BCSIR

Available online at www.banglajol.info

Bangladesh J. Sci. Ind. Res. **57(3)**, 149-162, 2022

BANGLADESH JOURNAL OF SCIENTIFIC AND INDUSTRIAL RESEARCH

E-mail: bjsir07@gmail.com

Mathematical modeling and simulation of control strategies for continuous stirrer tank reactor

H. G. Ibrahim

Marine Mechanical Engineering Department, Faculty of Marine Resources, Alasmarya Islamic University, Zliten city, Libya

Abstract

This study aims to establish a mathematical model for the Continuous Stirred Tank Reactor (CSTR) reactor that exhibits highly nonlinear dynamics and was carried out implemented by model-based conventional and non-conventional controllers for temperature control. The developed controllers were Proportional, Proportional-Integral, Proportional-Derivative, Proportional-Integral-Derivative, Two Degrees of Freedom, and Model Predictive Controller. Then, the controllers were simulated, tuning, and optimized using Matlab®/Simulink®. The response results were compared and the analysis performed. The results indicated that the performance of 2-DOF-PID and MPC controllers is better than other conventional controllers for nonlinear systems such as the CSTR process.

Received: 11 April 2021
Revised: 16 May 2022
Accepted: 05 June 2022

DOI: https://doi.org/10.3329/bjsir.v57i3.62017

Keywords: Continuous stirred tank reactor; Temperature control; MPC; PID; Simulink

Introduction

A primary aim of control theory is to respond in a certain way to the output of the dynamic operation. At some point, nearly every control system is subject to severe constraints in its operating space. State constraints are also the most critical challenges in the design, protection, and operation of control systems during process control. Requirements to steadily improve process system's economic efficiency, force process engineers to operate control systems at the boundaries of safe and feasible regions to achieve maximum efficiency. Such an operation practice carries the risk that important constraints may eventually be breached due to disturbances, with potentially severe safety-related consequences. Control systems must be designed to expressly respect these constraints (Bayer *et al*., 2011).

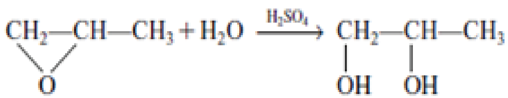
Continuous stirred tank reactors (CSTRs) have broad industrial applications and embody many characteristics of other reactor types. It is preferred use for highly exothermic reactions. The CSTR process is normally very complicated and deals with multiple aspects of the industry (Kishore *et al*., 2012). It consists of more than one process variable and manipulated variables, and shows very nonlinear dynamic behavior offering a variety of research in this area. Under such conditions, the nonlinearities may be complex and the performance of conventional control techniques suffers. All variables are correlated in that process, any changes in a single variable lead to undesirable behavior within the system (Åström and Hägglund, 1995). So, for controlling the system at the desired value, the control of all the variables is based on their relationship. For this process, a cascade controller is used in industries to get a more accurate control action (Rahmat *et al*., 2011). It is very complicated and a big challenge for engineers to design a controller for this process (Allwin *et al*., 2014).

*Corresponding author e-mail: h.ibrahim@asmarya.edu.ly

The main aim of this paper is the design a robustly stabilizing controller for the CSTR with the cooling in the jacket. So the novelty of this study is represented in the design of an algorithm of scheme controller based on Two Degrees of Freedom proportional- integral- derivative controller (2-DOF-PID) and Model Predictive Control (MPC) as alternative usage algorithm models for traditional controllers which are difficult to meet the requirements of temperature control for the system when using them. The comparison was done to find out which controllers will give a suitable control action for this process of CSTR temperature control by using Matlab®/Simulink®. The analysis of the final result was based on the performance index and time domain specifications by comparing the performance of controllers with one another.

Case study

An irreversible chemical reaction of propylene oxide (PO) reacts with water (W) to produce propylene glycol (PG) according to hydrolysis reaction with the presence of sulfuric acid and ethanol used as a case study. The reaction takes place readily at room temperature when catalyzed by sulfuric acid according to Eqn. (1) and the operating conditions mentioned by Fogler (2016);



(1)

The important constraint on the operation of propylene glycol production is propylene oxide has a rather low-boiling-point temperature, therefore, the operating temperature must not exceed 125 °F, to prevent oxide from vaporization through the vent system. All parameters and variables specified for the CSTR are presented by Fogler (2016).

Mathematical modeling

The mathematical model of the CSTR reactor comes from material and energy balances. The main assumptions were made to obtain the simplified modeling equations of a non-isothermal CSTR according presented by Seborg *et al.* (2011).

According to the assumptions, the unsteady-state mole balance for the CSTR is:

$$\frac{d(\rho V)}{dt} = \rho v_o - \rho v \quad (2)$$

Because V and ρ are constants, Eqn. (2) reduces to $v_o = v$; Thus, even though the inlet and outlet flow rate may change due to upstream or downstream conditions, Eqn. (2) must be satisfied at all times. In Fig. (1) flow rates are denoted by the symbol (v).

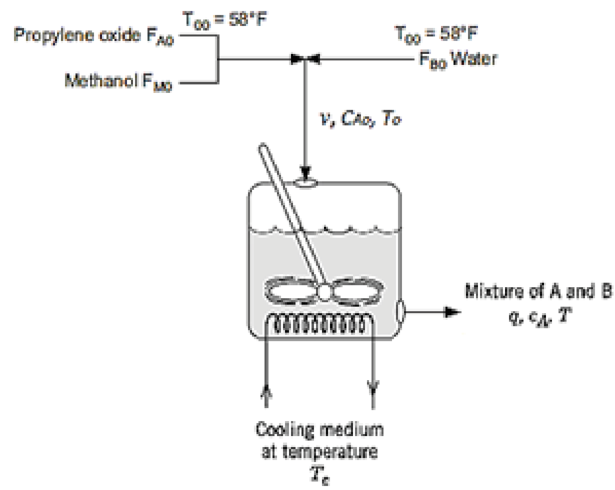


Fig. 1. Propylene Glycol production in a CSTR

The unsteady-state component balances for species *PO* (in molar units) is;

$$V\frac{dC_{PO}}{dt} = v(C_{POo} - C_{PO}) + Vr_{PO} \quad (3)$$

where C_{PO} is the product (effluent) concentration of component *PO* in the reactor and $-r_{PO}$ is the rate of disappearance of component *PO* per unit volume and given in first order as presented by Fogler (2016) for Eqn. (1);

$$-r_{PO} = k_o exp\left(\frac{-E}{RT}\right)C_{PO} \quad (4)$$

Also, the unsteady state energy balance equation for a non-isothermal CSTR is (Fogler, 2016);

$$\sum N_i C_{p_i}\frac{dT}{dt} = Ua(T_c - T) - \sum F_{io}Cp_i(T - T_o) + (-\Delta H)(-r_{PO}V) \quad (5)$$

Due to the reaction in liquid phase thus, $\sum N_i C_{pi} = N_{POo}Cp_s$ and $\sum F_{io}C_{pi} = F_{POo}Cp_s$; whereas

Cp_s is a specific heat of solution. So, Eqn. (5) becomes;

$$\frac{dT}{dt} = \frac{Ua(T_c - T) - F_{POo}Cp_s(T - T_o) + (-\Delta H)(-r_{PO}V)}{N_{POo}Cp_s} \quad (6)$$

where (ΔH) is the heat of reaction per mole of reacted *PO* is given as;

$$\Delta H = \Delta H^{o}_{rxn} + \Delta Cp(T - T_{Ref}) \quad (7)$$

U is the overall heat transfer coefficient, *a* surface area of the cooling coil, T_o is the feed temperature and T_c is the coolant temperature, and ΔC_p is the heat capacities for a chemical reaction.

