process.

Numerically, the statistical search method is used to determine the optimal values of the rate constants, Arrhenius constants and activation energies [39], which is a statistical search non-linear regression method, that agreed with the convergence criterion “If $F_{cal} > F_{tab}$ ” then, the values obtained from the simulations of the statistical models converges and the kinetic parameters values at 5% confidence interval fare optimal.

The optimization procedures followed the defined stated models as,

$$F_{cal} = \frac{\text{Mean of Square Erros}}{\text{Mean of Square Mean}} \quad (6)$$

where, F_{cal} is the calculated frequency distribution value. These square means are defined mathematically as,

$$\text{Mean of Square Erros} = \frac{\text{Sum of Square Mean}}{\text{parameters involved}} \quad (7a)$$

$$\text{Mean of Square Mean} = \frac{\text{Sum of Square Error}}{\text{iteration number} - \text{parameters involved}} \quad (7b)$$

The square means are defined as functions of fractional conversion and temperature obtained in the reactors' models reactors as,

$$\text{Sum of Square Mean} = \sum_p^n \{ (X_{i,cal} - X_i)^2 + (T_{j,cal} - \bar{T}_j)^2 \} \quad (8)$$

$$\text{Sum of Square Error} = \sum_p^n \{ (X_{i,cal} - X_{i,plant})^2 + (T_{j,cal} - T_{0,plant})^2 \} \quad (9)$$

where, $X_{i,cal}$, $\bar{X}_i$, $T_{j,cal}$, and $\bar{T}_j$ are the simulated and mean conversions and simulated and mean temperatures of the various runs generated respectively. $X_{i,plant}$ and $T_{0,plant}$ are the plant data for the conversion and temperature. The conversion and temperature means are defined as,

$$\bar{X}_i = \frac{\sum_{j=1}^n X_i}{n} \quad (10)$$

$$\bar{T}_j = \frac{\sum_{j=1}^n T_j}{n} \quad (11)$$

Suppose that the condition for acceptability of the parameters based on the criterion set as defined above met for convergence, then, the optimal kinetics are thus computed as,

$$E_i^{(j+1)} = E_i^j + \alpha \Delta \quad (12)$$

$$A_i^{(j+1)} = A_i^j + \alpha \Delta \quad (13)$$

where, $E_i^{(j+1)}$ and $A_i^{(j+1)}$ are the best values of energies of activation and pre-exponential constants obtained, E_i^j and A_i^j are the input or take off values for the energies of activation and pre-exponential (Arrhenius) constants, α is a scalar constant defined as $0.35 \leq \alpha \leq 0.95$ [38, 39], and Δ is the delta value determined mathematically as,

$$\Delta = -(m)^{-1} \cdot [n \ X \ p] \quad (14)$$

where, $(\mathbf{m})^{-1}$ is the matrix inverse, which comprises of the product of matrix and its transpose, and $[\mathbf{n} \ \mathbf{X} \ \mathbf{p}]$ is matrix originated from the iteration number by parameters involved. Then the refined rate constant is determined as,

$$\mathbf{k}_j = \mathbf{A}_i^{(j+1)} \exp \left\{ -\frac{\mathbf{E}_i^{(j+1)}}{\mathbf{RT}} \right\} \quad (15)$$

where, R is gas constant [J/mol. K]

2.3 Discretization of the Urea Reactors Models

The terms on the ODEs and PDEs models are non-linear; hence, Taylor's series approach is applied to linearized the non-linear terms on the right hand of the uncontrolled models 4 which powers of the variables are product and not 1. Linearity is key for control of the process and this effectively generate transfer functions for the processes and the loads. Higher powers of the variables in the series are truncated as the errors are negligible, hence the series used for the implementation of the linear term is shown in model 5.

$$\mathbf{f}(\mathbf{X}, \mathbf{T}) = \mathbf{f}(\mathbf{X}_j, \mathbf{T}_j) + \frac{\partial \mathbf{f}(\mathbf{X}_j, \mathbf{T}_j)}{\partial \mathbf{X}} (\mathbf{X} - \mathbf{X}_j) + \frac{\partial \mathbf{f}(\mathbf{X}_j, \mathbf{T}_j)}{\partial \mathbf{T}} (\mathbf{T} - \mathbf{T}_j) + \dots \quad (16)$$

where, $\mathbf{X}_j$ and $\mathbf{T}_j$ are steady state values of the conversion and temperature.

Applying model 16 to linearized models 3 and 4 coupled together give models 17 and 18 in terms of deviation variables respectively (see detailed of discretization in Appendix A and B).

$$\frac{d\mathbf{X}'}{d\tau} = -\mathbf{w}_2 \mathbf{X}' + \mathbf{w}_3 \mathbf{T}' + \mathbf{a}_2 \mathbf{T}'_0 + \mathbf{K}'_1 \quad (17a)$$

$$\frac{d\mathbf{T}'}{d\tau} = \mathbf{w} \mathbf{T}' + \frac{1}{\tau} \mathbf{T}'_1 + \mathbf{a}_1 \mathbf{T}'_0 + \frac{1}{\tau} \mathbf{T}'_{st} + \mathbf{w}_1 \mathbf{X}' + \mathbf{K}' \quad (17b)$$

where, $\mathbf{w}_2, \mathbf{w}_3, \mathbf{a}_2, \mathbf{K}'_1, \mathbf{w}, \mathbf{a}_1, \mathbf{w}_1$, and $\mathbf{K}'$ are constants defined appropriately (see appendix A in the supplementary document for clarity of the discretization method).

$$\frac{\partial \mathbf{X}'}{\partial \tau} + \mathbf{v} \frac{\partial \mathbf{X}'}{\partial z} = \mathbf{m} \mathbf{X}' + \mathbf{m}_1 \mathbf{T}' - \mathbf{m}_1 \mathbf{T}'_0 + \mathbf{d}' \quad (18a)$$

$$\frac{\partial \mathbf{T}'}{\partial \tau} + \frac{\partial \mathbf{T}'}{\partial z} = \mathbf{m}_{11} \mathbf{X}' + \mathbf{m}_{12} \mathbf{T}' + \mathbf{C}_1 \mathbf{T}'_0 - \frac{1}{\tau} \mathbf{T}'_{st} + \mathbf{d}'_1 \quad (18b)$$

where, $\mathbf{m}, \mathbf{m}_1, \mathbf{d}, \mathbf{m}_{11}, \mathbf{m}_{12}, \mathbf{C}_1$, and $\mathbf{d}_1$ are constants defined appropriately as shown in Appendix B in the supplementary document.

2.4 Transfer Functions Generation for the Processes and Loads

The generation of the transfer functions for the urea reactors are obtained from the Laplace Transform (LT) of the ODEs models for both reactors as the performance of the reactors must be based on same geometry, hence, the assumption was made to convert the PDEs (model 18) to ODEs. This is so because, control is time dependent, not distance. Thus, the differential terms approximate to zero (see Appendix C for clarity). The LT of models 17 and 18 to give models 19 and 20 respectively as,

$$(\mathbf{s} + \mathbf{w}_2) \bar{\mathbf{X}}'_{(s)} - \mathbf{w}_3 \bar{\mathbf{T}}'_{(s)} = \mathbf{a}_2 \bar{\mathbf{T}}'_{0(s)} + \frac{\mathbf{K}'_1}{\mathbf{s}} \quad (19a)$$

$$-w_1 \bar{X}_{(s)} + (s - w) \bar{T}'_{(s)} = \frac{1}{\tau} \bar{T}'_{i(s)} + a_1 \bar{T}'_{0(s)} + \frac{K'}{s} \quad (19b)$$

$$(s - m) \bar{X}'_{(s)} - m_1 \bar{T}'_{(s)} = -m_1 \bar{T}'_{0(s)} + \frac{d'}{s} \quad (20a)$$

$$m_{11} \bar{X}'_{(s)} + (s - m_{12}) \bar{T}'_{(s)} = C_1 \bar{T}'_{0(s)} = \frac{1}{\tau} \bar{T}'_{st(s)} + \frac{d'_i}{s} \quad (20b)$$

Detailed of the couple models 19 and 20 resolved are shown in appendix C in the supplementary document.

Each coupled algebraic models (19 and 20) consist of the conversion and temperature variables, resolved using Cramer's rule based on matrix form: $AX = b$ to give the transfer functions as shown respectively in models 22 and 26 for both reactors.

$$\begin{bmatrix} w_3 & (s + w_2) \\ (s - w) & -w \end{bmatrix} \begin{bmatrix} \bar{X}'_{(s)} \\ \bar{T}'_{(s)} \end{bmatrix} = \begin{bmatrix} a_2 \bar{T}'_{0(s)} + \frac{K'_1}{s} \\ \frac{1}{\tau} \bar{T}'_{i(s)} + a_1 \bar{T}'_{0(s)} + \frac{K'}{s} \end{bmatrix} \quad (21)$$

Model 21 is solved to give the transfer functions interms of conversion and temperature as,

$$\bar{X}'_{(s)} = \frac{w_3}{\tau P_{(s)}} \bar{T}'_{i(s)} + \frac{(a_2(s+w) + a_1 w_3)}{P_{(s)}} \bar{T}'_{0(s)} + \frac{(s+w) K'}{s P_{(s)}} + \frac{w_3 K'}{s P_{(s)}} \quad (22a)$$

$$\bar{T}'_{(s)} = \frac{(s+w_2)}{\tau P_{(s)}} \bar{T}'_{i(s)} + \frac{(a_1(s+w_2) + a_1 w)}{P_{(s)}} \bar{T}'_{0(s)} + \frac{(s+w_2) K'}{s P_{(s)}} + \frac{K'_1 w}{s P_{(s)}} \quad (22b)$$

where, $P_{(s)}$ is a polynomial of degree two (2), defined mathematically as,

$$P_{(s)} = s^2 - a's - w' \quad (23)$$

The transfer functions for the process and disturbance or load are obtained from models 22a and 22b as shown in model 24, Table 1, and Fig.1.

$$\begin{bmatrix} \bar{X}'_{(s)} \\ \bar{T}'_{(s)} \end{bmatrix} = \begin{bmatrix} G_{11(s)} & G_{12(s)} & G_{13(s)} \\ G_{21(s)} & G_{22(s)} & G_{23(s)} \end{bmatrix} \begin{bmatrix} \bar{T}'_{i(s)} \\ \bar{T}'_{0(s)} \\ K_{(s)} \end{bmatrix} \quad (24)$$

The transfer function matrix $G_{(s)} = \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \end{bmatrix}$ is presented in Table 1 for the various components as,

Table 1 Transfer Functions for the Indorama Urea Reactor (CSTR)

Output	Input	$G_{ij}(s)$ Element	Transfer Function
$\bar{X}'(s)$	$\bar{T}'_i(s)$ $\bar{T}'_0(s)$ $K'(s)$	G_{11} G_{12} G_{13}	$\frac{w_3/\tau P(s)}{[a_2(s-w) + a_1 w_3]/P(s)}$ $\frac{w_3/s P(s)}{[a_2(s-w) + a_1 w_3]/P(s)}$
$\bar{T}'(s)$	$\bar{T}'_i(s)$ $\bar{T}'_0(s)$ $K'(s)$	G_{21} G_{22} G_{23}	$\frac{(s+w_2)/\tau P(s)}{[a_1(s-w_2) + a_2 w]/P(s)}$ $\frac{(s+w_2)/s P(s)}{[a_1(s-w_2) + a_2 w]/P(s)}$

The transfer function for the CSTR process is also shown in Fig. 1.

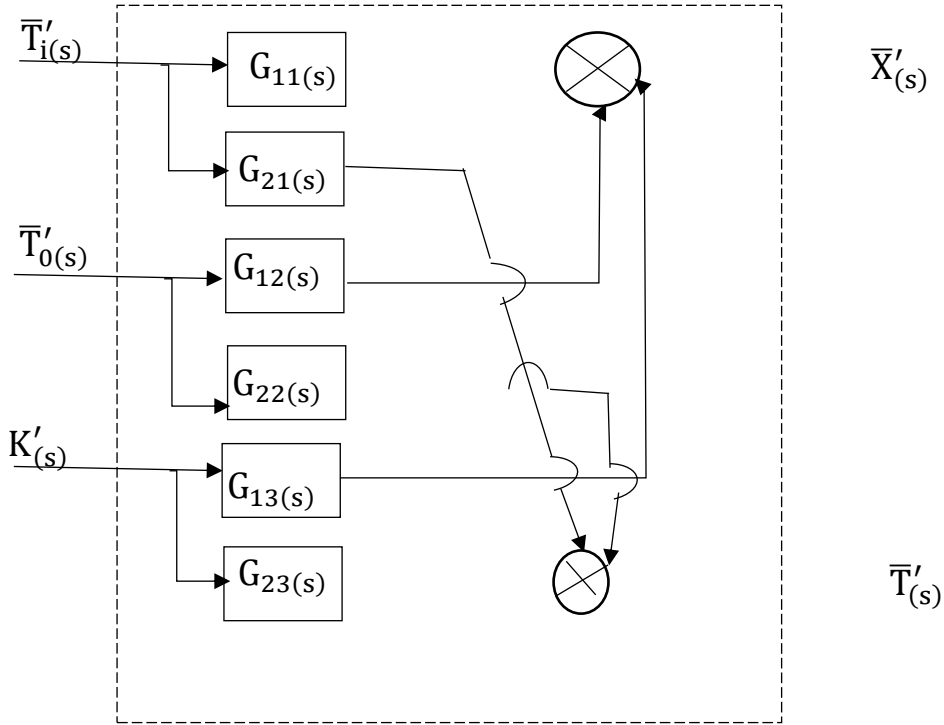


Fig. 1 Input-Output Transfer Functions for the CSTR Urea Process

Similarly, models 20a and 20b are resolved using Cramer's rule give $\bar{X}'_{(s)}$ and $\bar{T}'_{(s)}$ as,

$$\begin{bmatrix} s - m & -m_1 \\ -m_{11} & s - m_{12} \end{bmatrix} \begin{bmatrix} \bar{X}'_{(s)} \\ \bar{T}'_{(s)} \end{bmatrix} = \begin{bmatrix} \frac{d'}{s} - m_1 \bar{T}'_{0(s)} \\ c_1 \bar{T}'_{0(s)} - \frac{1}{\tau} \bar{T}'_{st(s)} + \frac{d'_1}{s} \end{bmatrix} \quad (25)$$

Using Cramer's rule on model 25 provides the solutions as,

$$\bar{\mathbf{X}}'_{(s)} = \frac{(\mathbf{m}' - \mathbf{m}_1 s) \bar{\mathbf{T}}'_{0(s)} - \frac{\mathbf{m}_1}{\tau} \bar{\mathbf{T}}'_{st(s)} + (s + \mathbf{n}) \frac{\mathbf{d}'_1}{s}}{\mathbf{P}_1(s)} \quad (26a)$$

$$\bar{\mathbf{T}}'_{(s)} = \frac{(s - \varphi) \bar{\mathbf{T}}'_{0(s)} - \frac{1}{\tau} (s - \mathbf{m}) \bar{\mathbf{T}}'_{st(s)} - (s + \varphi_1) \frac{\mathbf{d}'_1}{s}}{\mathbf{P}_1(s)} \quad (26b)$$

where, $\mathbf{P}_1(s)$ is a polynomial of degree 2 defined mathematically as,

$$\mathbf{P}_1(s) = s^2 - fs + f_1 \quad (27)$$

$\mathbf{n}$, φ , $\mathbf{f}$, f_1 , and φ_1 are constants defined accordingly as $\mathbf{m}_1 \mathbf{m}_{12}$, $\mathbf{m} + \mathbf{m}_1 \mathbf{m}_{11}$, $(\mathbf{m}_{12} + \mathbf{m})$, $\mathbf{m} \mathbf{m}_{12} - \mathbf{m} \mathbf{m}_{11}$, and $\mathbf{m}_{11} - \mathbf{m}$.

