

MATHEMATICAL MODELLING AND SIMULATION OF A CONTINUOUS STIRRED TANK REACTOR

Ioan NAȘCU, Silviu FOLEA, Paula RAICA

*Technical University of Cluj-Napoca, Automation Department
Ioan.Nascu@aut.utcluj.ro*

Abstract: This paper presents the relevant practical and theoretical aspects of the mathematical modelling and simulation of a chemical reactor. The model problem of a single, irreversible, exothermic reaction taking place in a perfectly mixed continuously stirred tank reactor (CSTR) is presented. The dynamic model consists of differential material and energy balance. A study of the dynamical behaviour of a CSTR will show that this system can exhibit rather complex and interesting behaviour. A short background on the theory of transient concentration and temperature behaviour in a CSTR is presented, followed by an analysis of the results. The analysis includes model simulations in MATLAB SIMULINK.

Key words: continuous stirred tank reactor, modelling, simulation

1. INTRODUCTION

Chemical reactors are very important parts of chemical industry installations. The processes that take place in these reactors are very complex because of the chemical and mass transformations with high quantities of heat exchanged.

Many authors have extensively studied the model problem of an irreversible, exothermic reaction, taking place in a perfectly mixed continuously stirred tank reactor, and its extensions. The early literature was presented by Douglas [1972]; more recent review articles are those of Razon and Schmitz [1987], detailing the multiplicity and dynamic behaviour of chemically reacting systems, and [Bequette 1991], dealing with the nonlinear control of chemical processes. The ultimate goal of this paper was to understand the dynamical behavior of the model for further development of advanced control algorithms (predictive control, adaptive control).

2. MODELLING

The main goal of this chapter is to determine the dynamic state behavior of an exothermic, perfectly mixed, continuous stirred tank reactor (figure 1).

Assumptions:

- level in the reactor will be considered constant;
- time delay introduced by the pipe transportation from the actuator to the reactor is neglected;
- Flow-rate of cooling agent is considered high enough so that the temperature of this agent will remain constant.

In the conditions given above, the variables used in figure 1 can be explained as follows:

- q – output flow-rate (evacuation or residual flow-rate) [m^3/s];
- q_i – input flow-rate (feed flow-rate) [m^3/s];
- c_i – molar concentration of component A in the feed line [mol/m^3];
- c – molar concentration of component A in residue (output line) [mol/m^3];
- m_m – molecular mass [kg/mol];
- T_i – temperature of the input component [K];
- T – temperature of the reactor mixture [K];
- T_r – temperature of the cooling agent [K];
- V – volume of the mixture in the reactor [m^3].

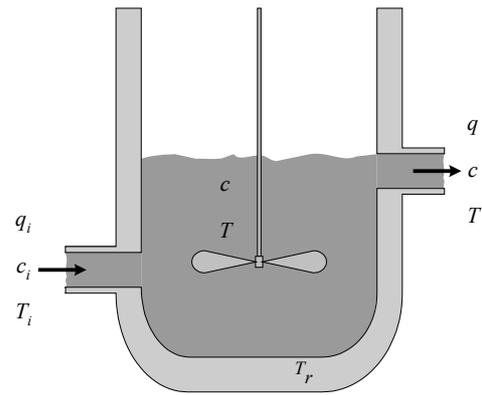


Figure 1

Considering that the reaction is isotherm ($T = \text{constant}$), the description of the reaction consists only of a mass balance:

$$d \frac{(m_m \cdot V \cdot c)}{dt} = m_m \cdot q \cdot c_i - m_m \cdot q \cdot c - m_m \cdot V \cdot r \quad (1)$$

or

$$V \frac{dc(t)}{dt} = q(t) \cdot c_i(t) - q(t) \cdot c(t) - V \cdot k \cdot c(t) \quad (2)$$

where $m_m V r$ is the production rate and $r = kc$ – reaction rate. $c_i(t)$ and $q(t)$ are considered inputs, while $c(t)$ is considered output.

