



e-ISSN: 2319-8753 | p-ISSN: 2347-6710

IJRSET

International Journal of Innovative Research in
SCIENCE | ENGINEERING | TECHNOLOGY

INTERNATIONAL JOURNAL OF INNOVATIVE RESEARCH

IN SCIENCE | ENGINEERING | TECHNOLOGY

Volume 11, Issue 12, December 2022

ISSN INTERNATIONAL
STANDARD
SERIAL
NUMBER
INDIA

Impact Factor: 8.118

 9940 572 462

 6381 907 438

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Laplace Representation of a Continuous Reactor

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ABSTRACT: Within industrial processes, especially in the organic chemical industry, the most widely used reactors are those that have a stirred tank that operates continuously, called continuous stirred tank type reactors. Among the applications of these reactors, we can highlight polymerization to produce plastics and paints, production of sodium acetate for the formation of soaps, production of nitrobenzene for explosives, production of ethyl glycol and propylene glycol for antifreeze, hydrolyzation of acetic anhydride for produce acetic acid. Due to the importance of these process units and the cost that their study from pilot plants implies this article focuses on the mathematical model of a continuously stirred tank type reactor scheme having computer simulation as a point of support.

KEYWORDS: Chemical reactor, Transfer function, Linear model, Steady state.

I. INTRODUCTION

A chemical reactor is a process designed in such a way that one or more chemical reactions take place inside it. This process is made up of a closed container, which has input and output lines for chemical substances, and is governed by a control algorithm.

Continuous stirred tank reactors (CSTR) are the most important process units in an industrial chemical process. In particular, the non-isothermal CSTR is the most widely applied reactor for many reactions of industrial interest.

Continuous stirred tank reactors (CSTR) work in a steady state, that is, their properties do not vary with time. This ideal model assumes that the reaction reaches maximum conversion at the instant the feed enters the tank, that is, that at any point in this equipment the concentrations are equal to those of the output stream.

In many situations, these ideal models are valid for real cases; otherwise, terms that reflect the deviation from ideality will have to be introduced in the material, energy and pressure balances. For example, the variation of the properties is due to phenomena of transport of matter or heat, the laws of Fick or Fourier can be introduced respectively. Like all chemical reactors, complete mix reactors (CSTR) have advantages and disadvantages, which we will see below:

Advantages

- They offer very good temperature control.
- They can be easily adapted to work with two phases.
- Its operating cost is low.
- They operate in stationary state, therefore, it is not required to stop production.
- They can be used in series.
- Its construction is simple.
- Ideal for processes that require homogenization.

Disadvantages

- Low conversion per unit volume.
- If possible, bypasses or extra channels are required, these will have poor agitation.
- They are not recommended for processes that are carried out at high pressures.
- Generally, they are used in the gas phase.

Paper is organized as follows. Section II describes some works about the treating of the mathematical model of continuous stirred tank reactor. The mathematical model development described by the balance of mass an energy is

given in Section III. Section IV presents experimental results showing the transfer function obtained. Finally, Section V presents conclusion.

II. PROCESS DESCRIPTION

The main functions of a chemical reactor are to ensure the type of contact or flow mode of the reactants inside the tank, to achieve a desired mix with the reactant materials; provide sufficient contact time between the substances and with the catalyst, to achieve the desired extension of the reaction; allow conditions of pressure, temperature and composition so that the reaction takes place to the degree and at the desired speed, taking into account the thermodynamic and kinetic aspects of the reaction.

The continuous stirred tank reactor (CSTR) consists of a nearly perfectly stirred tank, in which there is a continuous flow of reactant material, and from which reacted material is continuously emitted. The stirring condition is not that difficult to achieve as long as the liquid phase is not too viscous. The purpose of achieving good agitation is to achieve a good mixing of the materials inside the tank, to ensure that the entire volume of the container is used to carry out the reaction, and that there are no or remaining spaces. dead. It can be considered that the mixture is good, if the circulation time of a reactant element inside the tank is about one hundredth of the average time it takes for the same element to enter and leave the reactor. The schematic diagram of the reactor is shown in Fig.1.