The transfer function matrix $\mathbf{G}_{(s)}$, is obtained from model 9a and 9b, which serve as the transfer functions for the urea process and the disturbance described by the PFR and stated as,

$$\begin{bmatrix} \bar{\mathbf{X}}'_{(s)} \\ \bar{\mathbf{T}}'_{(s)} \end{bmatrix} = \begin{bmatrix} \mathbf{G}_{11(s)} & \mathbf{G}_{12(s)} & \mathbf{G}_{13(s)} \\ \mathbf{G}_{21(s)} & \mathbf{G}_{22(s)} & \mathbf{G}_{23(s)} \end{bmatrix} \begin{bmatrix} \bar{\mathbf{T}}'_{0(s)} \\ \bar{\mathbf{T}}'_{st(s)} \\ \mathbf{d}'_1 \end{bmatrix} \quad (28)$$

The transfer function matrix $\mathbf{G}_{(s)} = \begin{bmatrix} \mathbf{G}_{11} & \mathbf{G}_{12} & \mathbf{G}_{13} \\ \mathbf{G}_{21} & \mathbf{G}_{22} & \mathbf{G}_{23} \end{bmatrix}$ and the transfer functions for the input-output model of PFR is displayed in Table 2 and Fig.

2 as,

Table 2 Transfer functions for the Notore Urea Reactor (PFR)

Output	Input	$\mathbf{G}_{ij}(s)$	Transfer Function
$\bar{\mathbf{X}}'_{(s)}$	$\bar{\mathbf{T}}'_{0(s)}$ $\bar{\mathbf{T}}'_{st(s)}$ $\mathbf{d}'_{1(s)}$	$\mathbf{G}_{11}$ $\mathbf{G}_{12}$ $\mathbf{G}_{13}$	$(\mathbf{m}' - \mathbf{m}_1 s) / \mathbf{P}_1(s)$ $- \mathbf{m}_1 / \tau \mathbf{P}_1(s)$ $(s + \mathbf{n}) / s \mathbf{P}_1(s)$
$\bar{\mathbf{T}}'_{(s)}$	$\bar{\mathbf{T}}'_{0(s)}$ $\bar{\mathbf{T}}'_{st(s)}$ $\mathbf{d}'_{1(s)}$	$\mathbf{G}_{21}$ $\mathbf{G}_{22}$ $\mathbf{G}_{23}$	$(s + \varphi) / \mathbf{P}_1(s)$ $(s - \mathbf{m}) / \mathbf{P}_1(s)$ $-(s + \varphi_1) / s \mathbf{P}_1(s)$

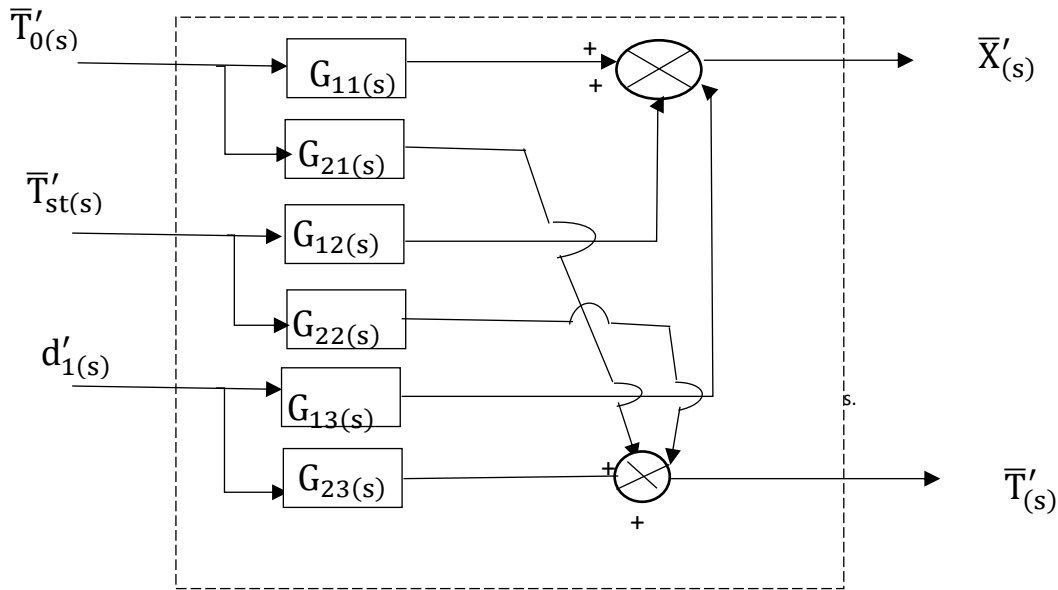


Fig. 2 Input-Output Transfer Functions for the PFR Urea Reactor

2.5 Control of the Urea Reactors using Fuzzy Logic Controller

The control models are transfer functions obtained from the urea reactors developed models. The fuzzy logic closed-loop system is built in such a way that the fuzzy logic controller controls the temperature fluctuations within the urea reactors via the integration of the fuzzy inference mechanisms [35]. The fuzzy block which is the replacement of the PID controller with the fuzzy mechanism (see Fig. 3), consist of fuzzy rules and the membership functions to implement the controller's objective as shown in the general block diagram of the closed-loop temperatures control system.

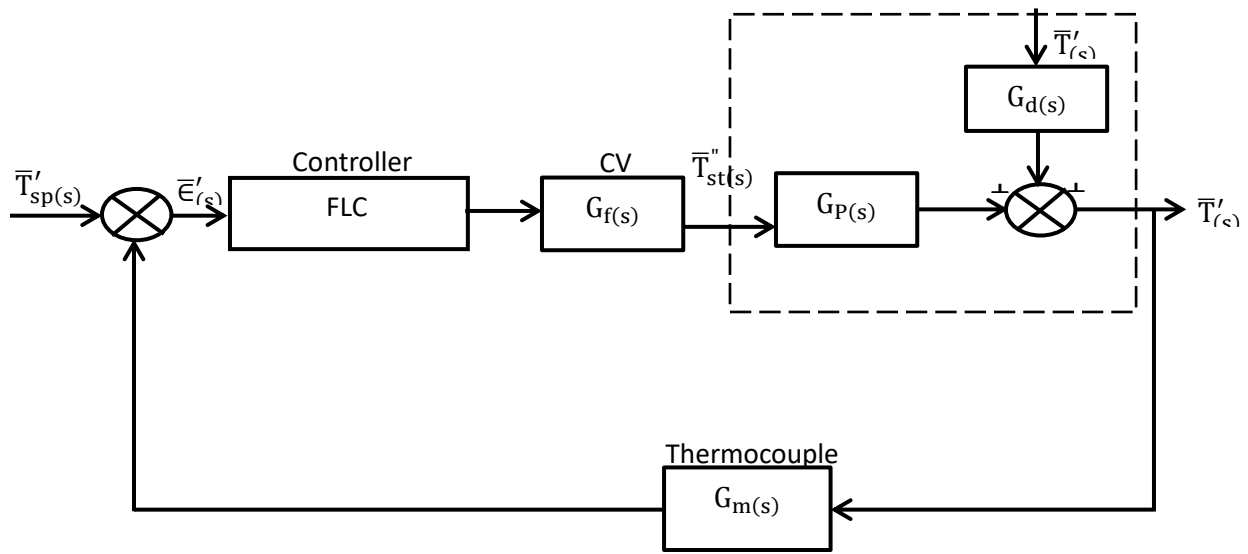


Fig.3 Generalized Fuzzy Logic Controller Block Diagram for a Closed-Loop Temperature Control of the Urea Reactors

where, CV is the control valve, $G_{f(s)}$, $G_{P(s)}$, $G_{d(s)}$, and $G_{m(s)}$ is the transfer function of the finite control element, the process, the load, and measuring instrument called the thermocouple of the first order function defined mathematically as,

$$G_{m(s)} = \frac{\bar{T}'_{m(s)}}{\bar{T}'_{(s)}} = \frac{1}{\tau_p s + 1} \quad (29)$$

$$G_{f(s)} = \frac{\bar{F}'_{(s)}}{\bar{C}'_{(s)}} = \frac{K_v}{\tau_v s + 1} \quad (30)$$

Models 29 and 30 are obtained from the LT of the thermocouple model [40] and final control element model [9]. Details of the developed models are shown in appendix D in the supplementary document.

The fuzzy rules are the most important design procedure of the fuzzy logic used to implement the fuzzy logic controller strategy on temperature control. The fuzzy rules create the fuzzy instructions to carry out the control function based on the membership functions of time and temperature.

The nine (9) fuzzy logic rules for the implementation of temperature control of the reactors [34, 41, 42] are stated as thus:

- i. If the input temperature is below the set point and time is moderate, then output temperature should be boosted.
- ii. If the input temperature is below the set point and time is fast, then output temperature is boosted.
- iii. If the input temperature is below the set point and time is moderate then, output temperature is boosted.
- iv. If the input temperature is accepted (at set point temperature) and time is slow, then output is control temperature.
- v. If the input temperature is accepted (set point temperature) and time is moderate, then output is control temperature.
- vi. If the input temperature is accepted (at set point) and time is fast, then output is control temperature.
- vii. If the input temperature is over (above the set point temperature) and time is slow, then output is normalizing temperature.
- viii. If the input temperature is over (above set point temperature) and time is moderate, then output is normalizing temperature.
- ix. If the input temperature is over (above set point) and time is fast, then output is normalizing temperature.

2.6 Input Data for Simulation

Tables 3 and 4 are input parameters from the CSTR and PFR Urea reactors respectively, which are obtained from the plants. The computational data used for the simulation also are presented in appendix E of the supplementary document. Table 5 present the literature data also used for the simulation process. The possibility of getting the data from the plants is due to collaborative support the Rivers State University have with the industries within the state, which was initiated by the Council for the Regulation of Engineering in Nigeria (COREN) during the outcome-based Education (OBE) awareness as one of the main criteria that the Engineering programs get partial or full accreditations by the body.

Table 3 Input parameters for the Indorama Plant (CSTR) [32a]

S/N	Parameter	Value	Unit
1.	T (Temperature)	184	°C
2.	P (Pressure)	155	[kg cm ⁻² . G]
3.	NH ₃ flow rate	93	[t h ⁻¹]
	CO ₂ flow rate	12	[t h ⁻¹]
	Carbamate flow rate	122	[t h ⁻¹]
4.	X (Conversion)	0.63 to 0.64	-
5.	T (Time)	3.7	[Min]
6.	N/C ratio	3.6	-
7.	H/C ratio	0.5	-
8.	Forward rate constant k ₁	0.691	[hr ⁻¹]
	Backward rate constant k ₂	0.596	[hr ⁻¹]
	Forward rate constant k ₃	1.2212.	[hr ⁻¹]
9.	E1	15	[kJ mol ⁻¹]
	Energies of activation: E2	15	
	E3	17.5	
10.	Reactor length	12	M
11.	A ₁	0.694	[hr ⁻¹]
	Pre-exponential constants: A ₂	0.598	[hr ⁻¹]
	A ₃	1.227	[hr ⁻¹]
12.	ΔH _r (Heat of reaction)	131.1	[kJ mol ⁻¹]
13.	Amount produced	4000	[MTPD]
14.	ρ (Density)	1323	[kg m ⁻³]
15.	C _p (Specific heat)	1.339	[kJ kg ⁻¹]

Table 4 Input or Plant data for Notore Plant (PFR) [33]

S/N	Parameter	Symbol	Value	Unit
1.	Temperature. T	T ₀	183	°C
2.	Pressure, P	P ₀	160	[kg cm ⁻² . G]
3.	Flow rate, F	F	61.23	[m ³ hr ⁻¹]
4.	Conversion, C	X	0.54	-
5.	Residence Time	t ₀	2.50	[min]
6.	Rate Constants	k ₁ , k ₂ , & k ₃	0.691, 0.596, & 1.2212	[hr ⁻¹]
7.	Activation Energy	E _{A1} , E _{A2} , & E _{A3}	15, 15, & 17.5	[kJ mol ⁻¹]
8.	Arrhenius Constant	A ₁ & A ₂ , & A ₃	0.694, 0.598, & 1.227	[hr ⁻¹]
9.	Reactor Capacity	V	1500	[MT]
10.	Heat of Reaction	ΔH _r	131.1	[kJ mol ⁻¹]
11.	Molar flow rate	C _{A0}	50.23	[Kmol m ⁻³]
12.	Nitrogen Carbon ratio	N/C	3	-
13.	Hydrogen Carbon ratio	H/C	3.1	-
14.	Ammonia Pressure	P ₁	210	[atm(g)]
15.	Equilibrium constant	K _p	115.94	-
16.	Carbon dioxide pressure	P ₂	200	[atm(g)]

17.	Density	P	1323	[kg m ⁻³]
18.	Specific heat	C _p	1.339	[kJ kg ⁻¹ .°C]
19.	Gibbs Free Energy	ΔG	-197.15	[kJ mol ⁻¹]
20.	Entropy	ΔS	-333.19	[kJ mol ⁻¹ °C]
21.	Enthalpy	ΔH	4.5	[kcal mol ⁻¹]

Table 5 Literature Data for the Urea Production Process [32b]

S/N	Parameter	Symbol	Value	Unit
1.	Feed Composition	CO ₂ , NH ₃ , H ₂ O, & (NH ₂) ₂ CO	31, 43, 21, & 5	%
2.	Temperature (°C)	T _i	172 – 178	°C
3.	Pressure	P _i	200	[atm, g]
4.	N ₂ Carbon ratio	N/C	4	-
5.	H ₂ Carbon ratio	H/C	0.64	-
6.	Conversion	X	0.64	-
7	Molar Concentration	CO ₂ , NH ₃ , H ₂ O, & (NH ₂) ₂ CO	0.018, 0.023, 0.011, & 0.003	[mol m ⁻³]

2.7 Solution Techniques

The uncontrolled models are the ODEs and PDEs developed which were numerically resolved with 4th order Runge-Kutta (R-K) and the finite difference approximation techniques (FDAT) respectively as stated clearly in the work of Ojong et al [2]. The kinetics parameters used for the simulation process were refined for proper control functionality [2,43]. The simulation is numerically conducted based on Simulink/MATLAB version 8.0 and it follows a clear flow chart shown in Fig.4.