From Eqns. (2-7), the mole and energy balance equations at unsteady state conditions are:

$$\frac{dC_{PO}}{dt} = \tau(C_{POo} - C_{PO}) - k_o exp\left(\frac{-E}{RT}\right) C_{PO} \quad (8)$$

$$\frac{dT}{dt} = \frac{Ua}{N_{POo}Cp_s}(T_c - T) - \tau(T - T_o) + \left(\frac{-\Delta HV}{N_{POo}Cp_s}\right) k_o exp\left(\frac{-E}{RT}\right) C_{PO} \quad (9)$$

where $\tau = V/v_O$.

At steady-state operating condition Eqns. (8 & 9) becomes;

$$0 = \tau(C_{POos.s.} - C_{POs.s.}) - k_o exp\left(\frac{-E}{RT_{s.s.}}\right) C_{POs.s.} \quad (10)$$

$$0 = \frac{Ua}{F_{POo}}(T_{cs.s.} - T_{s.s.}) - Cp_s(T_{s.s.} - T_o) + \left(\frac{-\Delta HV}{F_{POo}}\right) k_o exp\left(\frac{-E}{RT_{s.s.}}\right) C_{POs.s.} \quad (11)$$

where $C_{POs.s.}$, $T_{s.s.}$ and $T_{c.s.s.}$ are steady-state quantities of concentration of *PO*, temperature of outlet stream from the CSTR, and coolant temperate respectively.

The dynamic model of the non-isothermal CSTR is presented in Eqns. (8 and 9) is nonlinear as a result of the many product terms and the exponential temperature dependence of *k*. These equations are coupled and it is not possible to solve one equation independently of the other. For designing the controllers for such a nonlinear process, one of the approaches is to represent the nonlinear system as a family of local linear models.

Simulation and validity of the model

A comparison between outputs from the real system and simulated outputs demonstrates the validity of the mathematical model. If the difference between the real system and the model is unacceptable, it is necessary to jump back to modeling and cancel some simplifications. The goal is to find the simplest model with a satisfactory description of the real process (Vojtesek and Dostal, 2005).

Simulation studies were performed for the system at steady-state to find an optimal working point, where the product's concentration is maximal and the operating temperature must not exceed 125 °F, to prevent oxide from vaporization through the vent system.

Steady-state analysis for stable systems involves computing values of state variables in time $t \to \infty$ when changes of these variables are equal to zero. That means, the set of Eqns. (10 & 11) is solved with the operating conditions and the parameters given by Fogler (2016) after rearranged in forms *x* as a function of *T* as follows;

$$x_{MB} = \frac{2.084\times10^{12} e^{-16,306/T_{s.s.}}}{1+2.084\times10^{12} e^{-16,306/T_{s.s.}}} \quad (12)$$

$$x_{EB} = \frac{403.3(T_{s.s.}-535)+92.9(T_{s.s.}-545)}{36,400+7(T_{s.s.}-528)} \quad (13)$$

These two nonlinear simultaneous equations (NLE) have two unknowns, *x*, and *T*, which can solve with Polymath v.6.10. The exiting temperature and conversion are 103.7 °F (563.7 R) and 36.4%, respectively. This conversion is low, so could reduce the cooling by increasing T_c to raise the reactor temperature closer to 585 R, but not above this temperature as present in Table I.

Table I. Calculated values of NLE variables at different coolant temperature

$T_{cs.s.}$ (R)	$x_{s.s.}$(%)	$T_{s.s.}$ (R)
545	36.4	563.7
550	49.4	574.4
555	60.3	583.5
560	66.2	588.8

The reactor and coolant steady-state temperatures ($T_{s.s.}$=583.5 R, and $T_{cs.s.}$=555 R) respectively, and 60.3% of propylene oxide is converted to propylene glycol, so the propylene oxide and propylene glycol steady-state concentrations are 0.0524, and 0.0796 lb.mol/ft^3 respectively. This output temperature was used as the controlled variable in the control section and a change in the coolant temperature was considered a manipulated variable. So, the obtained results are satisfied with the results and constraints presented by Fogler (2016), which reveals the model of this system is satisfactory.

State-Space models

Dynamic models derived from typical physical principles consist of two ordinary differential equations (ODEs). It considers a general class of ODE models referred to as *linear state-space models* that provide a compact and useful representation of dynamic systems and provide the theoretical basis for the analysis of nonlinear processes (Seborg *et al.*, 2011). A linear state-space model is;

$$\left.\begin{array}{c}\dot{x} = Ax + Bu + Ed\\ y = Cx\end{array}\right\} \quad (14)$$

where x is the *state vector; u* is the input vector of manipulated variables (also called *control variables); d* is the disturbance vector, and y is the output vector of measured variables.

The elements of x are referred to as *state variables.* The elements of y are typically a subset of x, namely, the *state variables* that are measured. In general, x, u, d and y are functions of time. The time derivative of x is denoted by x (*=dx/dt);* it is also a vector. Matrices A, B, C, and E are constant matrices. The vectors in Eqn. (14) can have different dimensions (or "lengths") and are usually written as deviation variables. So the Eqns. (8 & 9) becomes;

$$\frac{d\bar{C}_{PO}}{dt} = \tau(\bar{C}_{POo} - \bar{C}_{PO}) - k_o exp\left(\frac{-E}{R\bar{T}}\right)\bar{C}_{PO} \quad (15)$$

$$\frac{d\bar{T}}{dt} = \frac{Ua}{N_{POo}Cp_s}(\bar{T}_c - \bar{T}) - \tau(\bar{T} - \bar{T}_o) + \left(\frac{-\Delta HV}{N_{POo}Cp_s}\right)k_o exp\left(\frac{-E}{R\bar{T}}\right)\bar{C}_{PO} \quad (16)$$

where $\bar{C}_{POo} = C_{POo} - C_{POos.s}$, $\bar{C}_{PO} = C_{PO} - C_{POs.s}$, $\bar{T} = T - T_{s.s}$ and $\bar{T}_c = T_c - T_{cs.s.}$. These variables resulting from subtracting Eqns. (8 & 9) from Eqns. (10 & 11). Because of the state-space model in Eqns. (15 & 16) may seem rather abstract, it is helpful to consider physical problems.

Linearization

At steady state condition Eqns. (15) and (16) becomes the standard state variable form as;

$$\frac{d\bar{C}_{PO}}{dt} = 0 = f_1(\bar{C}_{PO}.\bar{T}_{\square}) = \tau(\bar{C}_{POo} - \bar{C}_{PO}) - k_o exp\left(\frac{-E}{R\bar{T}_{\square}}\right)\bar{C}_{PO} \quad (17)$$

$$\frac{d\bar{T}}{dt} = 0 = f_2(\bar{C}_{PO}.\bar{T}_{\square}) = \frac{Ua}{N_{POo}Cp_s}(\bar{T}_c - \bar{T}_{\square}) - \tau(\bar{T}_{\square} - \bar{T}_o) + \left(\frac{-\Delta HV}{N_{POo}Cp_s}\right)k_o exp\left(\frac{-E}{R\bar{T}_{\square}}\right)\bar{C}_{PO} \quad (18)$$