Relation 2 is a nonlinear differential equation and therefore the solution of this equation is obtained through linearization around the steady state values of c_i^0, q^0 . The concentration of the input product in the residue is obtained $c^0 = (c_i^0 q^0) / (q^0 + V k)$ with the functional scheme given in figure 2.

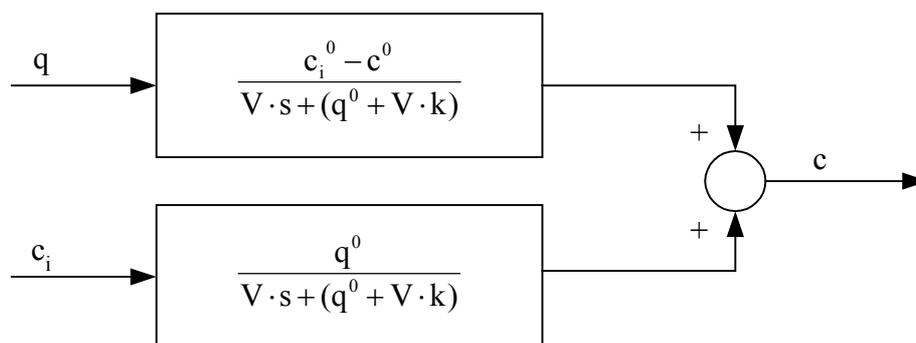


Figure 2.

In this linearized model the transfer functions of the two branches $c_i \rightarrow c$ and $q \rightarrow c$ are the equivalents of first order systems with time constant $\tau_1 = \tau / (1 + k \tau)$ and gain:

- $K_1 = (c_i^0 - c^0) / (q^0 + V k)$, for $q \rightarrow c$;
- $K_2 = q^0 / (q^0 + V k)$, for $c_i \rightarrow c$.

The $\tau = V/q$ constant is an important design parameter of a reactor, called the mixing time. In our case, the inertia of the chemical reactor is high and depends on the time given above and on the reaction rate. Two effects influence the dynamics of the process: mixing and chemical reaction. For low values of the reaction rate the most important

effect is given by the mixing delay. For a zero value of the reaction rate constant ($k=0$), meaning that no reaction takes place, all we have is a simple mixing process.

Static sensitivity of the output with respect to the input (given by the value of the static gain factor) decreases when the reaction rate increases. For $k=0$ we have $K_2=1$, and the output is completely sensitive to the input c_i .

Supposing that the reactor works in a non-isothermal state, besides mass balance, we have to take into consideration the energy balance. The thermal effects in these reactors are the result of the heat quantities introduced by the reactants, extracted through products and absorbed or generated during the reaction.

In the case of exothermic reactors, which we are going to analyze, the equation of heat balance is:

$$\rho \cdot V \cdot c_p \frac{dT(t)}{dt} = Q_p - Q_e \quad (3)$$

$$Q_p = (-\Delta H) \cdot V \cdot r = (-\Delta H) \cdot V \cdot k_0 \cdot e^{-E/RT(t)} \cdot c(t) \quad (4)$$

$$Q_e = \rho \cdot q(t) \cdot c_p \cdot T_i(t) - \rho \cdot q(t) \cdot c_p \cdot T(t) + k_T \cdot A \cdot [T_r(t) - T(t)] \quad (5)$$

where:

Q_p – heat evolved in chemical reaction [J/s],

Q_e – evacuated heat [J/s];

ρ – medium density of the product [kg/m^3];

c_p – medium specific heat [J/kgK];

ΔH – reaction enthalpy, specific to each mixture of reactants [J/mol];

$(-\Delta H) > 0$ for exothermic reaction

$(-\Delta H) < 0$ for endothermic reaction

A – thermal transfer surface of the cooling agent [m^2];

k_T – thermal transfer coefficient [$\text{W}/\text{m}^2\text{K}$].