Simulation of the system modelling design of the fuzzy inference system and then validation which involves the introduction of simulated temperature fluctuations, including sudden drops, to evaluate the controller's robustness based on time (mins) and temperature (°C) membership functions of range [0:1:8] and [84:250]. The Simulink/MATLAB of version 8.0 is the simulation environment for the implementation of controller strategy to control temperature disturbances within the urea reactors.

The 4th order-K algorithm used to resolve the ODEs is written as,

$$K_{1n} = hf(t_i; X_{ijp}; T_{ijp}) \quad (31a)$$

where, p takes values 0,1, 2, 3, ... n, m stands for 1 and 2.

$$K_{2n} = hf\left(t_i + \frac{1}{2}h; X_{ij,p} + \frac{1}{2}K_{11}; T_{ij,p} + \frac{1}{2}K_{12}\right) \quad (31b)$$

where, h is the step size for the iteration process.

$$K_{3n} = hf\left(t_i + \frac{1}{2}h; X_{ij,p} + \frac{1}{2}K_{21}; T_{ij,p} + \frac{1}{2}K_{22}\right) \quad (31c)$$

$$K_{4n} = hf(t_i + h_s; X_{ij,p} + K_{31}; T_{ij,p} + K_{32}) \quad (31d)$$

$$X_{ij,p+1} = h_i + \frac{1}{6}(K_{11} + 2K_{21} + 2K_{31} + K_{41}) \quad (31e)$$

$$T_{ij,p+1} = T_{ij,p} + \frac{1}{6}(K_{12} + 2K_{22} + 2K_{32} + K_{42}) \quad (31f)$$

$$t_{i+1} = t_i + h \quad (31g)$$

The FDAT used for the resolution of the PDEs developed are the central and forward FDAT applied for the time and the spatial domains of the functions respectively.

$$(a + 1)X(t, i) = y(t + 1, i) + ay(t, i + 1) - b \quad (32)$$

where, a is defined as $\frac{v\Delta t}{\Delta z}$, and b is defined as $(-r_4)\Delta t$

$$(1 - a + a_1)T(t, i) = aT(t, i + 1) + T(t + 1, i) - Jb + b_1 \quad (33)$$

where, b_1 is defined as $\Delta t T_C$

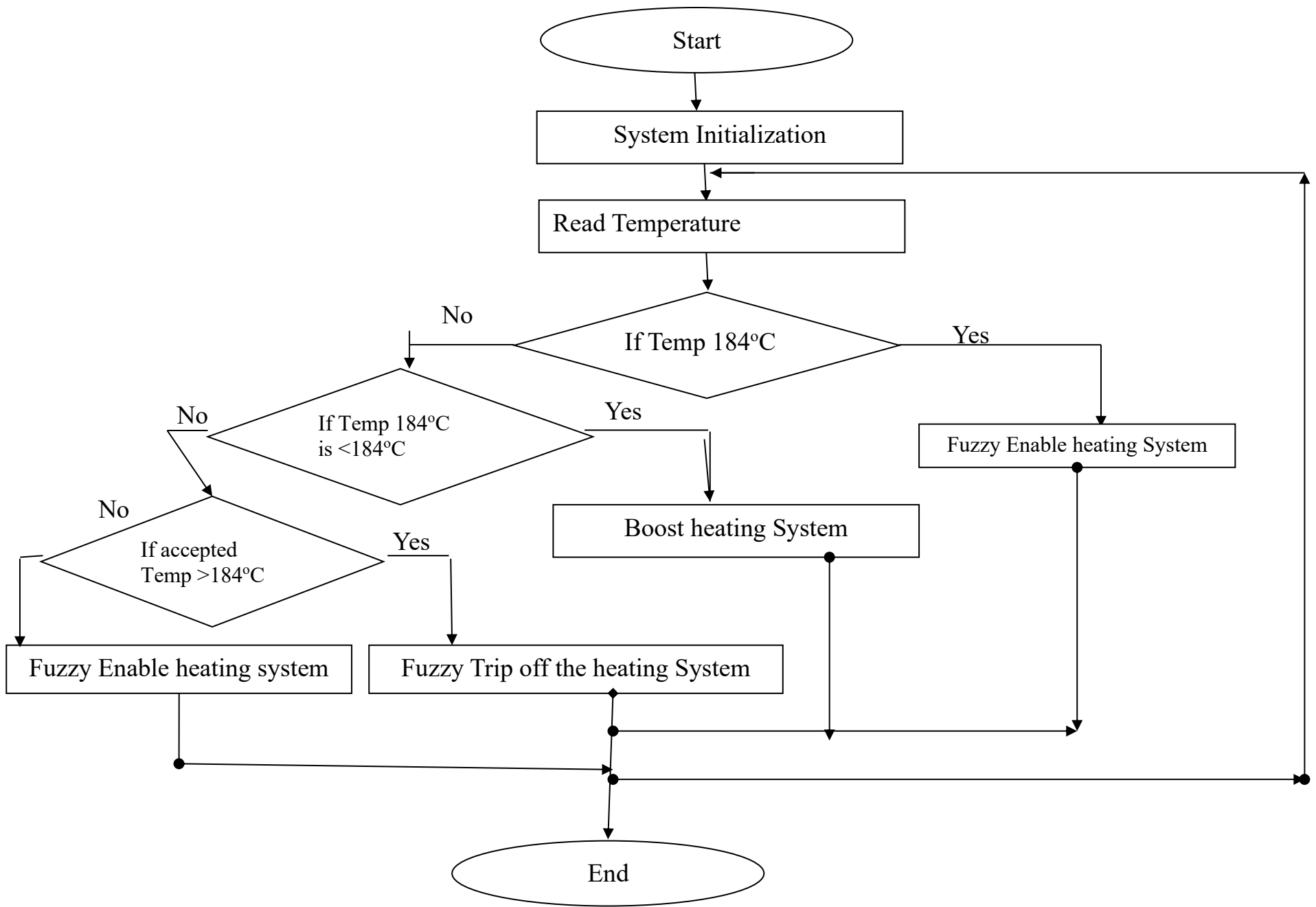


Fig.4 Flow Charts Implementation for the Fuzzy Logic Control Strategy for the Urea Reactors

2.8 Validation of the Models

The root means square error as the error analysis evaluation (rmse) displayed in model 34 [2, 38], is key for validation of the models as,

$$\text{rmse} = \sqrt{\left(\frac{\text{model-plant/literature}}{\text{iteration number}}\right)^2} \quad (34)$$

3 Results and Discussion

3.1 Uncontrol Reactors Models

The simulated conversion and temperature models developed for the urea reactors with sinusoidal inputs of $65.5\sin(0.4t)$ and $184\sin(0.4t)$, to ascertain the level of disturbance caused within the reactors, if there is a need for controller or not. Figs. 5 to 6 clearly indicated that controller is needed for the urea process.

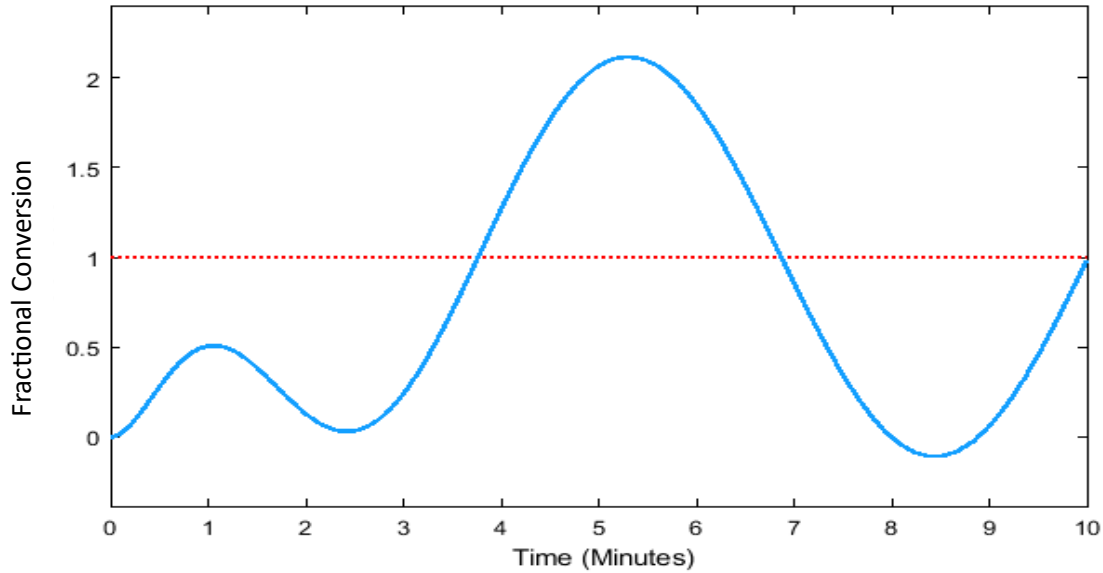


Fig.5a Effect of Sinusoidal Input on Fractional Conversion of CSTR urea process

The profile of fractional conversion against time generated when the model was simulated sinusoidally, produces more disturbances at output response of the urea reactor shown in Fig.5a, which agrees with literature trend [44, 45]. The profile has peak and trough values at 2.5 and 0 respectively and fluctuates in succession as time increases, indicating that the fluctuations of the fractional conversion value within the urea reactor is high and above the set point value of 1. This call for a proper and efficient controller mechanism, able to effectively and qualitatively control the output fluctuations for better quality and more urea produced.

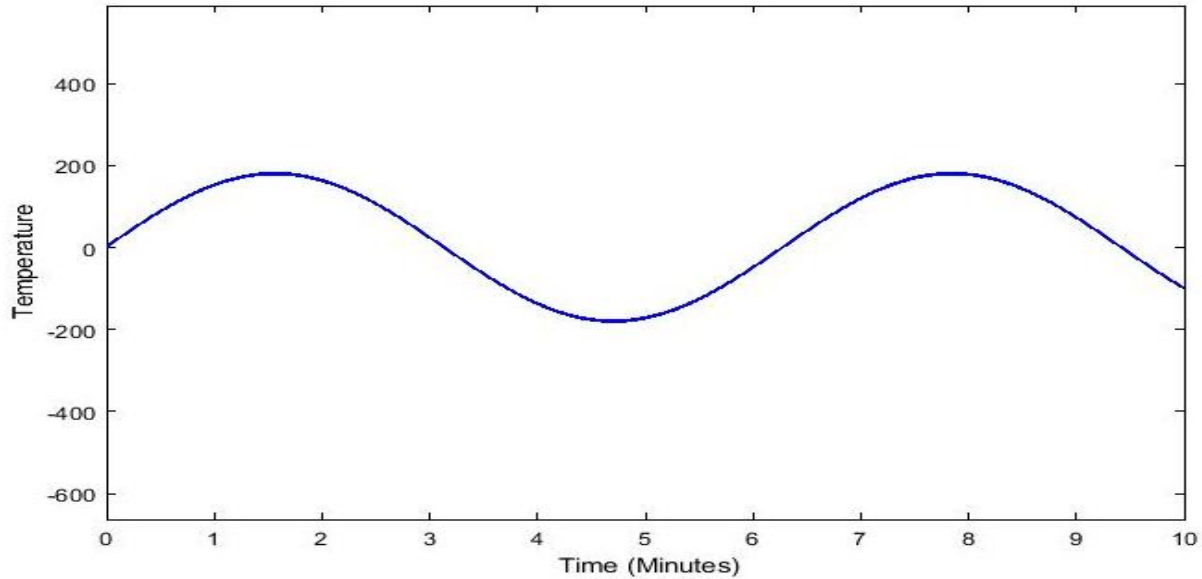


Fig.5b Effect of Sinusoidal Input on Temperature of CSTR urea process

The profile of temperature with time generated when the input parameter is sinusoidally disturbed the CSTR urea reactor is shown in Fig.5b. The temperature wave profile has peak and trough at values $\pm 200^{\circ}\text{C}$ respectively and fluctuates in succession as time increases, indicating that the fluctuations of the heat within the urea system is high and above the set point value of 184°C . This call for a proper and efficient controller mechanism, able to effectively and qualitatively control the temperature fluctuations for better quality and more yield of urea in the reactor in line with literatures [46, 47]. The step change behaviour of temperature input to the urea reactor makes no sense as there is sudden drop of temperature from the set point to 166°C .