For this situation, there are two input variables v *and* T_c, and two output variables C_{PO} and T. So, the linearized CSTR model in Eqns. (17 and 18) can be rewritten in vector-matrix form using deviation variables presented in Eqn. (14) as follows:

$$\left.\begin{array}{l}\dot{x} = Ax + Bu \;\Rightarrow\; \begin{bmatrix}\dot{x}_1\\ \dot{x}_2\end{bmatrix} = \begin{bmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix} + \begin{bmatrix}b_{11} & b_{12}\\ b_{21} & b_{22}\end{bmatrix}\begin{bmatrix}u_1\\ u_2\end{bmatrix}\\ y = Cx \;\Rightarrow\; \begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix}\end{array}\right\} \quad (19)$$

where $x_1 \equiv \bar{C}_{PO}$ and $x_2 \equiv \bar{T}$, and denote their time derivatives by x_1 and by x_2 and the feed volumetric flow rate $\bar{v}$ and coolant temperature $\bar{T}_c$ are considered to be a manipulated variables u_1 and u_2 respectively.

$$\left.\begin{array}{c}\begin{bmatrix}\frac{d\bar{C}_{PO}}{dt}\\ \frac{d\bar{T}}{dt}\end{bmatrix} = \begin{bmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{bmatrix}\begin{bmatrix}\bar{C}_{PO}\\ \bar{T}\end{bmatrix} + \begin{bmatrix}b_{11} & b_{12}\\ b_{21} & b_{22}\end{bmatrix}\begin{bmatrix}\bar{v}\\ \bar{T}_c\end{bmatrix}\\ \begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}\bar{C}_{PO}\\ \bar{T}\end{bmatrix}\end{array}\right\} \quad (20)$$

But according to the objective of this study, there is one input variable (manipulated, $\bar{T}_c$) and one output variable (controlled, $\bar{T}$). So, Eqn. (20) reduced into the final forms as follows;

$$\left.\begin{array}{c}\begin{bmatrix}\frac{d\bar{C}_{PO}}{dt}\\ \frac{d\bar{T}}{dt}\end{bmatrix} = \begin{bmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{bmatrix}\begin{bmatrix}\bar{C}_{PO}\\ \bar{T}\end{bmatrix} + \begin{bmatrix}0\\ b_{22}\end{bmatrix}\bar{T}_C\\ y_2 = \begin{bmatrix}0 & 1\end{bmatrix}\bar{T}\end{array}\right\} \quad (21)$$

The Jacobian matrix A is given as,

$$A = \begin{bmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{bmatrix} = \begin{bmatrix}\frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2}\\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2}\end{bmatrix} \quad (22)$$

The coefficients of Matrix A at steady-state operating conditions [presented by Eqns. (17 and 18)] are;

$$\begin{bmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{bmatrix} = \begin{bmatrix}-\tau - k_0 exp\left(\frac{-E}{RT_{S.S.}}\right) & -C_{POS.S.}k_0\left(\frac{E}{RT^2_{S.S}}\right)exp\left(\frac{-E}{RT_{S.S.}}\right)\\ \left(\frac{-\Delta HV}{N_{POo}Cp_s}\right)k_0 exp\left(\frac{-E}{RT_{S.S}}\right) & (-\tau) + \left(\frac{(-\Delta H)VC_{POS.S}}{N_{POo}Cp_s}\right)k_0\left(\frac{E}{RT^2_{S.S.}}\right)exp\left(\frac{-E}{RT_{S.S.}}\right) - \left(\frac{Ua}{N_{POo}Cp_s}\right)\end{bmatrix} \quad (23)$$

The Jacobiam matrix B is given by;

$$B = \begin{bmatrix}b_{11} & b_{12}\\ b_{21} & b_{22}\end{bmatrix} = \begin{bmatrix}\frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2}\\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2}\end{bmatrix} \quad (24)$$

where the coefficients of Matrix B at steady-state operating conditions [presented in Eqn. (18)] are;

$$\begin{bmatrix}0\\ b_{22}\end{bmatrix} = \begin{bmatrix}0\\ \frac{Ua}{N_{POo}Cp_s}\end{bmatrix} \quad (25)$$

By using the steady-state values and the CSTR parameters and substituting in Eqns. (23 and 25) gets on;

$$A = \begin{bmatrix} -12.5111 & -0.03109 \\ 3520.341 & 6.8377 \end{bmatrix} \quad (26)$$

$$B = \begin{bmatrix} 0 \\ 1.8738 \end{bmatrix} \quad (27)$$

The transfer function of the process that relates changes in the CSTR temperature $\bar{T}$ to the changes in the coolant temperature $\bar{T}_c$ is given as follow (Seborg *et al.*, 2011);

$$G_p = \frac{\bar{T}}{\bar{T}_c} = \frac{b_{22}*S - b_{22}*a_{11}}{S^2 - S*(a_{11}+a_{22}) + a_{11}*a_{22} - a_{21}*a_{12}} \quad (28)$$

By substitution in Eqn. (28) to gets;

$$\frac{\bar{T}}{\bar{T}_c} = \frac{1.874S+23.44}{S^2+5.673S+23.9} \quad (29)$$

Stability criterion for State-Space model

One important property of state-space models is *stability.* A state-space model is said to be stable if the response *x(t)* is bounded for all *u(t)* and *d(t)* that are bounded. [*i.e.* The state-space model in Eqn. (19) will exhibit abounded response *x(t)* for all bounded *u(t)* and *d(t)* if and only if all of the eigenvalues of *A* have negative real parts] (Seborg *et al.*, 2011). The stability is solely determined by *A,* the *B, C,* and *E* matrices do not affect. The corresponding values of *x* are the *eigenvectors* of *A.* The eigenvalues are the roots of the characteristic equation (Seborg *et al.*, 2011);

$$|\lambda I - A| = 0 \quad (30)$$

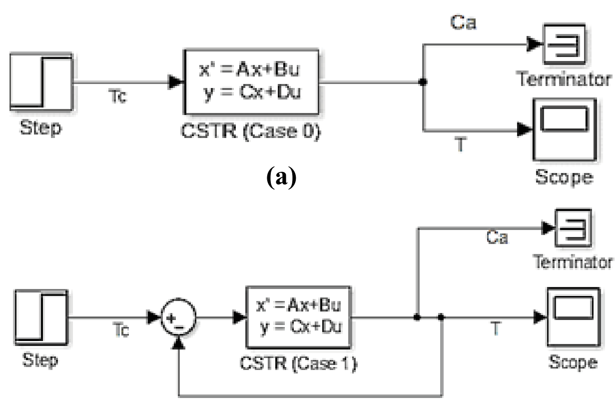
where *I* is the $n\times n$ identity matrix and $|\lambda I{-}A|$ denotes the determinant of the matrix $\lambda I{-}A$.

The stability criterion for state-space models indicates that stability is determined by the eigenvalues of *A.* They can be calculated using the MATLAB command, *eig,* after defining *A* as mentioned in Eqn. (26). The eigenvalues of *A* are -2.8367+3.9816*i*, and -2.8367-3.9816*i*. Because both Eigenvalues have negative real parts, the state-space model is stable, although the dynamic behavior will exhibit oscillation due to the presence of imaginary components in the eigenvalues.

Simulink model for CSTR

The operation of the CSTR is disturbed by external factors such as changes in the feed flow rate and temperature. So the control action to alleviate the impact of the changing disturbances and to keep *T* at the desired set point (SP) in this system, the manipulated temperature T_c is responsible to maintain the temperature *T* at the desired set-point. The reaction is exothermic and the heat generated is removed by the coolant, which flows in the jacket around the tank.

The continuous stirred tank reactor was modeled with Simulink according to Eqns. (26 & 27). The open and closed systems of CSTR are shown in Fig. (2a & b). Due to disturbance, the value of a controlled variable is increased. Without control, as shown in Fig. (2a), this variable continues to rise to a new final steady-state value. With regulation as shown in Fig. (2b), the control mechanism starts taking action to hold the controlled variable close to the value that existed before the disruption occurred (LeBlanc and Coughanowr, 2009). The control purpose is to affect the T_c (manipulated variable) and maintain the temperature of the system at the required value (controlled variable) so a controller must be used.