As a conclusion, for a irreversible, exothermic reaction taking place in a perfectly mixed continuously stirred tank reactor presented in figure 1 we can adopt the nonlinear mathematical model:

$$\begin{aligned} V \frac{dc(t)}{dt} &= q(t) \cdot c_i(t) - q(t) \cdot c(t) - V \cdot k_0 \cdot e^{-E/RT(t)} \cdot c(t) \\ \rho V c_p \frac{dT(t)}{dt} &= \rho q(t) c_p T_i(t) - \rho q(t) c_p T(t) + k_T A [T_r(t) - T(t)] + (-\Delta H) V k_0 e^{-E/RT(t)} c(t) \end{aligned} \quad (6)$$

3. ANALYSIS AND SIMULATION

In this stage of development an analysis of the steady state would be useful. The steady state corresponds to the state of dynamic systems where we have no variation with respect to time or where we have periodic variations. In the following, we will consider a steady-state analysis of the reactors when the state is constant with respect to time. In this case, the concentration and temperature of the mixture are maintained constant even if chemical modifications, mass transfers and heat exchanges take place. The steady state can be computed setting the derivatives to zero. If we have a steady state in temperature then $dT/dt = 0$ and equation (3) becomes:

$$Q_p = Q_e$$

In relation (5) we note that $Q_e(T)$ is a straight line. To obtain the representation $Q_p(T)$ conform with relation (4) let us note that in figure 2:

$$c(T) = K_2(T)c_i^0 = q^0/[q^0 + V k(T)]c_i^0 = q^0/(q^0 + V k_0 e^{-E/RT})c_i^0 \quad (7)$$

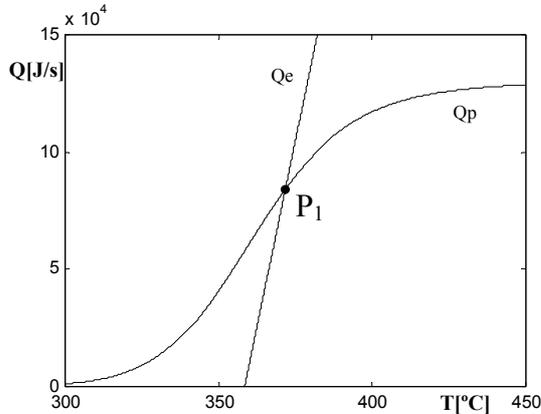


Figure 3.a.

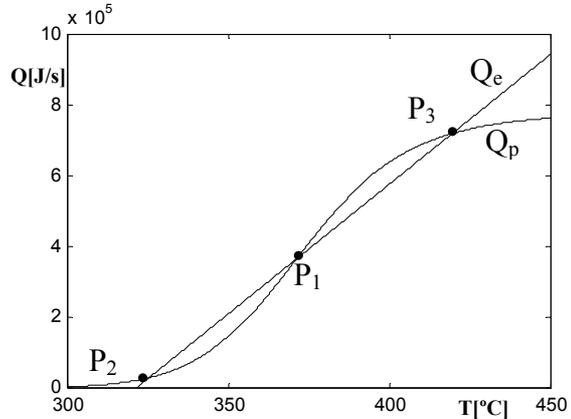


Figure 3.b.

The graphical representation of the two terms Q_e and Q_p is given in figure 3.a, while the independent variable is the temperature T of the mixture in the reactor. The following steady state values have been used:

$$\begin{aligned} r c_p = 1000, V = 1, k^0 = 10^{10}; E/R = 8330, hA = 5342, -\Delta H = 130, \\ q^0 = 1, c_i^0 = 1000, T_i^0 = 50 + 273, T_r^0 = 92 + 273. \end{aligned} \quad (8)$$