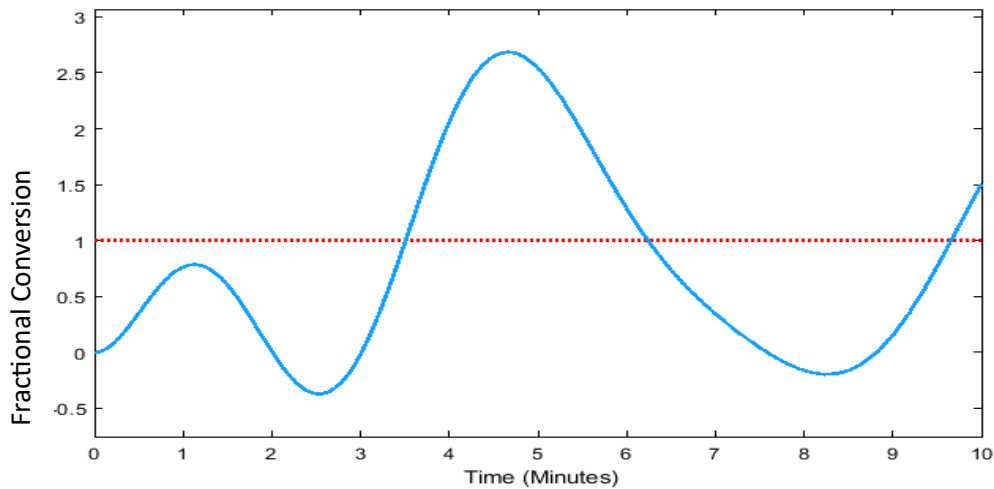


Fig.6a Effect of Sinusoidal Input on Fractional Conversion of PFR urea process

The fluctuations of the fractional conversion profile produced with time due to the variable input into the PFR urea reactor is shown in Fig.6a. The profile has peak and trough at values 2.8 and -0.4 respectively and fluctuates in succession as time increases, indicating that the urea reactor is highly unstable with

values above the set point value of 1. The input fractional conversion variation correspondingly disturbs the output values, causing the reactor not to perform optimally. This call for a proper and efficient controller mechanism, able to effectively and qualitatively control the output fluctuations for better quality and more yield of urea in the reactor.

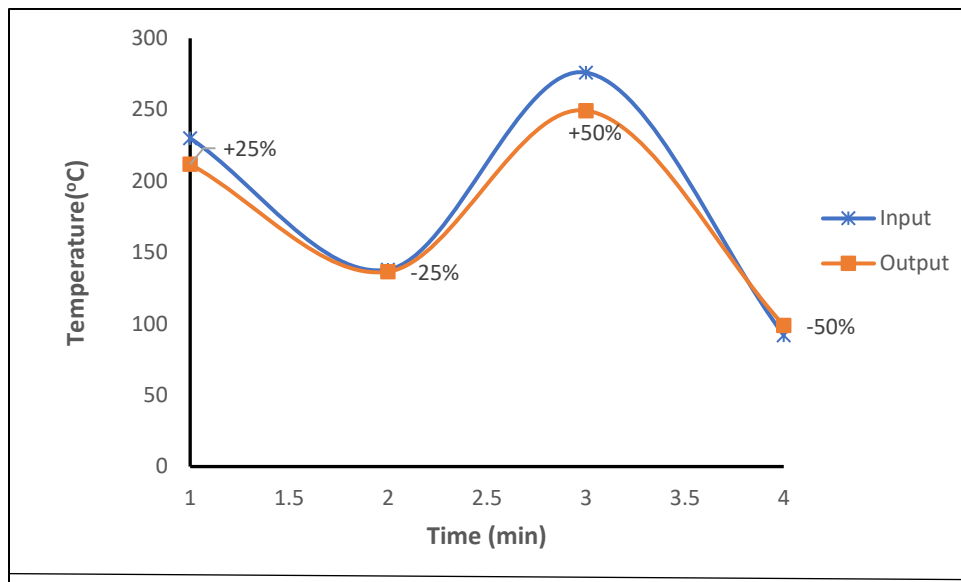


Fig.6b Effect of Sinusoidal Input on Temperature of PFR urea process

The sinusoidal temperature profile produced with time due to the variable input into the PFR urea reactor is shown in Fig.6b.

The temperature wave profile has peak and trough at values 250 °C and -150 °C respectively and fluctuates in succession with time increase, indicating that the fluctuations of the heat in the urea system are much and above the set point value of 184 °C (i.e., above the process condition value).

The input temperature variation causes disturbance of the output values which lead to poor performance of the reactor.

This call for a proper and efficient controller mechanism, able to effectively and qualitatively control the temperature fluctuations for better quality and more urea obtained.

3.2 Validation of the Urea Reactors Models

Table 6 presents the validation of the uncontrolled models results with plant and literature values.

The error analysis for the urea reactors models' results compared to plants and literature values gave negligible values from 9.0E-04 [-] to 0.010 [° C] and 7.0E04 [-] to 0.209 [° C] respectively for plant and literature values, indicate that the developed ODEs and PDEs that described the Indorama and Notore urea production process respectively can be reliable, good and should be acceptable.

This means that the models developed are good enough with minimal errors and assumptions made.

Table 6 Models Prediction and Performance Results

Urea Reactor	Plant Value	Literature Data	Model Result
Fractional Conversion (X)			
Indorama (CSTR)	0.63	0.64	0.683
RMSE absolute	0.0009 [-]	0.0007 [-]	-
Notore (PFR)	0.543	0.64	0.589
RMSE absolute	0.0008	0.00085	-
Temperature (T)			
Indorama (CSTR)	182 °C	175 °C	181.70°C
RMSE absolute	0.007 °C	0.163 °C	-
Notore (PFR)	184 °C	175 °C	183.57°C
RMSE absolute	0.010 °C	0.209 °C	-

3.3 Optimized and Validation of the Kinetic Parameters

Inline with Wordu et al. [38] and Wordu et al. [39], the optimized kinetic parameters shown in Table 7 gave negligible root mean squares error values when validated with plant data.

The errors indicated that the statistical optimization models are suitable and acceptable to produce best kinetic parameters, needed for the control and reactors design. I

t was observed that negligible errors showed a more robust and better models developed of the urea reactors, for good prediction of the process and may improve the functionality of the intended controller.

Table 7: Kinetic Parameters Validation with Plant Values.

S/N	Parameter	Plant Value	CSTR	PFR	RMSE Absolute	
					CSTR	PFR
1	Activation Energy (kJ/mol)	E ₁ 15	15.029185	15.0309	7.12e-04	7.54e-04
		E ₂ 15	15.02566	15.02716	6.0e-04	7.0e-04
		E ₃ 17.5	17.506899	17.507305	2.0e-04	2.0e-04
2	Arrhenius Constant (m ⁶ mol ⁻¹ s ⁻¹)	A ₁ 0.694	0.68723	0.687178	1.65e-04	1.66e-04
		A ₂ 0.598	0.592155	0.592123	1.42e-04	1.43e-04
		A ₃ 1.227	1.23038	1.21296	8.2e-05	3.4e-04
3	Rate Constant (m ⁶ mol ⁻¹ s ⁻¹)	k ₁ 0.691	0.723185	0.724902	7.85e-04	8.26e-04
		k ₂ 0.596	0.623655	0.625165	6.74e-04	7.11e-04
		k ₃ 1.2212	1.233899	1.234305	3.10e-04	3.20e-04

3.4 Simulation Results of Reactors with Fuzzy Logic Controller on Temperature Regulations and their Performance on Control Elements

The implementation of the FLC on the control of temperature fluctuations within the Indorama and Notore urea reactors via simulations and comparative performance of the controller strategy on both reactors is discussed in Figs. 7 to 9, and in line with works of [5, 42].

3.4.1 Temperature Regulations on the CSTR Urea Process

Figs 7 (a, b & c) indicate the influence of FLC on the regulation of low, moderate and high temperatures on urea synthesis within the CSTR considering other factors (such as flow rate, ratios of N/C & H/C, and concentrations) being constant.

The result showed that it took just 1.5 [s] and error of 0.144 °C to normalize the high temperature, while a delayed time of 5.59 [s] and error of 0.848 °C was needed to boost the low temperature by the controller. The moderate temperature of 184 °C takes 3.32 [s] with an error of 0.147 °C to be controlled for maximum performance of the reactor.

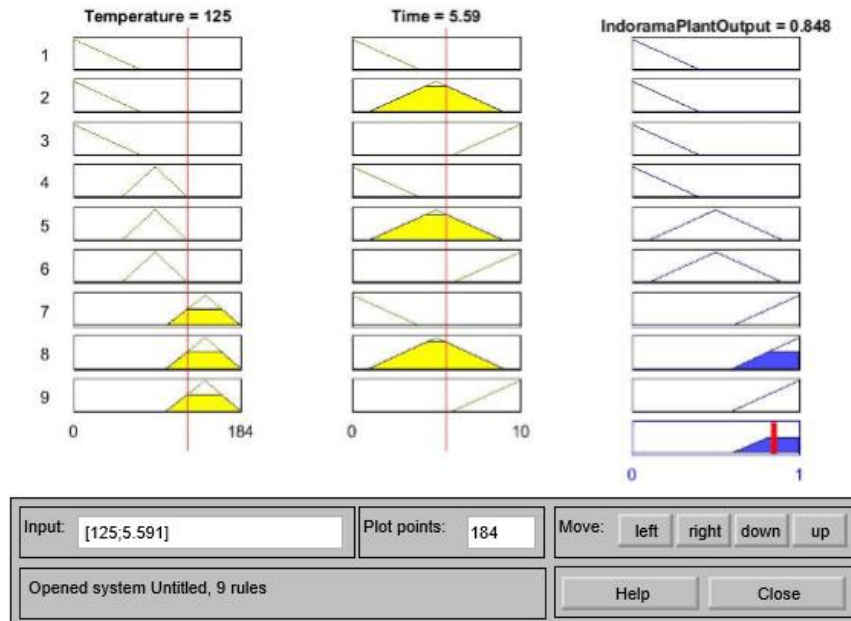


Fig.7a FL Boosting of Low Temperature (125 °C) Fluctuations within Indorama Urea Reactor to Setpoint

The input temperatures to the Indorama urea reactor are below (125 °C) the set point value of 184 °C as shown in Fig.7a.

The FLC respond, by boosting the temperature to setpoint value via control action of the valve to allow more heat into the reactor and delaying the time response to 5.59 [s] with errors of 0.848 °C.

That for low temperature input, the mechanism of the controller is placed to allow more heat into the system to properly maintain the process conditions (such as temperature) to setpoint value as in this case for stability, more production and quality of urea, which is in agreement with the work of Mendes et al. [35].

The quick intervention of the FL controller boosts the temperature to setpoint at shortest possible time of 5.59 [s] unlike the uncontrolled process, leading to less energy consumption and manpower as well as high market demand due to high quality and more yield.

At low temperatures, the CSTR urea reactor is not efficient and not productive, hence the delay of time to stabilize the temperatures to setpoint value. FL strategy is suited for this, to give good performance, effective control results leading to minimized energy wasted within the plant.

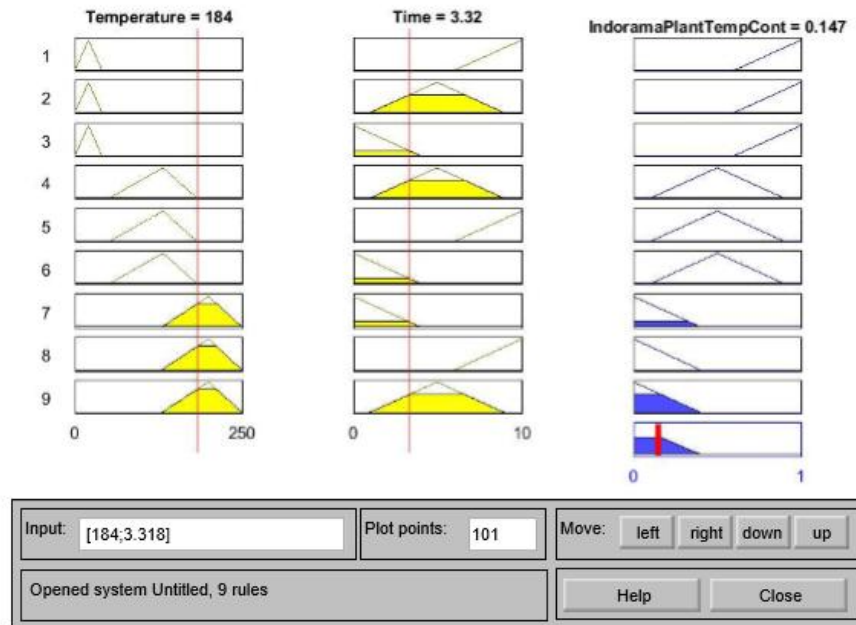


Fig.7b Control of Setpoint Temperature value within the CSTR Urea Reactor by FLC

The FLC controlled the input temperature value to setpoint output value when the input temperature to the CSTR is at setpoint value of moderated time 3.32 [s] and controller error of 0.147 °C.

The stability of the temperature occurs at shorter time of 3.32 [s] compared to low temperature as shown in Fig.7a.

It is believed that at this setpoint, there is normalcy within the reactor and this could improve the performance of the reactor to effectively and efficiently produce more and quality of the product since this is the optimal equilibrium temperature of the synthesis process. In this case, minimum energy is wasted within the plant, and also improves on the marketability of the product because of higher quality and more yield obtained.

The controlled error is small compared to the controlled error obtained from low temperature due to the temperature is the needed optimal process condition for the synthesis process. The error difference of 0.701 °C, is quite high, that can cause havoc within the reactor, which is in line with works from Ismael [9] where the fuzzy control system improved the control performance, reduced overshoot, adjustment time, and increased the reliability of the CSTR system.