(a)

(a)

Fig. 2. Simulink model for CSTR with set-point
a) Open system, and b) Closed system

Control Strategies of CSTR

A primary objective of control theory is to make the output of a dynamic process behave in a certain manner. The desired output of a system is called the reference (Set-Point). In the field of the control system, various control strategies and methods are implemented, devised, and experienced in the process control and other control applications (Kumar and Patel, 2015). The main controllers frequently used in industrial processes had been presented and discussed herein.

The actual electronic controller is but one of the components because the transducer and the converter will be lumped together with the controller for simplicity. The main goal of a controller used is to reduce the error between the process output (temperature of CSTR) and the temperature of cooling water. The controller works in a closed-loop system with a

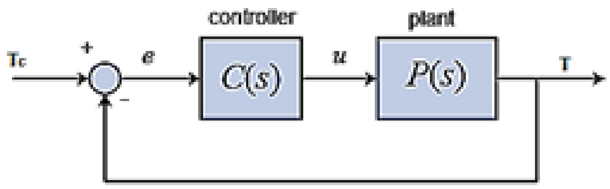


Fig. 3. Unity feedback control system of a process

process using the schematic shown in Fig. (3), the variable (ε) represents the tracking error, the difference between the desired output temperature (T_c) and the actual output temperature (T). This error signal (ε) is fed to the controller, and the controller computes the error to time. The effect of each of the controller parameters will be discussed on the dynamics of a closed-loop system and will demonstrate how to use a controller to improve a system's performance.

Proportional Controller (P)

The proportional controller has only one adjustable parameter, the proportional gain (K_P). This controller produces an output signal (current, or voltage for an electronic controller) that is proportional to the error (ε). This action may be expressed as a transfer function as follow*;*

$$\frac{u(s)}{\varepsilon(s)} = K_P \tag{31}$$

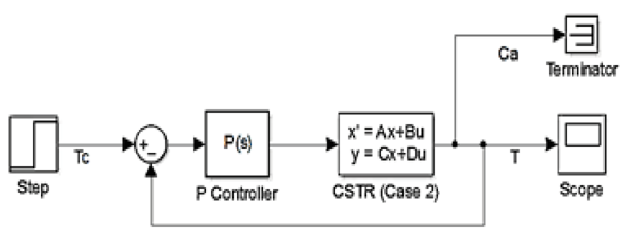


Fig. 4. Simulink model for CSTR with P controller

Fig. (4) presents the control system model by using a proportional controller. The default proportional gain value is 0.8.

Proportional-Integral Controller (PI)

This controller has two adjustable parameters the proportional gain (K_P) and the integral gain (K_I). Thus it is a bit more complicated than a proportional controller, but in exchange for the additional complexity, it reaps the advantage of no error at a steady state. This action may be expressed as;

$$\frac{u(s)}{\varepsilon(s)} = K_P + \frac{K_I}{S} \tag{32}$$

The proposed control model by using a proportional-integral controller is shown in Fig. (5). The default proportional and integral gain values are 0.8 and 1 respectively.

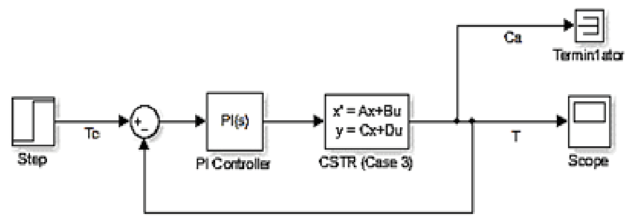


Fig. 5. Simulink model for CSTR with PI controller

Proportional-Derivative Controller (PD)

This controller has three adjustable parameters the proportional gain (K_P) the derivative gain (K_D) and the derivative filter coefficient (n). Proportional-derivative controller represented by;

$$\frac{u(s)}{\varepsilon(s)} = K_P + K_D \frac{n}{1+\frac{n}{S}} \tag{33}$$

The proposed control model by using a proportional-derivative controller is shown in Fig. (6). The default proportional and derivative gain values are 0.8 and 0.4, and the derivative filter coefficient is 100.

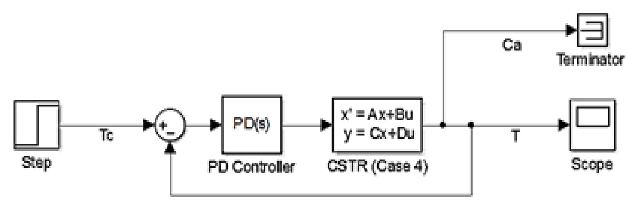


Fig. 6. Simulink model for CSTR with PD controller

Proportional-Integral-Derivative Controller (PID)

As implied by the name, a PID (proportional-integral-derivative) controller consists of three parts: the proportional part, the integral part, and the derivative part. The weighted sum of these three parts is used to adjust the process via a control valve. Usually, a PID is formulated as follows:

$$\frac{u(s)}{\varepsilon(s)} = K_P + \frac{K_I}{S} + K_D \frac{n}{1+\frac{n}{S}} \tag{34}$$

The proposed control model by using a proportional-integral-derivative controller is shown in Fig. (7), with default values of proportional, integral, and derivative gains are 0.8, 1, and 0.4 respectively, and the derivative filter coefficient is 100.

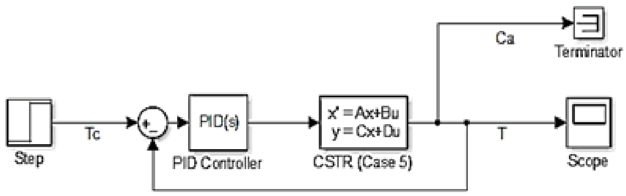


Fig. 7. Simulink model for CSTR with PID controller

Two Degree of Freedom-PID Controller (2-DOF-PID)

The degree of freedom of a control system is defined as the number of closed-loop transfer functions that can be adjusted independently (Araki and Taguchi, 2003). Two-degree-of-freedom (abbreviated as 2-DOF-PID) controller is capable of fast disturbance rejection without a significant increase of overshoot in set-point tracking. 2-DOF-PID controllers are also useful to mitigate the influence of changes in the reference signal on the control signal (Matlab website, 2020).

In the PID controller (2DOF) the set-point weights b and c determine the strength of the proportional and derivative action in the feed-forward compensator. The block of the 2-DOF-PID presented in Fig. (8) generates an output signal based on the difference between a reference signal (T_c) and a measured system output (T). The block computes a weighted difference signal for the proportional and derivative actions according to the set-point weights (b and c). The block output is the sum of the proportional, integral, and derivative actions on the respective difference signals, where each action is weighted according to the gain parameters K_P, K_I, and K_D. The default values of proportional, integral, and derivative gains are 0.8, 1, and 0.4 respectively, and the weights coefficients (b and c) are 1 and 1 respectively.