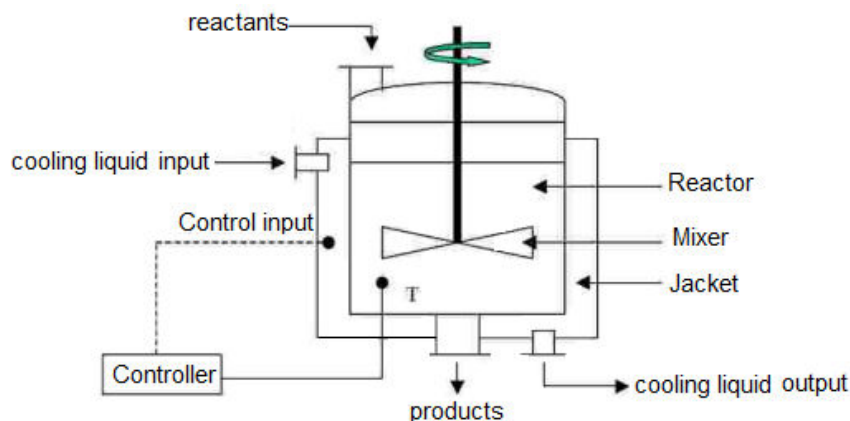


Fig1. 1. Schematic diagram of the reactor

Consider a CSTR in which an exothermic reaction ($A \rightarrow B$) takes place. The heat of the reaction is removed with water passing through a coil. The analysis of a CSTR reactor describes that the amount of heat generated by the exothermic reaction is a sinusoidal function of the temperature in the reactor (curve A) otherwise the heat removed by the cooling water is a linear function of the temperature. Consequently, when the CSTR is in a steady state, the heat produced by the reaction must be equal to that removed by the cooling water.

The three steady states of a CSTR are P1, P2, P3, where P1 and P3 are stable and P2 is unstable as shown in Fig. 2. To understand the concept of stability, let us consider the steady state P2. At this point the temperature is T_2 and the concentration of A is C_{A2} . If the feed temperature is increased, the temperature of the reaction mixture is T'_2 . At this temperature the heat generated by this reaction is (Q'_2) is more than the heat removed by the coolant (Q''_2), therefore the reactor temperature is higher, and the reaction rate increases. If the reaction rate is increased, the amount of heat produced by the exothermic reaction increases, leading to higher T and so on. Thus, a small increase in T_1 , the temperature of the reactor that was at point P2 goes to the steady state P3. Similarly, if T_1 decreases, the temperature of the reactor goes from point P2 to P1. In contrast, if we operate at steady states P3 and P1 and a disturbance is applied to the system, the reactor returns to its operating points P3 or P1.

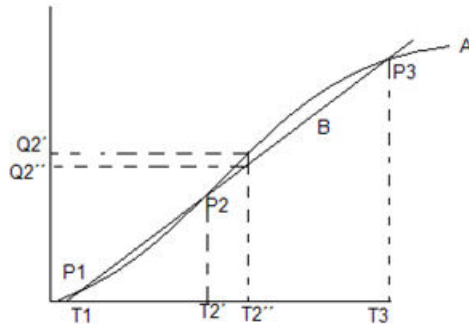


Fig. 2. Steady states for the CSTR

Generally, CSTRs operate in the unstable state, this is for the following reasons:

- At low temperatures, steady state P2, causes very low conversions because T1 is very low.
- At high temperatures, steady state P3, is very high, causing unsafe conditions, catalyst destruction for a catalytic reactor, product degradation etc.

In such cases, the reactor is operated at P2, and a controller is necessary to maintain the reactor at the steady state P2.

We consider a first-order, irreversible reaction $A \rightarrow B$ (with a rate constant k). The feed to the reactor contains C_{Ai} of A and an inlet temperature T_i and constant volumetric flow rate F . The product leaves at a flow rate equal to F . Mixing is assumed to be efficient, so the liquid content is homogeneous. This means that the composition and temperature are uniform throughout the reactor and the temperature and composition at the outlet of the reactor are T and C_A .

The mathematical model of this process is described by the balance of mass and energy of components A and B, however the amount of B present in the reactor is deduced from component A fed and that does not react with the reactor.

III. MODELING OF THE CSTR REACTOR

For the mass balance is required:

Accumulation rate of A in the reactor:

$$\frac{d(VC_A)}{dt}$$

Reactor Entry Velocity: FC_{Ai}

A muzzle velocity: FC_A

Rate of consumption of A per kVC_A chemical reaction

The balance per component of A is

$$\frac{d(VC_A)}{dt} = FC_{Ai} - FC_A - KVC_A$$

At constant reactor volume, equation (A) simplifies to:

$$\frac{dC_A}{dt} = -(K + \frac{1}{\theta})C_A + \frac{1}{\theta}C_{Ai}$$

where θ is the residence time of the reactor (D/F).