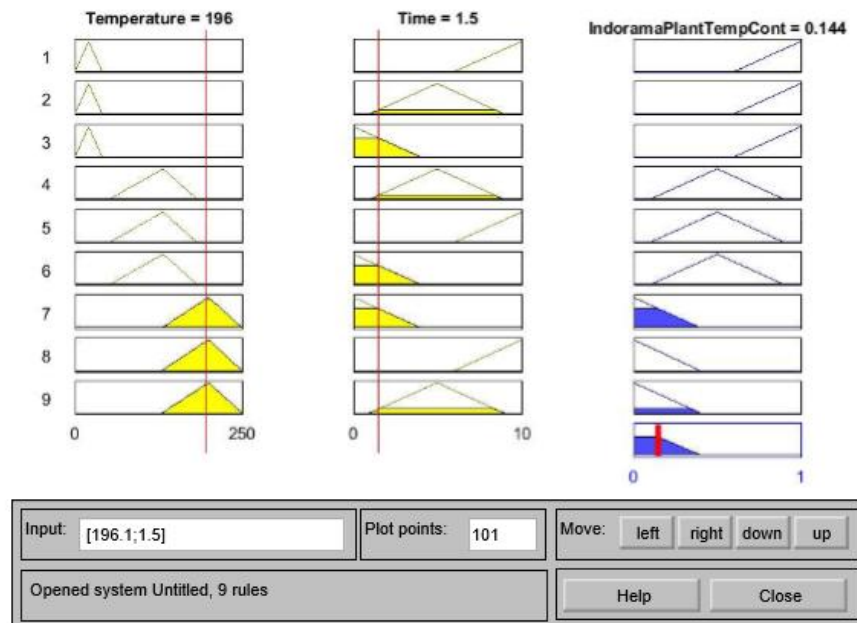


Fig.7c Fuzzy Logic Temperature Control for Input Temperature (196 °C) above the Setpoint Value of the CSTR Urea System

The temperature of the Indorama urea reactor when it exceeds the accepted temperature of 184 °C, (say 196 °C) as shown in Fig.7c will be normalized at fast time of 1.5 [s] at temperature-controlled error of 0.144 °C. This implies that at such high temperatures, above the acceptable reactor temperature, the urea reactor stabilizes at very short of 1.5 [s], thereby reducing wastage, product burn and improves on the quality and yield of the organic fertilizer but more energy cost.

The FLC strategy performs better, effectively and reliable, by normalizing the input temperature to setpoint value, thereby maintaining stability for optimal productivity. The work of Cheng et al. [48] made claims that fuzzy logic system was able to maintained a more stable temperature than a traditional PID control system at higher temperature.

3.4.2 Temperature Control of Notore (PFR) Urea Reactor using Fuzzy Logic Control

The production of urea within the PFR considering other factors (such as flow rate, ratios of N/C & H/C, and concentrations) being constant is dependent on the stability of the reactor, which is based on the controlling power of the controller to reduce the fluctuations of the temperature.

The result showed that it took 6.5 [s] and error of 0.50 °C to normalize the high temperature, while 5 [s] and error of 0.138 °C was needed to boost the low temperature to setpoint. The setpoint temperature of 184 °C was controlled in very less time of 1.05 [s] with an error of 0.138 °C for maximum performance of the reactor.

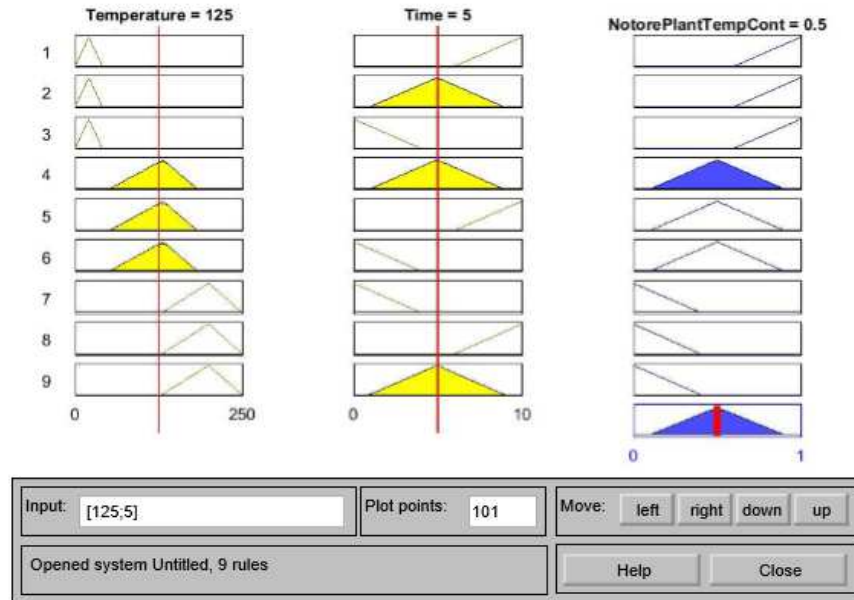


Fig.8a Fuzzy Logic Temperature Control Response to Low temperature (125 °C) Inputs into the PFR Urea System

Fig.8a displayed the output temperature response of the Notore urea reactor based on low input temperatures, shows that FLC strategy boosted the output value to setpoint at time of 5 [s] and controller errors of 0.5°C, compared to same low temperature within the CSTR.

The mechanism of boosting the temperature to desired setpoint value for efficient functioning of the reactor is due to the self-tuning and digital regulation with FLC. FLC gave better boost to the setpoint value for the Notore reactor than the Indorama reactor in less time and controlled error as achieved [49]. This mean that the PFR model developed and transformed into control models better describe the process compared to CSTR urea process.

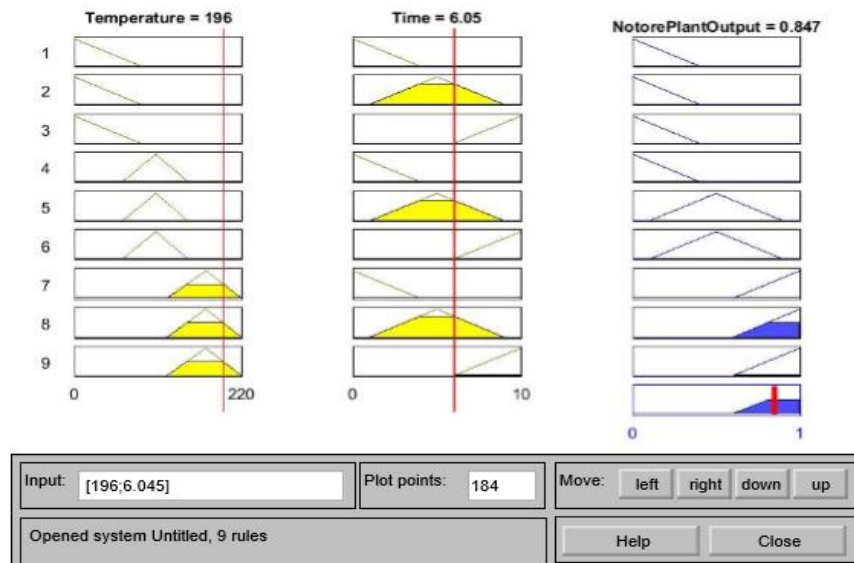


Fig.8b FLC Normalization of Low Temperature (196 °C) Changes in Notre Urea Reactor to Setpoint Value

The FLC strategy was able to normalize the high input temperatures (196°C) of the PFR urea reactor to accepted temperature of 184°C within the time of 6.05 [s] with errors of 0.847°C shown in Fig.8b, since at this temperature, the reactor becomes more turbulent compared to the CSTR urea reactor, hence much time is needed for normalization to setpoint.

The tendency to promptly regulate high temperature inputs within the reactor to optimal conditions of the process variables to avoid damages, gave the FLC an advantage over other controllers like the PID, in line with literature [50]. This study agrees with the literature result where the fuzzy logic controller system improved the energy efficiency of a heating process.

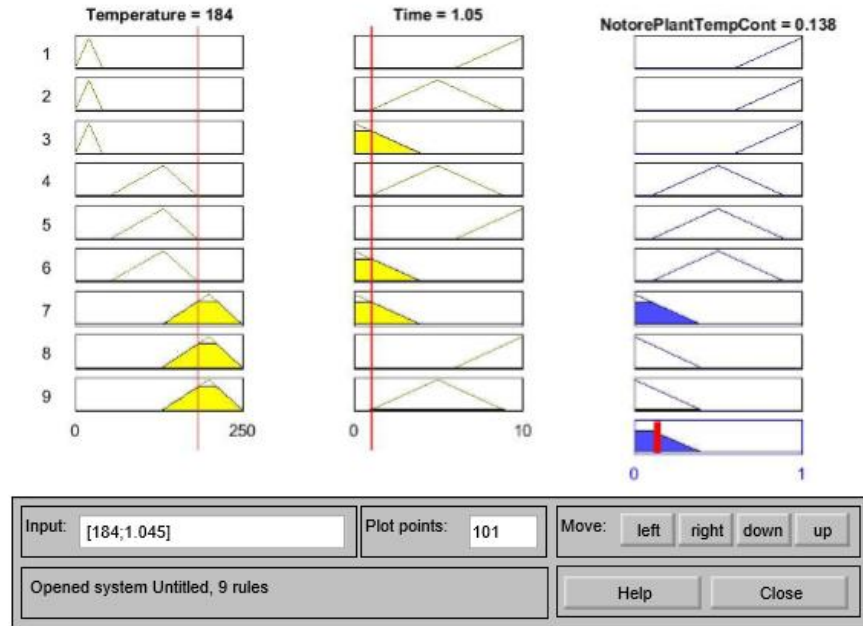


Fig.8c Fuzzy Logic Temperature Control Response for Input Temperature at Setpoint into the PFR Urea System

The FLC controls the input temperature within the PFR urea reactor at setpoint to stabilize it, by maintaining the setpoint value of 184°C at 1.05 [s] with a controlled error of 0.138°C , compared to the Indorama plant in Fig.8c where more time of 3.32 [s] and error of 0.147°C is needed for the same process.

FLC strategy was able and successfully controlled the temperature response of the Notore urea reactor within the acceptable temperature value at the shortest time of 1.05 [s] with controller error of 0.138°C [10, 51] compared to the Indorama reactor, indicating a better reactor capable of describing the urea process better.

FLC is the best controller which is reliable, acceptable and give desired values at the reactor temperature of 184°C . It should be noted and recommended that FLC is suitable for a PFR, since it takes shortest time and minimum error to stabilize the temperature fluctuations overall compared to CSTR. This is possible because the reactor models developed for the urea process were better than the CSTR urea system that described the process after being truncated to the same geometry for the control process.

3.4.3 Comparison of the Performance of FLC on the Urea Reactors

The comparison of the efficiency and effectiveness of the FLC on the control of temperatures disturbance within the CSTR and the PFR are shown in Fig. 9

Table 8 presents the PFR and CSTR settling time and temperature controlled-errors as a result of FLC to control the input temperatures values to setpoint value of 184 °C. Normalisation of temperatures to set point value takes more time for the PFR than the CSTR, while booting the temperature takes less time for the PFR compared to the CSTR. Controlling the input temperature at setpoint value to set point for the PFR is very fast and less error compared to CSTR. Overall, FLC performs effectively and efficiently for the PFR than the CSTR. This may be due to the process model and the level of disturbances produced for each reactor type.

Table 8: FLC Errors and Settling Time for PFR and CSTR Urea Reactors

Temp. (°C)	PFR Error (°C)	PFR Time (s)	CSTR Error (°C)	CSTR Time (s)
184	0.138	1.05	0.147	3.32
153	0.420	4.41	0.442	4.50
196	0.147	6.05	0.144	1.50
125	0.500	5.00	0.848	5.59
201	0.142	6.50	0.148	2.20

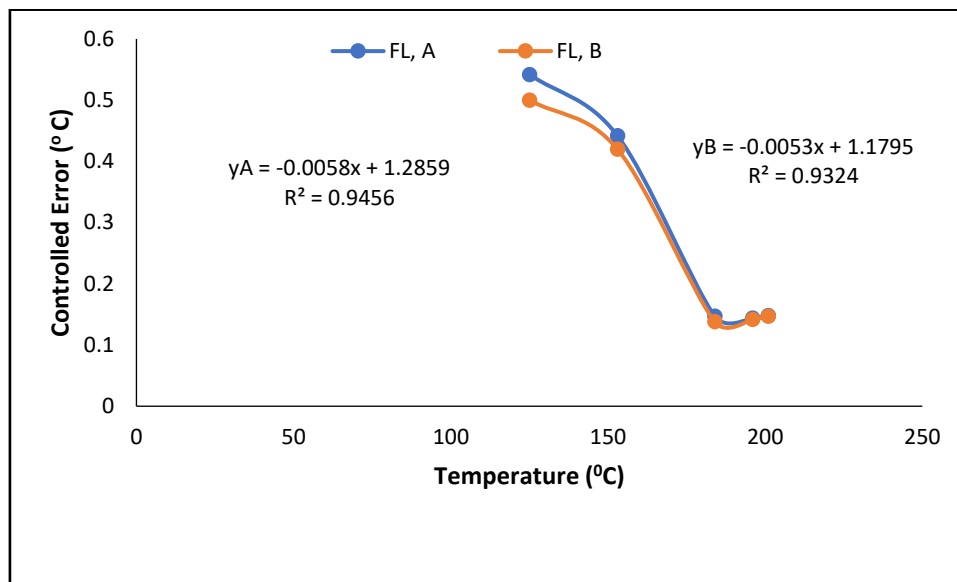


Fig.9a Effects of Temperature on the Control Errors within the Urea reactors due to Temperature Fluctuations

The temperature-controlled errors against the temperature for the urea reactors in Fig. 9a showed that higher errors are produced at lower temperatures (below the setpoint value), lower errors are obtained at setpoint and lower input temperatures when FLC controller is applied to control the temperature fluctuations within the reactors. Errors generally are minimized when the developed model is linear as this is evidence on the reactors models developed and discretized with CSTR model being more linear

compared to PFR (see the coefficient of determination values of $0.946 > 0.932$). Hence, the errors are lower for CSTR compared to PFR, in agreement with works by Karasakal et al. [34] and Mendes et al. [35].

This is because the model for the PFR developed produces more turbulence at lower or higher temperatures from setpoint, which could be the reason for low linearity.

The lower the errors, the sensitive the controller properties for effective and efficient control of temperature response within the urea reactor. However, the temperature-controlled error from the Notore urea reactor at setpoint is smaller to that of the value for the Indorama urea reactor.