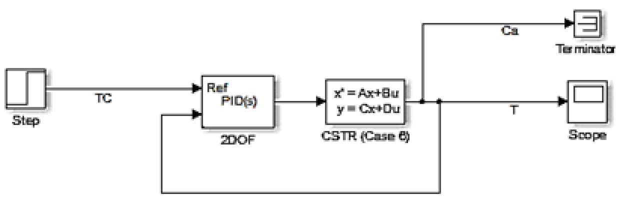


Fig. 8. Simulink model for CSTR with 2DOF-PID controller

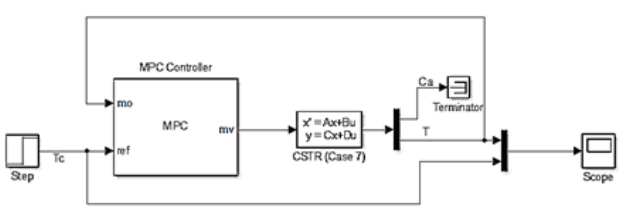


Fig. 9. Simulink model for CSTR with MPC controller

Model predictive controller (MPC)

A Model Predictive Controller used for control of temperature, concentration, and pH without a neural strategy for CSTR as presented by (Arivalagan *et al*., 2015; Shyamalagowri and Rajeswari, 2013; Hong and Cheng, 2012; Balaji and Maheswari, 2012). The MPC Controller block shown in Fig. (9) receives the current measured output signal (mo), and a reference signal (ref). The block computes the optimal manipulated variable (mv) by solving a quadratic programming problem using a system model then optimized at regular intervals concerning a performance. The control interval is chosen to be a 0.1-time unit. The Prediction horizon and Control Horizon are chosen as 5 and 1 intervals respectively.

Controllers tuning

The tuning of controllers is the main task for better performance of the system. The desired parameters for the controllers are the proportional gain (K_P) integral gain (K_I) and the derivative gain and filter coefficient (K_D and n) can be calculated by the Automatic controller tuning method in Simulink software (Simulink Tuner). Controller tuning refers to the selection of tuning parameters to ensure the best response of the controller. When a control system is properly tuned, the process variability is reduced, efficiency is maximized, energy costs are minimized, and production rates can be increased as mentioned by Buckbee (2009).

Simulink design optimization

Simulink® Design Optimization™ provides functions, interactive tools, and blocks for analyzing and tuning model parameters to determine the model's sensitivity, fit the model to test data, and tune it to meet requirements. The Simulink displays a warning if the signal violates the specified step

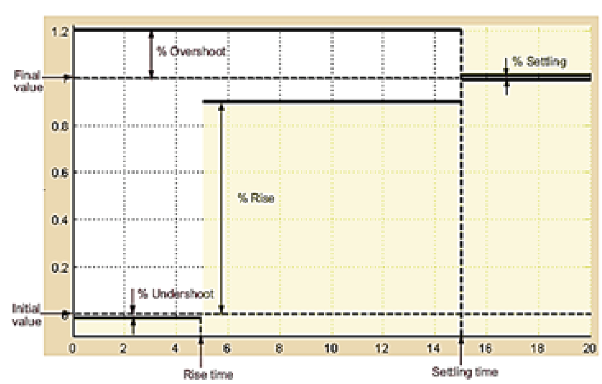


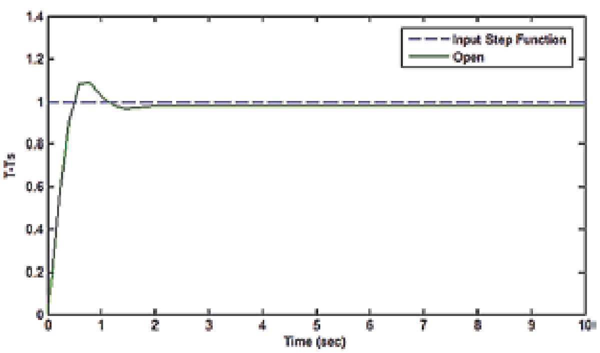
Fig. 10. The model verification of Simulink design optimization for a CSTR control system

response characteristics. The bounds also appear on the step response plot as shown in Fig. (10), and checked that a signal satisfies response bounds during the simulation. This block and the other blocks in the Model Verification library test that a signal remains within specified time-domain characteristic bounds.

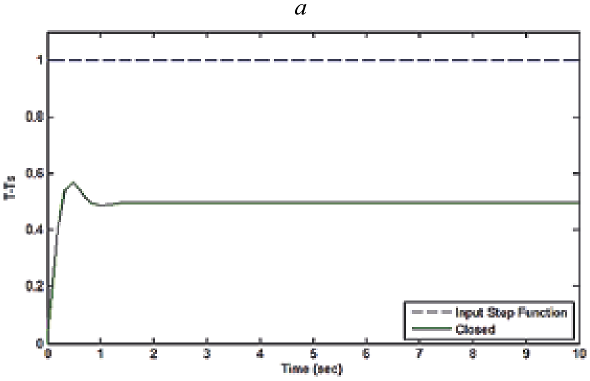
Results and discussion

Simulink models

The curves shown in Fig. (11a & b) represent the behavior of the controlled temperature of a CSTR system when it is subjected to a permanent step disturbance ($\overline{T}_c$). The values of the controlled temperature rise at time zero owing to the disturbance. The steady-state error for the open system (offset) reaches a new value up to 0.019 with a final temperature value reaching 124.481 ^{o}F. While the steady-state error for the closed-loop system (offset) also reaches a new value up to 0.505. Generally, the closed-loop system is better than an open system due to it has small values of rising time, peak time, and settling time as shown in Table II. But, it has a high overshoot percentage then it settles at a lower stable value with a more restricted final temperature value that reaches 123.995 ^{o}F compared with the open system.



a



b

Fig. 11. CSTR temperature response of uncontrolled systems a) Open-loop system, and b) Closed-loop system

Comparative the responses of the CSTR model with the different controllers

The comparative analysis of the control strategies results had been used for the control response of a CSTR by Simulink. In all the simulation runs, the process is simulated using the State-Space Model of the CSTR presented through Eqns. (26-27). The control models designed for this process were done by using various controllers P, PI, PD, PID, 2-DOF-PID, and MPC. For the controllers' design default values for parameters have been used to find the system response. A set-point of 1 ^{o}F is given as a step input at t= 0 sec.

With no control, the controlled variable (T) continues to rise to a new steady-state value as seen previously. But with control after some time, the control system begins to take action to try to maintain the controlled variable close to the value that is required. With a proportional controller, the block temperature response of CSTR shown in Fig. (12), the control system can arrest the rise of the controlled temperature and ultimately bring it to rest at a new steady-state value with short time-domain responses as presented in Table II.

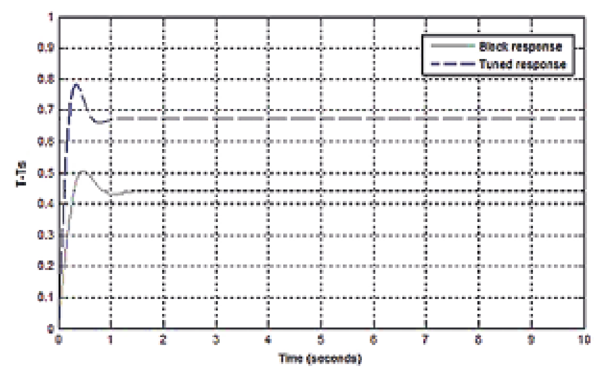


Fig. 12. Temperature responses of CSTR with P controller; a) Block and b) Tuned

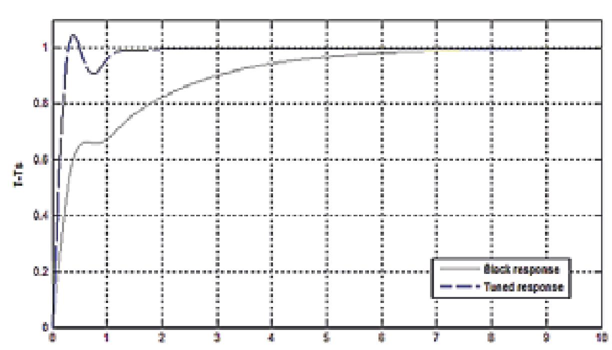


Fig. 13. Temperature responses of CSTR with PI controller; a) Block and b) Tuned

The time values of responses include rise time, peak time, and settling time are around 0.2299, 0.5376, and 0.8199 sec respectively; with an overshoot of 14.147% (overshoot value reaches 0.5019 ^{o}F). The steady-state error for the process with P controller (offset) reaches 0.56, and the final value of the response reaches 123.94 ^{o}F; this value has a smaller offset than that obtained by an uncontrolled process in a closed-loop system (Final temperature value reached 123.995 ^{o}F). So, as shown in Fig. (12), block proportional control produces an overshoot followed by the oscillatory response, which levels out at a value that does not equal the set-point; this ultimate displacement from the set-point is the offset.