Modifying:

$$q^0 = 2, c_i^0 = 3000, T_r^0 = 48 + 273 \quad (9)$$

we obtain the graphics from figure 3.b. The measurement units are the standard ones. In steady state, the working point (P) results at the intersection of line $Q_e(T)$ with curve $Q_p(T)$. This point is stable only if the slope of $Q_e(T)$ is higher than the one of curve $Q_p(T)$, case in which the reactor can be cooled and brought back to the initial point when the temperature rises accidentally ($\Delta T > 0$) because $Q_e(T) > Q_p(T)$, the evacuated caloric flow-rate is higher than the produces one. If the slope of line $Q_e(T)$ at the intersection point is lower than the one of curve $Q_p(T)$ when the temperature rises accidentally ($\Delta T > 0$), $Q_p(T) > Q_e(T)$, respectively the produced caloric flow-rate is higher than the evacuated one, the temperature keeps rising. In consequence, the chemical reactions are intensified (considering exothermic reactions) and the temperature will rise and the working point will move to a new position where the slope of $Q_e(T)$ is higher than the one of curve $Q_p(T)$. Therefore, for picture 3.a results an intersection in point P1 ($T^0 = 371.6$) that is stable, while for figure 3.b, the working point P1 ($T^0 = 370.2$) is unstable and points P2 ($T^0 = 325.4$) and P3 ($T^0 = 419.5$) are stable.

In order to change the straight line (5) the following modifications can be made: either the temperature T_r of the cooling agent can be changed (a family of curves results, obtained through horizontal translation of the line), either the flow-rate of the same agent can be changed.

Returning to CSTR model given by relations (6) we will take into consideration the following bloc scheme:

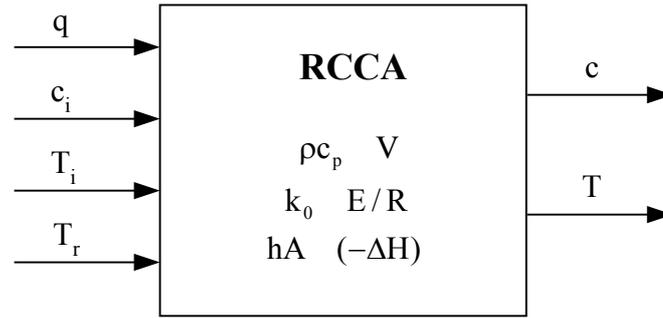


Figure 4

The output variables (controlled variables) are c (concentration of the component in the residue) and T (temperature of the mixture in the reactor), while perturbation variables are $\{q, c_i, T_i\}$ and T_r is the control variable.

In steady state, linearizing for instance around the working point P_1 from figure 3.a (numerical values given by (8)), we can obtain a state-space model of the form:

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y &= Cx + Du \end{aligned} \quad (10)$$

with $x^T = y^T = [c \ T]$, $u^T = [q \ c_i \ T_i \ T_r]$ and matrices A, B, C, D of the form:

$$A = \begin{bmatrix} -\frac{q^0}{V} - k_0 \cdot e^{-E/RT^0} & -k_0 \cdot e^{-E/RT^0} \frac{E c^0}{R T^{0^2}} \\ \frac{(-\Delta H)}{\rho c_p} k_0 \cdot e^{-E/RT^0} & -\frac{q^0}{V} - \frac{k_T A}{\rho V c_p} + \frac{(-\Delta H)}{\rho c_p} k_0 \cdot e^{-E/RT^0} \frac{E c^0}{R T^{0^2}} \end{bmatrix} = \begin{bmatrix} -2.8477 & -39.1244 \\ 0.2402 & -1.2558 \end{bmatrix}$$

$$B = \begin{bmatrix} \frac{c_i^0 - c^0}{V} & \frac{q^0}{V} & 0 & 0 \\ \frac{T_i^0 - T^0}{V} & 0 & \frac{q^0}{V} & \frac{k_T A}{\rho V c_p} \end{bmatrix} = \begin{bmatrix} 648.8340 & 1.0000 & 0 & 0 \\ -48.6770 & 0 & 1.0000 & 5.3420 \end{bmatrix}$$