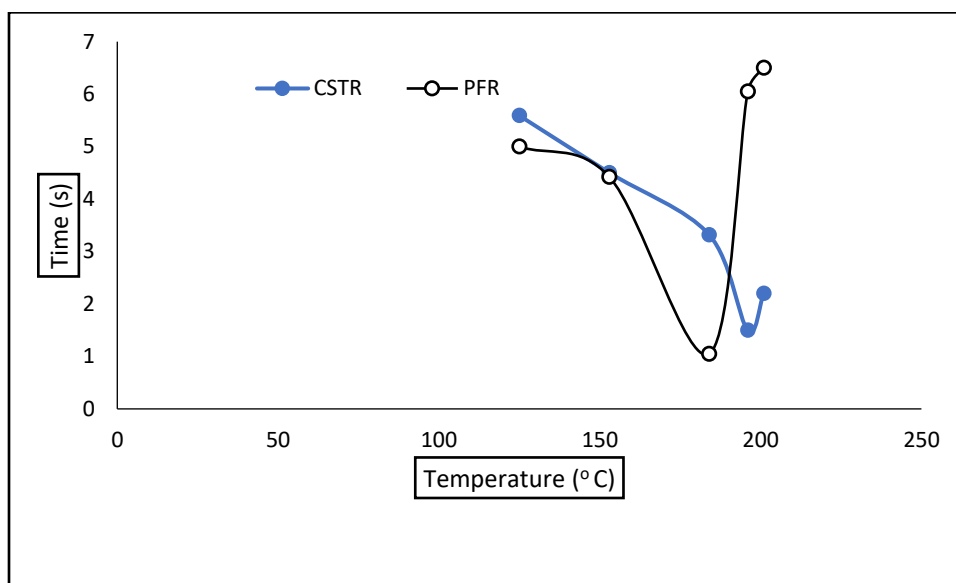


Fig.9b Comparative effect on stabilizing temperature using FLC as a function of time

The temperature regulation within the urea reactor using fuzzy logic controller is dependent on time. As shown in Fig.9b, PFR gave lowest time of 1.05 [s] at setpoint temperature of 184 °C compared to CSTR while at higher temperatures, it normalizes the temperature almost the same settling time for the reactors. Though, the errors obtained from the CSTR are almost linearly related compared to PFR due to the highly turbulent nature of the reactor compared to CSTR. This agrees with literatures studies [52, 53]. Generally, the settling time values are relatively lower for the PFR compared to CSTR, due to FLC response to temperature control for PFR better compared to CSTR urea process of similar geometry.

4. Conclusion

- (i) The fractional conversion and temperature responses from the reactors simulations were unstable and gave damped oscillations (exponential fluctuations of the profiles), an indication that the two systems are uncontrolled and unstable due to external disturbances. Hence, the need of an appropriate controller to regulate the urea reactors for better and quality urea product.
- (ii) The validation of the reactors models' results with plant and literature values gave negligible root mean square errors ranged $7.0\text{e-}04$ to $8.5\text{e-}04$ and $7.0\text{e-}03$ °C to $2.1\text{e-}01$ °C for both reactors, an indication that the models are properly developed and good for the study of the urea production process.
- (iii) The kinetic parameters optimization and validation showed that negligible root mean square errors of ranged $2.0\text{e-}4$ to $7.5\text{e-}4$ kJ/mol, $1.43\text{e-}4$ to $8.2\text{e-}4$ $\text{m}^6\text{mol}^{-1}\text{s}^{-1}$ and $3.1\text{e-}4$ to $8.3\text{e-}4$ $\text{m}^6\text{mol}^{-1}\text{s}^{-1}$ respectively for activation energies, pre-exponential constants and rate constants are as a result of a better optimal kinetic parameters obtained for the controlling process.

- (iv) The Fuzzy Logic Controller functions on the CSTR and PFR urea reactors as practicalized in the Indorama and Notore plants stabilize the temperatures fluctuations within the reactors to setpoint value of 184 °C with smaller temperature-controlled errors and settling time values 0.147 °C and 3.32 [s], and 0.138 °C and 1.05 [s] respectively. The FLC on the Notore plant is more efficient and effective compared to the Indorama plant due to smaller settling time and temperature-controlled errors.
- (v) The controller responds to PFR urea model better than CSTR urea model with same geometry, as evidenced in smaller temperature controlled-errors and settling time values for the former to the later urea process. But as conditions are below and above the operating limits, the CSTR process responds better with the controller, since the PFR become more turbulent and unpredictable behaviour than the CSTR.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this study.

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Data availability

The data used in this manuscript are provided.

Author's Contribution

The study of the work was successfully contributed by the authors, specifically, **O.E. Ojong:** Conceptualization, software and simulation, validation, writing – review & editing. **C.O. Wosu:** Formatting, editing and review. **Patrick Sedi:** Introduction and review, editing and assisted in financing the research actualization, and **K.N. Dollah:** Provide financial assistance and conceptual design for this manuscript.

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Appendix AA: Schematics Diagrams for CSTR and PFR urea reactors as applicable in Indorama and Notore Plants/Reactors

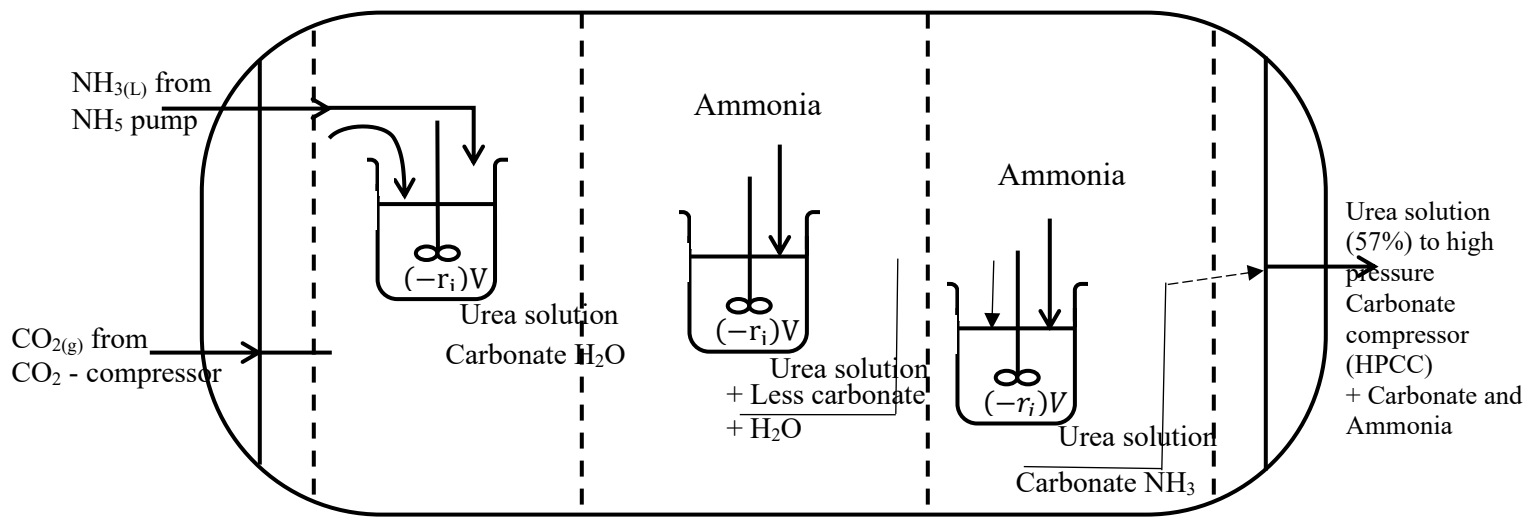


Fig. A Series of CSTR in a Vertical Column for Urea Production

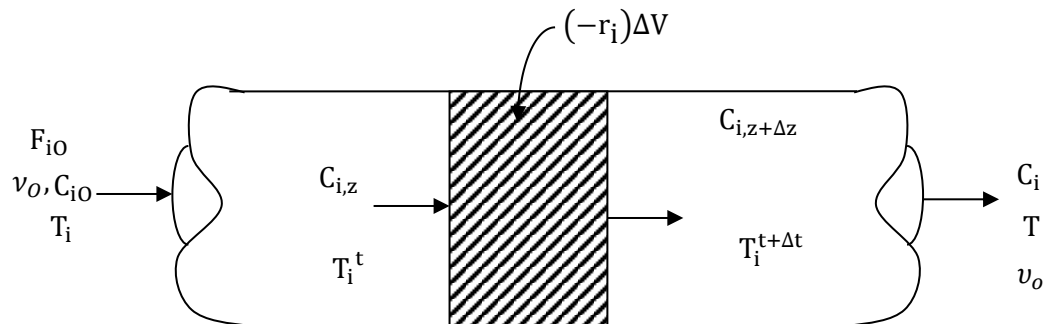


Fig. B Schematic Diagram of a PFR indicating Material and Energy Flow for Urea Production

Appendix A: Discretization of the ODEs (Models 3a and 3b)

The ODE model 3b which has a non-linear term in the right-hand side (RHS) of model A1 is discretized using Taylor's series as shown below

$$\frac{dT_i}{d\tau} = \frac{1}{\tau}(T_0 + T_C - 2T_i) + jP_T^3 y_{2,0}^3 \{ (k_2 - k_1)(\theta - X)^2(1 - X) \} + jk_3 P_T \theta_1 y_{2,0} X \quad (A1)$$

Model A1 contains rate constants expressed in terms of Arrhenius equation for non-isothermal condition in A2.

$$\begin{aligned} \frac{dT}{d\tau} = & \frac{1}{\tau}(T_0 + T_C - 2T) + jP_T^3 y_{2,0}^3 \left\{ k_{20} \exp\left(\frac{-E_2}{RT}\right) - k_{10} \exp\left(\frac{-E_1}{RT}\right) \right\} (\theta_1 - X)^2(1 - X) \\ & + \frac{1}{\tau}(T_{st} - T) + a \exp\left(\frac{-E_3}{RT}\right) X \end{aligned} \quad (A2)$$

Further expansion and arrangement give,

$$\begin{aligned} \frac{dT}{d\tau} = & \frac{1}{\tau}(T_0 + T_C - 2T) + jP_T^3 y_{2,0}^3 k_{20} \exp\left(\frac{-E_2}{RT}\right) (\theta - X)^2(1 - X) - jP_T^3 y_{2,0}^3 k_{10} \exp\left(\frac{-E_1}{RT}\right) (\theta - X)^2(1 - X) \\ & + \frac{1}{\tau}(T_{st} - T) + a \exp\left(\frac{-E_3}{RT}\right) X \end{aligned} \quad (A3)$$

where, $\frac{F_i}{V} = \frac{1}{\tau} = \frac{UA_t}{\rho C_P V}$, $j = \frac{(-\Delta H_F)}{\rho C_P}$; and $a = \theta_1 y_{20} P_T k_{30}$

Taylor's approximation technique is applied to model A3 to linearize the non-linear term as given as

$$f(X, T) = f(X_0, T_0) + \frac{\partial f(X_0, T_0)}{\partial X} (X - X_0) + \frac{\partial f(X_0, T_0)}{\partial T} (T - T_0) + \dots \quad (A4)$$

Hence, the terms " $\exp\left(\frac{-E_2}{RT}\right) (\theta - X)^2(1 - X)$ " and " $\exp\left(\frac{-E_1}{RT}\right) (\theta - X)^2(1 - X)$ " are non-linear discretized to give

$$\begin{aligned} \exp\left(\frac{-E_2}{RT}\right) (\theta - X)^2(1 - X) \equiv & \exp\left(\frac{-E_2}{RT}\right) (\theta - X_0)^2(1 - X_0) (X - X_0) \left\{ \exp\left(\frac{-E_2}{RT}\right) 2\theta(-1)(1 - X_0) + \right. \\ & \left. \exp\left(\frac{-E_2}{RT_0}\right) (\theta - X_0)^2(-1) \right\} + (T - T_0) \left\{ \frac{E_2}{RT_0^2} \exp\left(\frac{-E_2}{RT_0}\right) (\theta - X_0)^2(1 - X_0) \right\} \\ & + \left((T - T_0) \left\{ \begin{aligned} & aX_0 \left(\frac{-E_3}{RT_0^2}\right) \exp\left(\frac{-E_2}{RT_0}\right) \\ & + (X - X_0)a \exp\left(\frac{-E_3}{RT_0}\right) \end{aligned} \right\} \right) \end{aligned} \quad (A5)$$

Initial conversion $X_0 = 0$, then, model A5 is resolved to give

$$f(X, T) = \exp\left(\frac{-E_2}{RT_0}\right) (\theta^2)(1) + X \left\{ \exp\left(\frac{-E_2}{RT_0}\right) (-2\theta) - \theta^2 \exp\left(\frac{-E_2}{RT_0}\right) \right\} + (T - T_0) \left(\frac{E_2}{RT_0^2} \exp\left(\frac{-E_2}{RT_0}\right) \theta^2 \right) \quad (A6)$$

Defining the terms,

$$K = \exp\left(\frac{-E_2}{RT_0}\right) \theta^2; K'_\theta = \exp\left(\frac{-E_2}{RT_0}\right) (2\theta); K_T = \frac{E_2}{RT_0^2} \exp\left(\frac{-E_2}{RT_0}\right) \theta^2, K_\theta = \theta^2 \exp\left(\frac{-E_2}{RT_0}\right)$$

then, equation (A6) gives,

$$f(X, T) = X(-2K'_\theta - K_\theta) + (T - T_0)(K_T) + K_\theta \quad (A7)$$

$$f(X, T) = K''_\theta X + K_T(T - T_0) + K_\theta \quad (A8)$$

where, $2K'_\theta - K_\theta = K''_\theta$

Similarly,

$$\exp\left(\frac{-E_1}{RT}\right)(\theta - X)^2(1 - X) \equiv X(-2(K'_{1\theta} - K_{1\theta})) + (T - T_0)(K_{T1}) + K_{1\theta} \quad (A9)$$

where, $K'_{1\theta} = \exp\left(\frac{-E_1}{RT_0}\right)(2\theta)$; $K_{1\theta} = \exp\left(\frac{-E_1}{RT_0}\right)\theta^2$; and $K_{T1} = \frac{E_1}{RT_0^2} \exp\left(\frac{-E_1}{RT_0}\right)\theta^2$