As shown in Fig. (13), the block response of CSTR temperature by using the PI controller, the addition of integral action eliminates the offset; the controlled temperature ultimately goes to the required value. This advantage of integral action is balanced by the disadvantage of more oscillatory behavior. For the system with the PI controller, the domain-time responses were 2.918, 10, and 5.655 sec for rising time, peak time, and settling time respectively. There is no overshoot percentage in the response (the overshoot value reaches 0.998 ^{o}F). The steady-state error for the process with PI controller (offset) reaches an excellent value up to 0.002, and the final value of the temperature response reaches 124.498^{o}F. Compared with the previous systems without a controller (closed-loop system) and with a proportional controller, the temperature settles at lower stable values (Final temperature values reached 123.995 and 123.94 ^{o}F for each one respectively). The main disadvantage is that it has a high value of settling time compared to other systems. In this case, the block response has no overshoot; and the response returns to the approximated set-point (offset=0.002) after a relatively long settling time. The most beneficial of the integral action in the controller is reducing the offset.

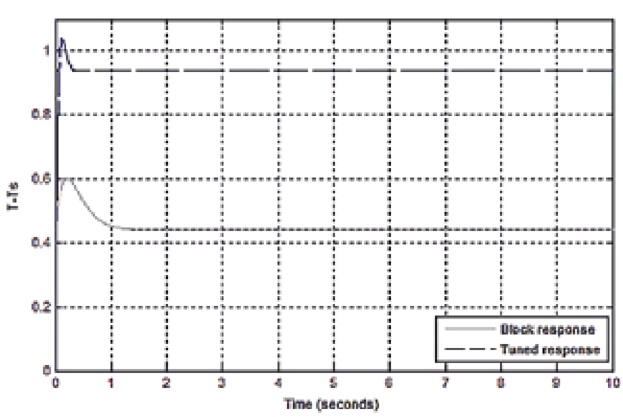


Fig. 14. Temperature responses of CSTR with PD controller; a) Block and b) Tuned

For the system with a PD controller shown in Fig. (14), the block response exhibits a smaller period of oscillation compared to the block response for proportional control. The rise time, peak time, and settling time are around 0.0113, 0.2049, and 1.0987 sec respectively, and a high overshoot of 36.731% in the block response (overshoot value reaches 0.6012 ^{o}F). The offset that remains is the same that for portioned control (reaches 0.56), the final value of the block response reaches (123.94 ^{o}F). Compared with a process without a controller (closed-loop system) the temperature settles at the same stable value faster than a PD controller.

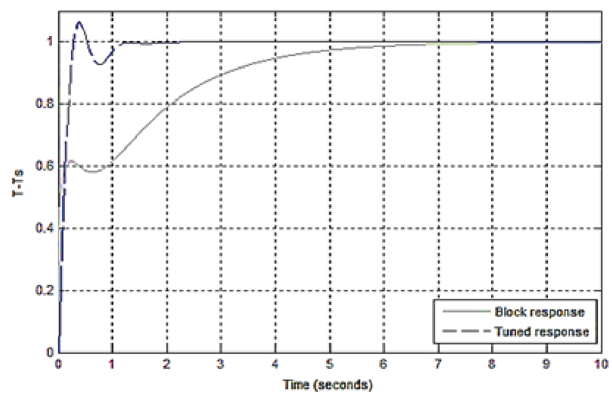


Fig. 15. Temperature responses of CSTR with PID controller; a) Block and b) Tuned

The addition of derivative action to the PI action gives a definite improvement in the block response. The rise of the controlled variable is arrested more quickly, and it is returned rapidly to the original value with little or no oscillation. For the block system with PID controller shown in Fig. (15), the rise time, peak time, and settling time are around 3.0859, 10, and 5.3737 sec respectively. The block response has a lower overshoot of 0.09%, in which the peak value reaches 0.9991 ^{o}F. The steady-state error for the process with PID controller (offset) reaches an excellent value more than the PI controller (reaches 0), and the final value of the block response reaches (124.5 ^{o}F). The main advantage of the PID controller is that it has small values of offset and overshot compared to other controllers, with acceptable values of settling time, rise time, and peak time.

The used 2-DOF-PID shown in) for control of the system generates a low-value overshoot (0% with a peak value reaching 0.999 ^{o}F), where rise time, peak time, and settling time were recorded at 3.2805, 9.95, and 5.5674 sec respectively. It has been found that 2-DOF-PID performs best in terms of overshoot and settling time reduction and suppressing the effect of the applied perturbation on the system.

In this case, the overshoot has been reduced to 0% and has the same settling time recorded by conventional PID with default parameters (about 5.3737 sec).

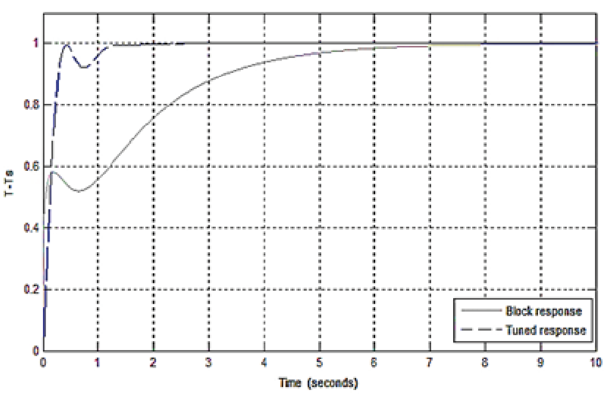


Fig. 16. Temperature responses of CSTR with 2 DOF -PID controller; a) Block and b) Tuned

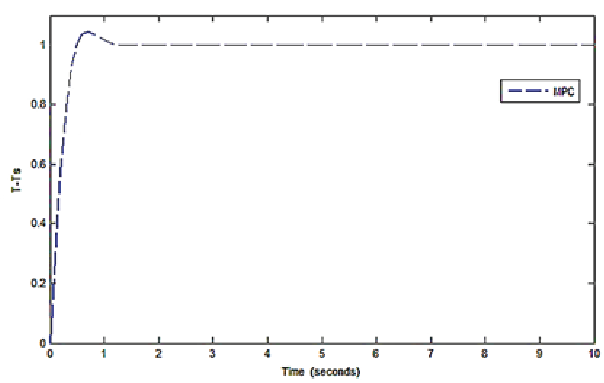


Fig. 17. Temperature response of CSTR with MPC controller

The simulation results with the MPC controller as shown in Fig. (17), prove that the MPC control method is a more effective way to enhance the stability of the time-domain performance of the temperature of the CSTR process. It is shown that the proposed model predictive control design yields better improvement with significantly better response, peak, and settling times than the PID controller in their forms of conventional and 2-DOF as mentioned in Table II. The time values of responses include; rise time, peak time, and settling time are around 0.383, 0.7, and 0.919 sec respectively, and the overshoot value reaches 1.04 ^{o}F with 4%. The more the overshoot gives the transients in the response though gives a short rise time, the stability of the system to keep in mind (Deulkar and Patil, 2015). In these simulation results, the MPC controller yields a better and more stable response. There are no offset reaches, and the final value of the response reaches (124.5 ^{o}F).