For the energy balance is required:

Speed of accumulation of Energy in the reactor:

$$\rho C_p \frac{d}{dt} [V(T - T^*)]$$

Input Energy Velocity:

$$\rho FC_p (T_i - T^*)$$

Output Energy Velocity:

$$\rho FC_p (T - T^*)$$

Rate of Heat Transfer through the refrigerant: QC



Rate of Heat Generation by Reaction: $(-\Delta H) kVC_A$

The density and heat capacity of the reacting material are represented by ρ and C_p , they are constant. T is a temperature data, and ΔH is the heat of reaction.

The energy balance is:

$$\frac{VdT}{dt} = F(T_i - T) + \frac{(-\Delta H_r)rV}{\rho C_p} - \frac{Q_c}{\rho C_p}$$

It amplifies to:

$$\frac{dT}{dt} = -\frac{1}{\theta}T + \beta k C_A + \frac{1}{\theta}T_i - X$$

where

$$\beta = \frac{-\Delta H}{\rho C_p}, \quad X = \frac{Q_c}{\rho C_p V}, \quad Q_c = \frac{UA_T}{\rho C_p V}(T - T_{H2O})$$

If the Arrhenius equation is introduced to the previous equations, it remains:

$$\frac{dC_A}{dt} = -\frac{1}{\theta}C_A - k_o e^{-\frac{E}{RT}} C_A + \frac{1}{\theta}C_{Ai}$$

$$\frac{dT}{dt} = -\frac{1}{\theta}T + \beta k_o e^{-\frac{E}{RT}} C_A + \frac{1}{\theta}T_i - X$$

Both equations contain nonlinear functions on T and C_A ; they are coupled and in this sense it is not possible to solve them independently.

This mode is nonlinear due to the presence of the nonlinear term $e^{-\frac{E}{RT}} C_A$, to linearize two equations, the nonlinear term is linearized around the term $(C_{Ao}$ and T_0).

$$e^{-\frac{E}{RT}} C_A \cong e^{-\frac{E}{RT_0}} C_{Ao} + \left[\frac{\partial(e^{-\frac{E}{RT}} C_A)}{\partial T} \right]_{(T_0, C_{Ao})} (T - T_0) + \left[\frac{\partial(e^{-\frac{E}{RT}} C_A)}{\partial C_A} \right]_{(T_0, C_{Ao})} (C_A - C_{Ao}) =$$

$$e^{-\frac{E}{RT_0}} C_{Ao} + \left(\frac{E}{RT_0^2} e^{-\frac{E}{RT_0}} C_{Ao} \right) (T - T_0) + e^{-\frac{E}{RT_0}} (C_A - C_{Ao})$$

Substituting the above approximation into equations, the linearized model for a non-isothermal CSTR reactor is obtained:

$$\frac{dC_A}{dt} = \frac{1}{\theta}(C_{Ai} - C_A) - k_o \left[e^{-\frac{E}{RT}} C_{Ao} + \frac{E}{RT_0^2} e^{-\frac{E}{RT}} C_{Ao} (T - T_0) + e^{-\frac{E}{RT}} (C_A - C_{Ao}) \right]$$

$$\frac{dT}{dt} = \frac{1}{\theta}(T_i - T) + \beta k_o \left[e^{-\frac{E}{RT}} C_{Ao} + \frac{E}{RT_0^2} e^{-\frac{E}{RT}} C_{Ao} (T - T_0) + e^{-\frac{E}{RT}} (C_A - C_{Ao}) \right] - \frac{UA_T}{\rho C_p V} (T - T_{H2O})$$

Deviation variables are made, assuming that T_0 and C_{Ao} are the steady state conditions for the CSTR by the input conditions C_{Ai0} , T_{i0} and T_{H2O} then equations become:

$$0 = \frac{1}{\theta}(C_{Ai} - C_{Ao}) - k_o e^{-\frac{E}{RT}} C_{Ao}$$

$$0 = \frac{1}{\theta}(T_{i0} - T_0) + \beta k_o e^{-\frac{E}{RT}} C_{Ao} - \frac{UA_T}{\rho C_p V} (T_0 - T_{H2O})$$