Substituting equations (B3.9) and (B3.10) into equation (B3.4) gives,

$$\begin{aligned} \frac{dT}{d\tau} = & \frac{1}{\tau}(T_0 + T_C - 2T) + jP_T^3 y_{2,0}^3 k_{2,0} \{X(-2K'_\theta - K_\theta) + (T - T_0)K_T + K_\theta\} \\ & - jP_T^3 y_{2,0}^3 k_{10} \{(-2K'_{1\theta} - K_{1\theta})X + (T - T_0)K_{T1} + K_{1\theta}\} + \frac{1}{\tau}(T_{st} - T) + a \exp\left(\frac{-E_3}{RT_0}\right)X \end{aligned} \quad (A10)$$

$$\frac{dT}{d\tau} = \frac{1}{\tau}(T_0 + T_C - 2T) - K''_\theta X + K'_T(T - T_0) + K'_\theta + K''_{1\theta}X - K'_{T1}(T - T_0) + K'_{1\theta} + \frac{1}{\tau}(T_{st} - T) \quad (A11)$$

where, $K''_\theta = jP_T^3 y_{2,0}^3 k_{20}(2K'_\theta + K_\theta)$; $K'_T = jP_T^3 y_{2,0}^3 k_{20}K_T$; $K'_\theta = jP_T^3 y_{2,0}^3 k_{20}K_\theta$;

$K''_{1\theta} = jP_T^3 y_{2,0}^3 k_{10}(2K'_{1\theta} + K_{1\theta})$; $K'_{T1} = jP_T^3 y_{2,0}^3 k_{10}K_{T1}$; $K'_{2\theta} = jP_T^3 y_{2,0}^3 k_{10}K_{1\theta}$; and $K_a = a \exp\left(\frac{-E_3}{RT_0}\right)$

$$\frac{dT}{d\tau} = (K'_T - 3/\tau - K'_{T1})T + \frac{1}{\tau}T_i + (K'_{T1} - K'_T + \frac{1}{\tau})T_0 + \frac{1}{\tau}T_{st} + (K''_{1\theta} + K''_\theta - K_a)X + K'_\theta + K'_{1\theta}$$

$$\frac{dT}{d\tau} = \mathbf{w}T + \frac{1}{\tau}\mathbf{T}_i + \mathbf{a}_1\mathbf{T}_0 + \frac{1}{\tau}\mathbf{T}_{st(s)} + \mathbf{w}_1\mathbf{X} + \mathbf{K} \quad (A12)$$

where, $\mathbf{w} = K'_T - 3/\tau - K'_{T1}$; $\mathbf{a}_1 = K'_{T1} - K'_T + \frac{1}{\tau}$; $\mathbf{w}_1 = K''_{1\theta} + K''_\theta - K_a$; and $\mathbf{K} = K'_\theta + K'_{1\theta}$

Model A12 is the discretized temperature model for non-isothermal process in a CSTR which is to be resolved analytically with Laplace Transform (LT). Before the equation is resolved with LT, it is transformed to deviation variables as,

At steady-state,

$$\mathbf{0} = \mathbf{w}\mathbf{T}_s + \frac{1}{\tau}\mathbf{T}_{i(s)} + \mathbf{a}_1\mathbf{T}_{0(s)} + \frac{1}{\tau}\mathbf{T}_{st(s)} + \mathbf{w}_1\mathbf{X}_s + \mathbf{K}_s \quad (A13)$$

Subtracting equation (A14.) from equation (A15) in-terms of deviation variables give,

$$\frac{d}{dt}(T - T_s) = \mathbf{w}(T - T_s) + \frac{1}{\tau}(\mathbf{T}_i - \mathbf{T}_{i(s)}) + \mathbf{a}_1(\mathbf{T}_0 - \mathbf{T}_{0(s)}) + \mathbf{w}_1(\mathbf{X} - \mathbf{X}_s) + (\mathbf{K} - \mathbf{K}_s)$$

where, $T - T_s = T'$; $T_i - T_{i(s)} = T'_i$, $T_{st} - T_{st(s)} = T'_{st}$, $T_0 - T_{0(s)} = T'_0$, $X - X_s = X'$, and $K - K_s = K'$

Suppose $w = K'_T - 3/\tau - K'_{T1}$; $a_1 = K'_{T1} - K'_T$; $w_1 = K''_{1\theta} - K''_\theta + K_a$; $K = K'_\theta - K'_{1\theta}$, then Temperature ODE model in terms of deviation variable becomes,

$$\frac{dT'}{d\tau} = wT' + \frac{1}{\tau}T'_i + a_1T'_0 + \frac{1}{\tau}T'_{st} + w_1X' + K' \quad (A14)$$

The ODE model 3a describing the conversion process within the Indorama urea reactor is shown in model A15

$$\frac{dX}{dt} = \frac{1}{\tau_1}\theta + \frac{1}{\tau_2} + P_T^3 y_{2,0}^2 \{(k_2 - k_1)(\theta - X)^2(1 - X)\} + k_3 \theta_1 P_T X \quad (A15)$$

Model (A1) is a non-linear non-isothermal ODE fractional conversion, which is linearized by applying model A4 as,

$$\begin{aligned} \frac{dX}{dt} = & \frac{1}{\tau_1}\theta + \frac{1}{\tau_2} + P_T^3 y_{2,0}^2 k_{20} \{(2K'_\theta + K_\theta)X + K_T(T - T_0) + K_\theta\} \\ & - P_T^3 y_{2,0}^2 k_{10} \{-(2K'_{1\theta} + K_{1\theta})X + K_{T1}(T - T_0) + K_\theta\} + b \exp\left(\frac{-E_3}{RT_0}\right) X \end{aligned} \quad (A16)$$

$$\frac{dX}{dt} = \frac{1}{\tau_1}\theta + \frac{1}{\tau_2} - a_{12}X + K_{T12}(T - T_0) + K_{\theta 2} + a_{11}X - K_{T11}(T - T_0) - K_{\theta 11} + b_1X \quad (A17)$$

where, $a_{12} = P_T^3 y_{2,0}^2 k_{10} (2K'_\theta + K_\theta)$; $K_{T12} = P_T^3 y_{2,0}^2 k_{20} K_T$; $K_{\theta 2} = P_T^3 y_{2,0}^2 k_{20} K_\theta + \frac{1}{\tau_1}\theta + \frac{1}{\tau_2}$;
 $a_{11} = P_T^3 y_{2,0}^2 k_{10} (2K'_{1\theta} + K_{1\theta})$; $K_{T11} = P_T^3 y_{2,0}^2 k_{10} K_{T1}$; $K_{\theta 11} = P_T^3 y_{2,0}^2 k_{10} K_{1\theta}$; $b_1 = b \exp\left(\frac{-E_3}{RT_0}\right)$;
and $b = \theta_1 y_{20} P_T k_{30}$

$$\frac{dX}{d\tau} = -\left(\frac{1}{\tau} + a_{12} - a_{11} - b_1\right)X + (K_{T12} - K_{T11})T + (K_{T11} + K_{T12})T_0 + K_{\theta 2} - K_{\theta 11} \quad (A18)$$

Defining the constants in model A18, $w_2 = \frac{1}{\tau} + a_{12} - a_{11} - b_1$; $w_3 = K_{T12} - K_{T11}$; $a_2 = K_{T11} + K_{T12}$;
and $K_1 = K_{\theta 2} - K_{\theta 11}$, then, model become,

$$\frac{dX}{d\tau} = -w_2X + w_3T + a_2T_0 + K_1 \quad (A19)$$

Interms of deviation variables, model A19 is transformed to,
At steady state,

$$0 = -w_2X_{(s)} + w_3T_s + a_2T_{0(s)} + K_{1(s)} \quad (A20)$$

Subtracting the steady state model A20 from the dynamic model A19 to give,

$$\frac{d}{d\tau}(X - X_s) = -w_2(X - X_s) + w_3T' + C_{12}(T_0 - T_{0(s)}) + (K_1 - K_{1(s)}) \quad (A21)$$

Defining the deviation variables terms in model A21 as,

$X' = X - X_s$, $T' = T - T_s$, $T'_0 = T_0 - T_{0(s)}$, and $K'_1 = K_1 - K_{1s}$, then, model A21 becomes,

$$\frac{dX'}{dt} = -w_2 X' + w_3 T' + a_2 T'_0 + K'_1 \quad (A22)$$

Appendix B: Discretization of the PDEs (Models 4a and 4b)

The fractional conversion model 4a describing the urea production process in the Notore urea reactor is shown in B1

$$\frac{\partial X}{\partial \tau} + v \frac{\partial X}{\partial z} = k_2 P_T^3 y_{20}^2 (\theta - X)^2 (1 - X) - k_1 P_T^3 y_{20}^2 (\theta - X)^2 (1 - X) + k_3 P_T \theta_1 y_{20} X \quad (B1)$$

Discretization of model B1 using Taylor series expansion model A4

$$\frac{\partial X}{\partial \tau} + v \frac{\partial X}{\partial z} = P_T^2 y_{20}^2 k_{20} \{-(2K'_\theta + K_\theta)X + K_T(T - T_0) + K_\theta\} - P_T^2 y_{20}^2 k_{10} \{-(2K'_{1\theta} + K_{1\theta})X + K_{T1}(T - T_0) + K_{1\theta}\} + k_{30} \exp\left(-E_3/RT_0\right) X$$

$$\frac{\partial X}{\partial \tau} + v \frac{\partial X}{\partial z} = -b_{11}X + b_{12}(T - T_0) + K_{11} + b_{13}X - b_{14}(T - T_0) - K_{12} + b_{15}X \quad (B2)$$

$$\frac{\partial X}{\partial \tau} + v \frac{\partial X}{\partial z} = (b_{15} + b_{13} - b_{11})X + (b_{12} - b_{14})(T - T_0) + K_{11} - K_{12} \quad (B3)$$

where, $b_{11} = P_T^3 y_{20}^2 k_{20} (2K'_\theta + K_\theta)$; $b_{12} = P_T^3 y_{20}^2 k_{20} K_T$; $K_{11} = P_T^3 y_{20}^2 k_{20} K_\theta$

$b_{13} = P_T^3 y_{20}^2 k_{10} (2K'_{1\theta} + K_{1\theta})$; $b_{14} = P_T^3 y_{20}^2 k_{10} K_{T1}$; $b_{15} = k_{30} \exp\left(-E_3/RT_0\right) P_T y_{20} \theta_1$, and

$K_{12} = P_T^3 y_{20}^2 k_{10} K_{1\theta}$.

Defining the constants $m = b_{15} + b_{13} - b_{11}$; $m_1 = b_{12} - b_{14}$; $d = K_{11} - K_{12}$, then model B3 becomes,

$$\frac{\partial X}{\partial \tau} + v \frac{\partial X}{\partial z} = mX + m_1 T - m_1 T_0 + d \quad (B4)$$

Interms of deviation variables, the steady state of model B5 is subtracted from model B4 to give,
At steady state,

$$0 + \left(\frac{v \partial X}{\partial z}\right)_{(s)} = mX_s + m_1 T_s - m_1 T_{0(s)} + d \quad (B5)$$

Subtracting model B5 from model B4, defined the deviation variable PDE model as,

$$\frac{\partial X'}{\partial \tau} + v \frac{\partial X'}{\partial z} = mX' + m_1 T' - m_1 T'_0 + d' \quad (B6)$$

where, $d' = d - d_{(s)}$

The temperature model 4b describing the urea synthesis in a PFR is a PDE model shown as model B7 which the non-linear terms in the RHS of the model are discretized to give,

$$\frac{\partial T}{\partial \tau} + v \frac{\partial T}{\partial z} = j(k_2 - k_1)P_T^2 y_{20}^2 (\theta_1 - X)^2 (1 - X) + jk_3 X + \frac{1}{\tau} (T - T_{st}) \quad (B7)$$

Applying the discretization of the non-linear terms form in the RHS of the temperature model gives,

$$\begin{aligned} \frac{\partial T}{\partial \tau} + v \frac{\partial T}{\partial z} = & jk_{20} P_T^2 y_{20}^2 \{-X(2K'_\theta + K_\theta) + K_T(T - T_0) + K_\theta\} \\ & - jk_{10} P_T^2 y_{20}^2 \{-(2K'_{1\theta} + K_{1\theta})X + K_{T1}(T - T_0) + K_{1\theta}\} + jk_{30} \exp\left(\frac{-E_3}{RT_0}\right) \times + \frac{1}{\tau} (T - T_{st}) + C_{17} \end{aligned} \quad (B8)$$

$$\frac{\partial T}{\partial \tau} + v \frac{\partial T}{\partial z} = -C_{11}X + C_{12}(T - T_0) + C_{13} + C_{14}X - C_{15}(T - T_0) + C_{16}X + \frac{1}{\tau} (T_{st} - T) - C_{17}$$

$$\frac{\partial T}{\partial \tau} + v \frac{\partial T}{\partial z} = (C_{14} - C_{11} + C_{16})X + \left(C_{12} - C_{15} + \frac{1}{\tau}\right)T + (C_{15} - C_{12})T_0 - \frac{1}{\tau}T_{st} + (C_{13} - C_{17})$$

$$\frac{\partial T}{\partial \tau} + v \frac{\partial T}{\partial z} = m_{11}X + m_{12}T + C_1 T_0 - \frac{1}{\tau} T_{st} + d_1 \quad (B9)$$

where, $C_{11} = jk_{20} P_T^3 y_{20}^2 (2K'_\theta + K_\theta)$; $C_{12} = jk_{20} P_T^3 y_{20}^2 K_T$; $C_{13} = jk_{20} P_T^3 y_{20}^2 K_\theta$;
 $C_{14} = jk_{10} P_T^3 y_{20}^2 (2K'_{1\theta} + K_{1\theta})$; $C_{15} = jk_{10} P_T^3 y_{20}^2 K_{T1}$; $C_{16} = jk_{30} \exp\left(\frac{-E_3}{RT_0}\right) P_T y_{20} \theta_1$;
 $C_{17} = jk_{10} P_T^3 y_{20}^2 K_{1\theta}$; $m_{11} = C_{14} - C_{11} + C_{16}$; $m_{12} = C_{12} - C_{15} + \frac{1}{\tau}$; $C_1 = C_{15} - C_{12}$; and $d_1 = C_{13} - C_{17}$

Interms of deviation variables, model B10 is transformed to model B11 as

At steady state, model B9 becomes,

$$0 + v \left(\frac{\partial T}{\partial \tau}\right)_s = m_{11}X_s + m_{12}T_s + C_1 T_{0(s)} - \frac{1}{\tau} T_{st(s)} + d_{1(s)} \quad (B10)$$