(11)

$$C = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad D = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Given these conditions we will have:

$$\frac{C(s)}{T_r(s)} = \frac{-209}{s^2 + 4.103s + 12.973} \quad \frac{T(s)}{T_r(s)} = \frac{5.342s + 15.212}{s^2 + 4.103s + 12.973} \quad (12)$$

If the nonlinear model given by relations (6) is considered, there are two ways to simulate its dynamic behavior:

1. Using *ode* functions from MATLAB[®] (*cstrode.m* program)
2. Implementing in SIMULINK[®] the nonlinear model (*ctr.mdl* file – fig 5).

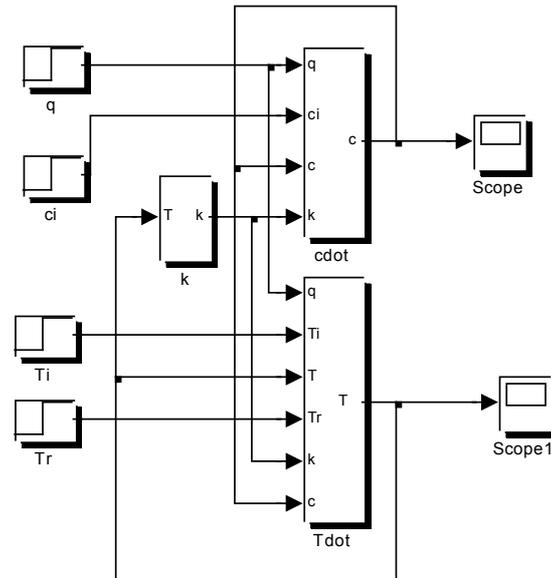
cstrode.m

```
tspan=0:0.01:5;
[tplo,Y]=ode23('rcca',tspan,[400; 105+273]);
plot(tplo,Y);
function Xdot=rcca(tplo,X);
```

```

rcp=1000; V=1; k0=10^10; EdR=8330; kTA=5342; mdH=130;
q=1; ci=1000; Ti=50+273; Tr=92+273;
c=X(1); T=X(2); if c<0, c=0; end;
k=k0*exp(-EdR/T);
cdot=(q*(ci-c)-V*k*c)/V;
Tdot=(rcp*q*(Ti-T)+kTA*(Tr-T)+mdH*V*k*c)/(rcp*V);
Xdot=[cdot;Tdot];
    
```

cstr.mdl



4. CONCLUSION

The purpose of this paper was to analyze the dynamical behavior of an irreversible, exothermic reaction in a continuous stirred tank reactor (CSTR). In general, CSTR are operated at steady state, but when certain specific parameters attain threshold values, the behavior of the reactor becomes transient. The most important reason for studying the dynamic behaviour of a CSTR is to understand the mechanisms by which thermal runaway occurs, so as to eliminate these phenomena in industry. The risk of thermal runaway may be reduced by using a good control strategy that changes one of the inflow parameters, e.g. the inflow temperature, inflow velocity, or inflow concentration, as a function of the outflow variables, usually the outflow temperature.

5. REFERENCES

- [1] Douglas J.M, [1972], Process Dynamics and control, Prentice Hall, Vol 1, pp.57;
- [2] Razon L.F, and Schmitz R.A, [1987], Multiplicities and instabilities in chemically reacting systems. A Review. Chemical Engineering Science, 42(5), pp.1005-1047
- [3] Bequette R.W, [1991], Nonlinear control of chemical processes: A review. Ind. Eng. Chem., 30, pp.1391-1413;
- [4] Sexton M.J, Forbes L.K, and Gray B.F, [1997], A study of the dynamics of a continuously stirred tank reactor with feedback control of the temperature. Dynamics and Stability of Systems, 12(2), pp. 89—107;