Substituting equations, we obtain:

$$\frac{dC_A}{dt} = \frac{1}{\theta} [(C_{Ai} - C_{Ai0}) - (C_A - C_{Ao})] - k_o \frac{E}{RT_0^2} e^{-\frac{E}{RT}} C_{Ao} (T - T_0) - k_o e^{-\frac{E}{RT}} (C_A - C_{Ao})$$



$$\frac{dT}{dt} = \frac{1}{\theta} [(T_i - T_{io}) - (T - T_o)] + \beta k_o \left[\frac{E}{RT_o^2} e^{-E/RT_o} C_{Ao} (T - T_o) + e^{-E/RT_o} (C_A - C_{Ao}) \right] - \frac{UA_t}{\rho C_p V} [(T - T_o) - (T_{H2O} - T_{io})]$$

Defining the derivation variables:

$$C_A' = C_A - C_{Ao} \quad C_{Ai}' = C_{Ai} - C_{Aio}$$

$$T' = T - T_o \quad T_i' = T_i - T_{io}$$

$$T_{H2O}' = T_{H2O} - T_{H2Oo}$$

Substituting:

$$\frac{dC_A'}{dt} = \frac{1}{\theta} (C_{Ai}' - C_A') - \left[\frac{k_o E}{RT_o^2} e^{-E/RT_o} C_{Ao} \right] T' - \left[k_o e^{-E/RT_o} \right] C_A'$$

$$\frac{dT'}{dt} = \frac{1}{\theta} (T_i' - T') + \beta k_o \left[\left(\frac{E}{RT_o^2} e^{-E/RT_o} C_{Ao} \right) T' + e^{-E/RT_o} C_A' \right] - \frac{UA_t}{\rho C_p V} (T' - T_{H2O}')$$

Rearrange the terms and you get:

$$\frac{dC_A'}{dt} + \left[\frac{1}{\theta} + k_o e^{-E/RT_o} \right] C_A' + \left[\frac{k_o E}{RT_o^2} e^{-E/RT_o} C_{Ao} \right] T' = \frac{1}{\theta} C_{Ai}'$$

$$\frac{dT'}{dt} + \left[\frac{1}{\theta} - \beta \frac{K_o E}{RT_o^2} e^{-E/RT_o} C_{Ao} + \frac{UA_t}{\rho C_p V} \right] T' - \left[\beta K_o e^{-E/RT_o} \right] C_A' = \frac{1}{\theta} T_i' + \frac{UA_t}{\rho C_p V} T_{H2O}'$$

Simplifying the notation:

$$a_{11} = \frac{1}{\theta} + K_o e^{-\frac{E}{RT_o}}$$

$$a_{12} = \frac{K_o E}{RT_o^2} e^{-\frac{E}{RT_o}} C_{Ao}$$

$$a_{21} = -\beta K_o e^{-\frac{E}{RT_o}}$$

$$a_{22} = \frac{1}{\theta} - \frac{\beta K_o E}{RT_o^2} e^{-\frac{E}{RT_o}} C_{Ao} + \frac{UA}{\rho C_p V}$$

$$b_1 = \frac{1}{\theta}$$

$$b = \frac{UA_t}{\rho C_p V}$$

The equations are transformed:

$$\frac{dC_A'}{dt} + a_{11} C_A' + a_{12} T' = b_1 C_{Ai}'$$

$$\frac{dT'}{dt} + a_{21} C_A' + a_{22} T' = b_1 T_i' + b_2 T_{H2O}'$$

The initial conditions are:

$$C_A'(0) = T'(0) = 0$$

The Laplace transform is applied:

$$(S + a_{11}) \bar{C}_A'(s) + a_{12} \bar{T}' = b_1 \bar{C}_{Ai}'(s)$$

$$a_{21} \bar{C}_A'(s) + (S + a_{22}) \bar{T}' = b_1 \bar{T}_i' + b_2 \bar{T}_{H2O}'$$

It reduces for $\bar{C}_A'(s)$ and \bar{T}'



$$C_A'(s) = \frac{b_1(s+a_{22})}{P(s)} C_{Ai}(s) - \frac{a_{12}b_1}{P(s)} \bar{T}_i(s) - \frac{a_{12}b_2}{P(s)\bar{T}_c(s)}$$

$$T'(s) = \frac{-a_{21}b_1}{P(s)} C_{Ai}(s) + \frac{b_1(s+a_{11})}{P(s)} T_i'(s) + \frac{b_2(s+a_{11})}{P(s)} T_{H_2O}'(s)$$

where

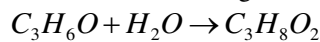
$$P(s) = s^2 + (a_{11} + a_{22})s + (a_{11}a_{22} - a_{12}a_{21})$$