Controllers tuning

The tuning of controllers was done by using the Controller Tuner provided by Simulink which is powered by Matlab. The results of tuned control systems (tuned response) are shown in Figs. (12-16), and the values presented in Table III better performance and reduction of error in the majority of all control cases than the results of the systems that have default parameters of controllers (block response) presented in Table II.

The MPC controller gave the optimized tuning parameters directly, this behavior was confirmed by the results of Jibril *et al*. (2020) for study the continuous stirred tank reactor with the MPC controller has a better response in minimizing the overshoot and tracking the desired value with the effect of the disturbance makes the output with small fluctuations and it is better than the continuous stirred tank reactor with PID controller. The MPC controller incorporates a way better reaction in terms of minimizing overshoot and following the temperature required by the system. Even in the event of a failure, a CSTR with an MPC controller provides better response behavior than a CSTR with traditional control technology, which is the optimal value of the controller parameters generated, as mentioned by Prabhu *et al*. (2021).

Tuning with actuator constraints

The method of tuning with constraints optimization is based on the minimization of a global objective function that incorporates local objective functions. With this approach, it is possible to consider uncertainties of the model, several control algorithms, and different types of disturbances. The proposed method does not place any kind of restriction on the characterization of the process. So, even nonlinear models can be used. Moreover, any type of controller can be implemented (Neto and Embirucu, 2000). So, by using the *Simulink Design optimization tool* that includes checking step response characteristics. The constrained bounds values of step response characteristics are specified including rising time, settling time as 5 and 7 seconds, and the percentage of settling, overshoot, and rise is specified as 2%, 10%, and 90%. By starting the optimization of the controller parameters with the initial values of K_P, K_I, K_D, n, b, and c mentioned previously where the response is not satisfactory, the optimization process is iterating to meet the requirement. The obtained process response must not be out of the envelope. The optimized response satisfied with the constrained requirements is plotted by the thickest line of response in the scheme of optimization progress of the response of a CSTR control system with the controllers shown in Fig. (18). The comparison between the final values of gains of the used tuned and optimized controllers are presented in Table IV.

Table II. Comparative Analysis of CSTR using various Controllers with default parameters

Data	Unit	Open	Closed	P	PI	PD	PID	2DOF	MPC
Rise time	sec	0.3375	0.2167	0.2299	2.918	0.0113	3.0859	3.2805	0.383
Overshoot	%	10.649	15.112	14.147	0	36.731	0.09	0	4
Peak value	ºF	1.0853	0.57	0.5019	0.998	0.6012	0.9991	0.999	1.04
Peak time	sec	0.7902	0.484	0.5376	10	0.2049	10	9.95	0.7
Settling time	sec	1.1368	0.7678	0.8199	5.655	1.0987	5.3737	5.3737	0.919
Final value	ºF	0.981	0.495	0.44	0.998	0.44	1	0.999	1
Offset	ºF	0.019	0.505	0.56	0.002	0.56	0	0.001	0
T	ºF	124.481	123.995	123.94	124.498	123.94	124.5	124.499	124.5

Table III. Comparative analysis of CSTR temperature response with various tuned controllers by using Simulink Tuner

Data	Unit	Open	Closed	P	PI	PD	PID	2DOF	MPC
Rise time	sec	0.3375	0.2167	0.153	0.214	0.0471	0.207	0.253	0.383
Overshoot	%	10.649	15.112	16.4	4.58	10.9	6.44	0	4
Peak value	ºF	1.0853	0.57	0.783	1.05	1.04	1.06	1	1.04
Peak time	sec	0.7902	0.484	0.346	0.384	0.118	0.384	2.56	0.7
Settling time	sec	1.1368	0.7678	0.596	1.12	0.259	1.06	1	0.919
Final value	ºF	0.981	0.495	0.673	1	0.937	1	1	1
Offset	ºF	0.019	0.505	0.327	0	0.063	0	0	0
T	ºF	124.481	123.995	124.173	124.5	124.437	124.5	124.5	124.5

Table IV. Comparison between the final values of gains of the tuned and optimized responses of the used controllers

Parameter	Controller Type									
	P		PI		PD		PID		2-DOF-PID	
	Tuned	Optimized	Tuned	Optimized	Tuned	Optimized	Tuned	Optimized	Tuned	Optimized
K_P	2.0945	55.54	1.942	0.8	15.291	61.549	1.819	0.8	1.819	0.8
K_I	-	-	6.1337	1	-	-	7.272	1	7.272	1
K_D	-	-	-	-	100	3.508	0.018	0.4	0.0318	0.4
n	-	-	-	-	-	749.75	9.298	100	9.298	100
c	-	-	-	-	-	-	-	-	0.83	0.83
b	-	-	-	-	-	-	-	-	1	1