Subtracting model B10 from model B9 and defining in-terms of deviation variables gives,

$$\frac{\partial T'}{\partial \tau} + \frac{\partial T'}{\partial z} = m_{11}X' + m_{12}T' + C_1 T'_0 - \frac{1}{\tau} T'_{st} + d'_1 \quad (B11)$$

Appendix C: Analytical Integration of the Discretized Models

Model (A14) is resolved analytically using LT to give the transfer functions as,

$$\mathcal{L}\left(\frac{dT'}{d\tau}\right) = w\mathcal{L}\{T'\} + \frac{1}{\tau}\mathcal{L}\{T'_i\} + a_1\mathcal{L}\{T'_0\} + \frac{1}{\tau}\mathcal{L}\{T'_{st}\} + w_1\mathcal{L}\{X'\} + K'\mathcal{L}\{1\}$$

$$\begin{aligned}
s\bar{T}'_{(s)} - T'_{(0)} &= w\bar{T}'_{(s)} + \frac{1}{\tau}\bar{T}'_{i(s)} + a_1\bar{T}'_{0(s)} + \frac{1}{\tau}\bar{T}'_{st(s)} + w_1\bar{X}'_{(s)} + \frac{K'}{s} \\
(s-w)\bar{T}'_{(s)} - w_1\bar{X}'_{(s)} &= \frac{1}{\tau}\bar{T}'_{i(s)} + a_1\bar{T}'_{0(s)} + \frac{K'}{s}
\end{aligned} \tag{C1}$$

Model C1 is algebraic s-domain linear equation with variables $\bar{T}'_{(s)}$ and $\bar{X}'_{(s)}$ where, $T'_{(0)} = \bar{T}'_{st(s)}$

LT on the model A22 and further simplification gives,

$$\begin{aligned}
\mathcal{L}\left(\frac{dX'}{dt}\right) &= -w_2\mathcal{L}\{X'\} + w_3\mathcal{L}\{T'\} + a_2\mathcal{L}\{T'_0\} + K'_1\mathcal{L}\{1\} \\
s\bar{X}'_{(s)} - X'_{(0)} &= -w_2\bar{X}'_{(s)} + w_3\bar{T}'_{(s)} + a_2\bar{T}'_{0(s)} + \frac{K'_1}{s}
\end{aligned}$$

But $X'_{(0)} = 0$, further re-arranging gives,

$$-w_3\bar{T}'_{(s)} + (s + w_2)\bar{X}'_{(s)} = a_2\bar{T}'_{0(s)} + \frac{K'_1}{s} \tag{C2}$$

LT of model B6 to resolved the PDE to simple linear s-domain algebraic model as,

$$\begin{aligned}
\mathcal{L}\left(\frac{\partial X'}{\partial \tau}\right) + v\mathcal{L}\left\{\frac{\partial X'}{\partial z}\right\} &= m\mathcal{L}\{X'\} + m_1\mathcal{L}\{T'\} - m_1\mathcal{L}\{T'_0\} + d'\mathcal{L}\{1\} \\
s\bar{X}'_{(s)} + v\frac{d\bar{X}'_{(s)}}{dz} &= m\bar{X}'_{(s)} + m_1\bar{T}'_{(s)} + m_1\bar{T}'_{0(s)} + \frac{d'}{s}
\end{aligned} \tag{C3}$$

For control strategy implementation, $\frac{d\bar{X}'_{(s,z)}}{dz} = 0$

$$(s - m)\bar{X}'_{(s)} - m_1\bar{T}'_{(s)} = -m_1\bar{T}'_{0(s)} + \frac{d'}{s} \tag{C4}$$

Model C4 is algebraic s-domain linear equation obtained from the resolution of linearized PDE model B6.

LT of model B11 gives,

$$\begin{aligned}
\mathcal{L}\left\{\frac{\partial T'}{\partial \tau}\right\} + v\mathcal{L}\left\{\frac{\partial T'}{\partial z}\right\} &= m_{11}\mathcal{L}\{X'\} + m_{12}\mathcal{L}\{T'\} + C_1\mathcal{L}\{T'_0\} - \frac{1}{\tau}\mathcal{L}\{T'_{st}\} + d'_1\mathcal{L}\{1\} \\
s\bar{T}'_{(s)} - T'_{(0)} + v\frac{d\bar{T}'_{(s)}}{dz} &= m_{11}\bar{X}'_{(s)} + m_{12}\bar{T}'_{(s)} + C_1\bar{T}'_{0(s)} - \frac{1}{\tau}\bar{T}'_{st(s)} + \frac{d'_1}{s}
\end{aligned}$$

But $\frac{d\bar{T}'_{(s,z)}}{dz} = 0$, for control

$$m_{11}\bar{X}'_{(s)} + (s - m_{12})\bar{T}'_{(s)} = C_1\bar{T}'_{0(s)} = \frac{1}{\tau}\bar{T}'_{st(s)} + \frac{d'_1}{s} \tag{C5}$$

Appendix D: Thermocouple and Final Control Element Models and Related Transfer Functions

The transient thermocouple model is developed based on the energy balance taking place in Fig.D1

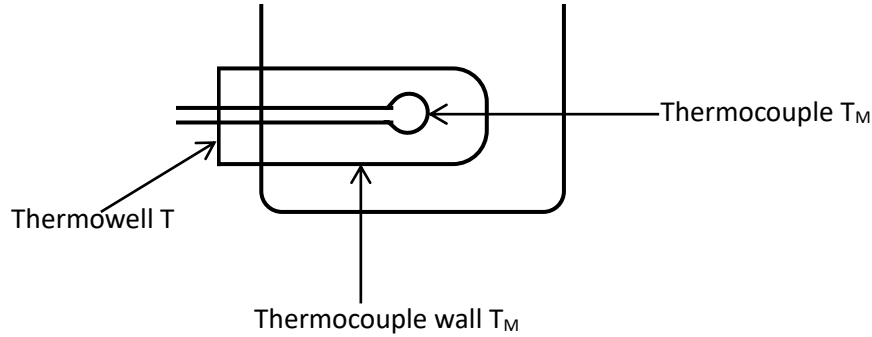


Fig. D1 Thermocouple Arrangement used as Temperature Sensor

The thermocouple shown in Fig. D1 is modelled as a first order system based on the energy balance model D1 applied to give the ODE.

$$\left\{ \begin{array}{l} \text{Rate of Accumulation} \\ \text{of energy within the} \\ \text{thermocouple} \end{array} \right\} = \left\{ \begin{array}{l} \text{Rate of Inflow of energy} \\ \text{into the thermocouple} \end{array} \right\} - \left\{ \begin{array}{l} \text{Rate of Outflow} \\ \text{of energy from} \\ \text{the thermocouple} \end{array} \right\} - \left\{ \begin{array}{l} \text{Rate of Consumption} \\ \text{of energy within the} \\ \text{thermocouple due to} \\ \text{Chemical Reaction} \end{array} \right\} + \left\{ \begin{array}{l} \text{Rate of addition of} \\ \text{Energy into the} \\ \text{thermocouple system} \end{array} \right\} \quad (D1)$$

Model D1 is analyzed mathematically and the thermocouple process is a physical and a measuring instrument to give the first order model of a thermocouple as,

$$V_t C_p \rho_t \frac{dT_m}{dt} = v_{0,t} C_p \rho_t T - v_{0,t} C_p \rho_t T_m \quad (D2)$$

where, V_t is the volume of the thermocouple, $C_p \rho_t$ is the product of the specific capacity at constant pressure and the density of the thermocouple, T_m is the measured temperature, known as the output temperature, $v_{0,t}$ is the volumetric flow rate of the thermocouple, and T is the input temperature into the thermocouple.

Further simplification of model D2 gives the thermocouple model as,

$$\tau_p \frac{dT_m}{dt} + T_m = T \quad (D3)$$

where, τ_p is the time constant defined mathematically as,

$$\tau_p = \frac{V_t}{v_{0,t}} \quad (D4)$$

Model D4 is an ODE model of the thermocouple, resolved analytically using Laplace Transform in terms of deviation variables to give the s-domain algebraic model of the measuring device as,

$$\tau_p \mathcal{L}\left\{\frac{dT'_m}{dt}\right\} + \mathcal{L}\{T'_m\} = \mathcal{L}\{T'\} \quad (D5)$$

where, T'_m and T' the deviation variables of the measured variable and the temperature is defined mathematically as,

$$T'_m = T_m - T_{m,s} \text{ and } T' = T - T_s$$

$$\tau_p s \bar{T}'_{m(s)} - T'_{m(0)} + \bar{T}'_{m(s)} = \bar{T}'_{(s)} \quad (D6)$$

where $T'_{m(0)} = 0$

$$(\tau_p s + 1) \bar{T}'_{m(s)} = \bar{T}'_{(s)} \quad (D7)$$

$$G_{m(s)} = \frac{\bar{T}'_{m(s)}}{\bar{T}'_{(s)}} = \frac{1}{\tau_p s + 1} \quad (D8)$$

Model D8 is the transfer function of the thermocouple (measuring device) for the first-order system (Jean-Pierre, 2018).

Transfer Function for the Control Valve (Final Control Element)

The transfer function of the final control element (FCE) depends on the type of the actuating signals, adjustable according to the manipulated variable value. The pneumatic valve is the most common FCE, modelled as in D9 (Stephanopoulos, 2008; Ismael, 2020)

$$F = K f(x) \sqrt{\frac{\Delta P}{G}} \quad (D9)$$

where, F is the flow rate [m^3/s], ΔP is pressure drop across the pneumatic valve, K is constant depending on the valve size, G is the specific gravity of the flowing liquid (relative to water), and $f(x)$ is the valve flow characteristic curve.

Assuming the control valve have a transfer function after linearization and substitution from D10 as,

$$G_{f(s)} = \frac{\bar{F}'_{(s)}}{\bar{C}'_{(s)}} = \frac{K_v}{\tau_v s + 1} \quad (D10)$$

where, $G_{f(s)}$ is the transfer function for the FCE, K_v is the control value constant, and τ_v is the time constant of the valve.

APPENDIX E: Computational Data used for the Simulation Process

Table E1a Calculated or Derived Constants and their Values

S/N	Constant	Value	Unit
1.	V	0.0013	m/s
2.	Θ	1.265	-
3.	J	0.074	$\text{m}^3 \cdot \text{K} \cdot \text{mol}^{-1}$
4.	$K_{\Theta}, K_{1\Theta}$	0.0520, 0.0352	$\text{m}^3 \cdot \text{K} \cdot \text{mol}^{-1} \text{hr}^{-1}$
5.	$K'_{\Theta}, K'_{1\Theta}$	0.035, 0.0519	$\text{m}^3 \cdot \text{K} \cdot \text{mol}^{-1} \text{hr}^{-1}$
6.	$K_T = K_{T1}$	0.000304	$\text{m}^3 \cdot \text{K} \cdot \text{mol}^{-1} \text{hr}^{-1}$
7.	T	3.7	min^{-1}
8.	$K''_{\Theta}, K''_{1\Theta}$	0.00059, 0.00078	$\text{m}^3 \text{Khr}^{-1}$
9.	K'_T, K'_{T1}	1.48e-6, 1.71e-6	hr^{-1}
10.	$k'_{\Theta}, k'_{2\Theta}$	2.53E-4, 1.986e-4	-
12.	w, w ₁	-0.0134, 3.80e-4	-
13.	a ₁ , a ₂	0.0042, 1.394e-4	-
14.	K, K _a	0.026, 1.886e-4	$^{\circ}\text{Khr}^{-1}$
15.	B	0.018	$^{\circ}\text{Kmol}^{-1} \text{hr}^{-1}$
16.	a, a ₁₂	0.0189, 0.0128	$^{\circ}\text{Kmol}^{-1} \text{hr}^{-1}$
17.	K_{T12}, K_1	6.453e-5, 0.0522	hr^{-1}
18.	$K_{\Theta11}, K_{\Theta2}$	8.658e-3, 0.0322	$^{\circ}\text{Khr}^{-1}$
19.	a ₁₁ , K'	0.0342, 0.0522	$^{\circ}\text{Kmol}^{-1} \text{hr}^{-1}$
20.	K_{T11}	7.485e-5	hr^{-1}
21.	b ₁	1.887e-4	$^{\circ}\text{Kmol}^{-1} \text{hr}^{-1}$
22.	w ₂	-0.0358	hr^{-1}
23.	w ₃	-1.032e-5	$\text{molK}^{-1} \text{hr}^{-1}$

Table E1b Calculated or Derived Constants and their Values

S/N	Constant	Value
24.	d, f	0.00266, 0.0166
25.	f_1	1.981e-4
26.	m_{11}	0.0255
27.	m_{12}	0.0063
28.	c_{11}	0.0021
29.	c_{12}	0.00238
30.	c_{13}	8.877e-4
31.	c_{14}	0.00276
32.	c_{15}	0.00276
33.	c_{16}	1.407e-5
34.	m'	-3.44e-5
35.	n	3.244e-5
36.	c_{17}	0.008
37.	b_{11}	0.0282
38.	K_T, b_{12}	0.1382, 0.0322
39.	b_{13}	0.0372
40.	b_{14}	0.0374
41.	b_{15}	1.901e-4

Table E1c Calculated or Derived Constants and their Values

S/N	Constant	Value	Unit
42.	m	0.00914	-
43.	m_1	-0.00516	-
44.	d_1	1.903e-4	[°Khr ⁻¹]
45.	c_1	0.0004	[°Kmol ⁻¹ hr ⁻¹]
46.	Φ, v	0.240, 0.0182	[hr ⁻¹], [m.s ⁻¹]
47.	φ_1	0.01638	[hr ⁻¹]
48.	$P_{(s)}$	$s^2 + 0.0492s - 0.0005$	
49.	$P_{1(s)}$	$s^2 - 0.0166s + 0.0002$	
50.	K_{11}	0.012	[hr ⁻¹]
51.	a_2	1.394e-4	[molK ⁻¹ hr ⁻¹]
52.	K_1	0.0235	[molK ⁻¹ hr ⁻¹]
53.	a'	-0.0492	[hr ⁻¹]
54.	w'	4.799e-4	[hr ⁻¹]
55.	ξ_1	0.1602 or 0.1973	-
56.	ξ_2	0.3204 or 0.3946	-
57.	K_{12}	0.00934	[°Kmol ⁻¹ hr ⁻¹]