In matrix form:

$$\begin{bmatrix} C_A'(s) \\ T'(s) \end{bmatrix} = \begin{bmatrix} G_{11}(s) & G_{12}(s) & G_{1B}(s) \\ G_{21}(s) & G_{22}(s) & G_{23}(s) \end{bmatrix} \begin{bmatrix} C_{Ai}(s) \\ T_i(s) \\ T_{H_2O}(s) \end{bmatrix}$$

IV. EXPERIMENTAL RESULTS

Consider the following exothermic reaction



It is a first order reaction, irreversible and elementary. The reaction rate from this equation is:

$$r_{C_3H_6O} = k_0 e^{-E/RT_0} C_{C_3H_6O}$$

where:

The activation energy is

$$E = 74426.8 \frac{kJ}{Kgmol}$$

The rate constant is

$$K_0 = 1.3235 \times 10^{14}$$

The gas constant is

$$R = 8.134 \frac{kJ}{Kgmol^\circ K}$$

The operating temperature

$$T_0 = 298.15K$$

The heat transfer coefficient

$$U = 1495 \frac{W}{m^2 \cdot K}$$

transfer area

$$A_t = 0.335m^2$$

The density

$$\rho = 36.14 \frac{Kgmol}{m^3}$$

The heat capacity

$$C_p = 84.57 \frac{kJ}{Kgmol^\circ K}$$

With these parameters the values of a_{11} , a_{12} , a_{21} , a_{22} are

$$a_{11} = 25.776$$

$$a_{12} = 1.634 \times 10^{-5}$$

$$a_{21} = -355.64$$

$$a_{22} = 0.1391$$

$$Gp(s) = \frac{13.837(s + 25.776)}{s^2 + 39.613s + 356.688}$$

The parameters that were used to find the transfer function are of a stable state, so this system under these conditions does not require a controller, since as mentioned above a CSTR has three stationary states. We remove a zero from this transfer function, leaving the following equation.

$$Gp(s) = \frac{13.837}{s^2 + 39.613s + 356.688}$$

In Fig. 3. it shows the step response the obtained transfer function in Laplace, we can observe that the system tends to steady state with quickly settle time.

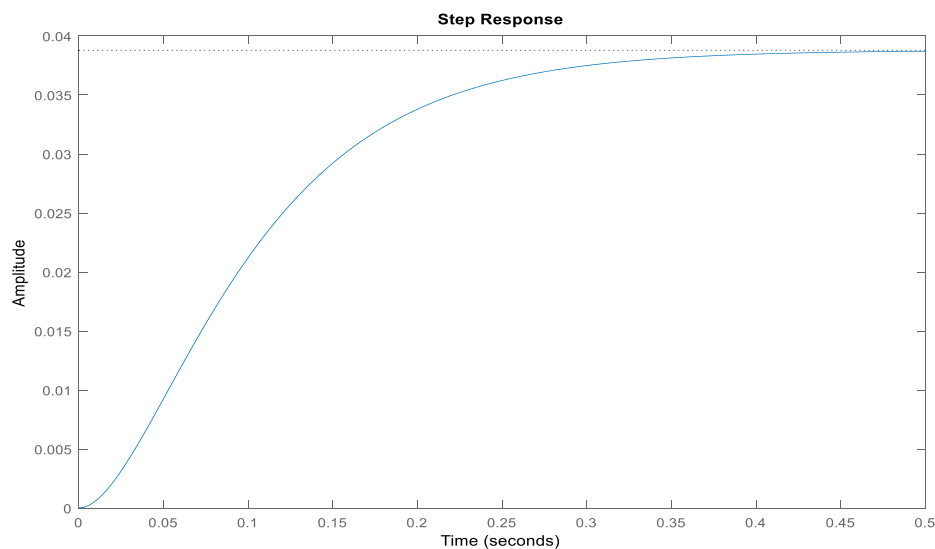


Fig.3.Step response of the reactor

V. CONCLUSION

The mathematical model of a CSTR type reactor was obtained through the differential equations that represent its dynamics; The reactor dynamics were fixed in its stable region and a feedback loop was applied to later simulate its response to a disturbance. A next stage of study would be to control the system in the unstable steady state to observe the behavior of the PID controller. In the case of the Bioreactor, the reaction speed of the microorganism would be non-linear and the model would have to be linearized and other parameters would be taken into account, such as the growth medium.

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