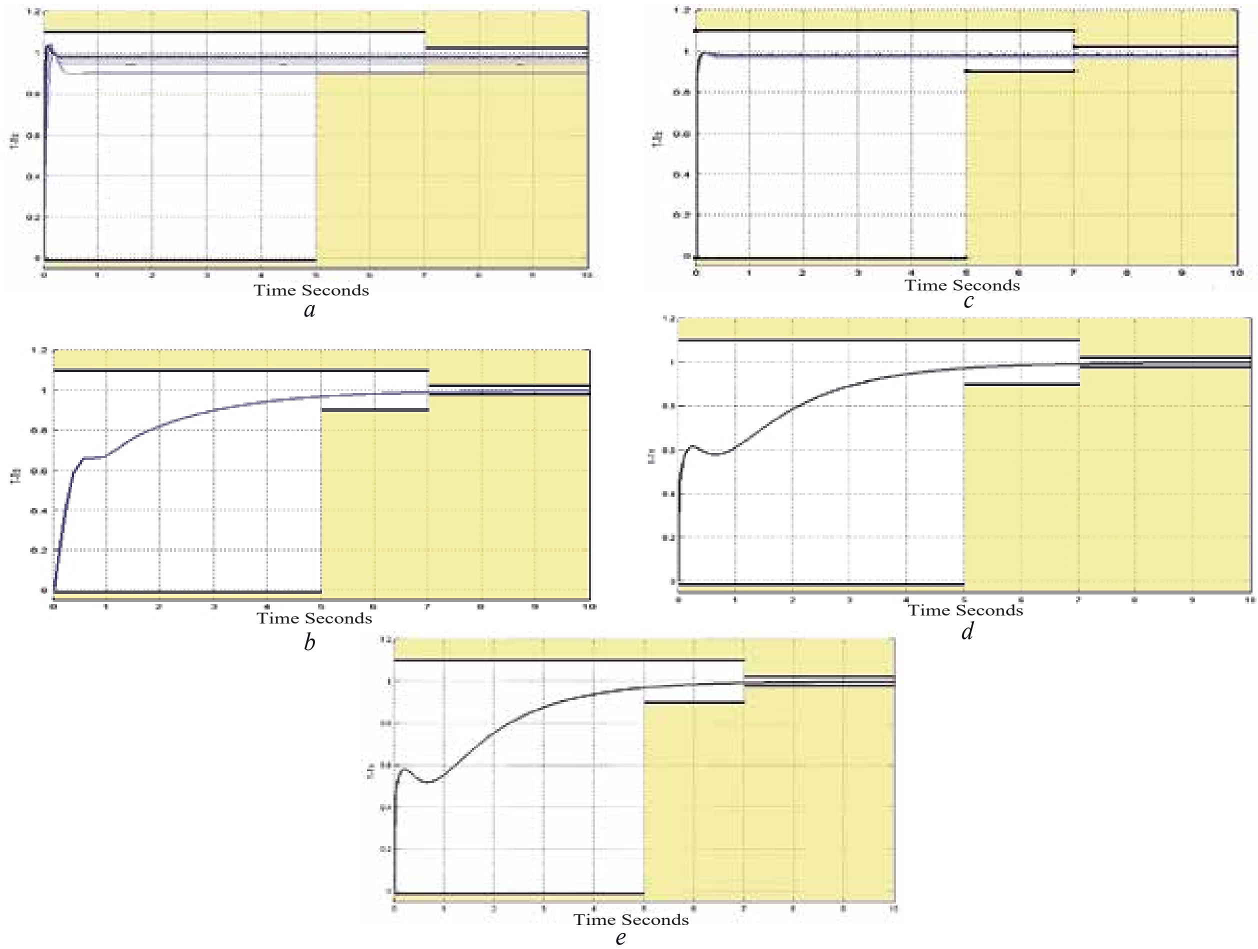


Fig. 18. The optimization progression of the temperature response of the CSTR control system with; a) P, b) PI, c), PD, d) PID, and e) 2-DOF-PID controllers

Table V. Comparative analysis of CSTR temperature response with various tuned controllers by using constraints optimization

Data	Unit	P	PI	PD	PID	2DOF	MPC
Rise time	sec	0.0172	2.918	0.0047	3.0859	3.2805	0.383
Overshoot	%	5.21	0	0.716	0.09	0	4
Peak value	ºF	1.03	0.998	0.991	0.9991	0.999	1.04
Peak time	sec	0.0509	10	0.115	10	9.95	0.7
Settling time	sec	0.131	5.655	0.0562	5.3737	5.3737	0.919
Final value	ºF	0.982	1	1	1	1	1
Offset	ºF	0.018	0	0.016	0	0	0
T	ºF	124.482	124.5	124.484	124.5	124.5	124.5

Also, the results presented in Table V clearly show that the method of tuning with constraints optimization of controllers efficiently provides temperature control for CSTR more than a Simulink tuner (presented in Table III) with small overshoot, good rise and settling times, and achieves the set-point without offset. It can be verified that due to imposed restriction the process presented a slower closed-loop response and a variation in the variable manipulated softer.

Conclusion

The CSTR process was extremely nonlinear and the modeling of the CSTR process was defined and applied. The model has been determined by empirically determining the method that extracts the actual process from the data. In the event of an uncontrolled process response, an enormous amount of steady-state error is made. To control the temperature inside the reactor different controllers (P, PI, PD, PID, 2-DOF-PID, and MPC) were implemented in this study. To monitor the servo response, the simulations had implemented, and the results are plotted. It has been found that MPC performs are best on the system with default gain parameters in terms of rising time, settling time, and offset.

Optimization of controller parameters by using Simulink Tuner and tuning with a method of optimizing constraints to get quick responses. The design having a 2-DOF-PID control has far-ranging implications as seen from the tests and study. Under two-DOF PID control, the system performs better with a very low percentage overshoot and good load disturbance rejection with a minimum settling time, both compared to traditional controllers. Also, as it is compared to other conventional controllers used in this study, the MPC controller has an overshoot of 4 percent and the minimum rise and settling times. It is found that the performance of 2-DOF-PID and MPC controllers is better than other conventional controllers for nonlinear systems such as the CSTR process. Besides, it must be pointed out that no issues in the convergence of the tuning method were faced, even though using a weak initial estimate. In this case, the use of tuning with constraints optimization method is strongly recommended to improve the time domain output stability of the controlled variable and to get quick responses.

Declaration of Competing Interest

The author declared no conflict of interests.

References

Allwin S, Biksha SN, Abirami S, Kala H and Udhaya AP (2014), Comparison of conventional controller with model predictive controller for CSTR process, *IJAREEIE* **3**(9): 11934-11941.

Araki M and Taguchi H (2003), Two-degree-of-freedom PID controllers, *IJCAS* **1**(4): 401-411.

Arivalagan M, Panda RC, Sivamani R and Dheepak R (2015), Design of MPC controller for CSTR, *IJAER*, **10**(33): 26251- 26254.

Åström KJ and Hägglund T (1995), PID controllers: theory, design, and tuning, 2nd Ed., Research Triangle Park, NC: Instrument society of America, pp 1-12.

Balaji V and Maheswari E (2012), Model predictive control techniques for CSTR using Matlab, *IJEET* **3**(3): 121-129.

Bayer F, Bűrger M, Guay M and Allgöwer F (2011), On state-constrained control of a CSTR, *IFAC Proceedings Volumes* **44**(1): 6079-6084. https://-doi.org/10.3182/20110828-6-IT-1002.02532

Buckbee G (2009), Best practices for controller tuning. PlantTriage, Exper Tune, Inc., p 2.

Deulkar AM, and Patil AB (2015), Temperature control of continues stirred tank reactor using model predictive controller, *IJIEEE* **3**(8): 57-60.

Fogler HF (2016), Elements of chemical reaction engineering. 5th Ed. (Pearson Education, Inc. NJ), pp 568-569.

Jibril M, Tadesse M and Alemayehu E (2020), Comparison of PID and MPC controllers for continuous stirred tank reactor (CSTR) Concentration control, *IRJMETS* **2**(4): 133-140.

Kishore C, Vandhana T, Hussain S and Raju SS (2012), Implementation of model predictive control and auto tuning based PID for effective temperature control in CSTR, *GRET* **1**(1): 84-89. doi.org/10.47893/ GRET. 2013.1018

Kumar M and Patel VV (2015), Tuning of two degree of freedom PID controller for second order processes, *IJSETR* **4**(5): 1543-1546.

LeBlanc SE and Coughanowr DR (2009), Process systems analysis and control, 3rd Ed., McGraw-Hill- Chemical Engineering Series, NY, p 7.

Hong M and Cheng S (2012), Nonlinear model predictive control based on LS-SVM, *GCIS*, **8**(4): 1373-1381.

Matlab website, *Two-Degree-of-Freedom PID Controllers*. Available online at: [https:// www. mathworks. com/help/control/ug/two-degree-of-freedom-2-dof-pid-controllers.html], Accessed on; 28/05/2020.

Neto CA and Embirucu M (2000), Tuning of PID controllers: An optimization-based method, *IFAC Proceedings Volumes* **33**(4): 367-372. doi.org/10.1016/S1474-6670 (17)38271-X

Prabhu K, Dharani P, Vijayachitra S and Kavya C (2021), Design Of Fuzzy–Pid Controller For Continuous Stirred Tank Reactor Plant, *NVEO-NATURAL VOLATILES & ESSENTIAL OILS Journal* **8**(5): 199-205.

Rahmat MF, Yazdani AM, Movahad MA and Zadeh SM (2011), Temperature control of a continuous stirrer tank reactor by means of two different intelligent strategies, *International Journal on Smart Sensing and Intelligent System* **4**(2): 244-267.

Seborg DE, Edgar TF, Mellichamp DA and Doyle III FJ (2011), Process dynamics and control, 3rd Ed., John Wiley & Sons, NJ, p 103.

Shyamalagowri M and Rajeswari R (2013), Modeling and simulation of non linear process control reactor-continuous stirred tank reactor, *IJAET* **6**(4): 1813-1818.

Vojtesek J and Dostal P (2005), From steady-state and dynamic analysis to adaptive control of the CSTR reactor. Procceding of 19th European Conference on Modeling and Simulation, Riga, Latvia, pp 591-598.