MODELING AND SIMULATION OF NON LINEAR PROCESS CONTROL REACTOR - CONTINUOUS STIRRED TANK REACTOR

M. Shyamalagowri[1], R. Rajeswari[2]
[1]Research Scholar, Assistant Professor Selection Grade-II / EEE, Erode Sengunthar Engineering College, Thudupathi, Erode, India
[2]Asst Prof (Senior) / EEE, Government College of Technology, Coimbatore, India

ABSTRACT
Chemical reactors are the most influential and therefore important units that a chemical engineer will encounter. To ensure the successful operation of a Continuous Stirred Tank Reactor (CSTR) it is necessary to understand their dynamic characteristics. A good understanding will ultimately enable effective control systems design. The aim of this paper is to introduce some basic concepts of chemical reaction systems modeling and develop simulation models for CSTR's. The descriptions of the non-linear and linear systems are derived. To describe the dynamic behavior of a CSTR mass, component and energy balance equations must be developed. This requires an understanding of the functional expressions that describe chemical reaction. A reaction will create new components while simultaneously reducing reactant concentrations. The reaction may give off heat or my require energy to proceed.

KEYWORDS: *CSTR (Continuous Stirred Tank Reactor), MATLAB, Modeling, Simulation, Nonlinearity.*

I. INTRODUCTION

Continuous Stirred Tank Reactor (CSTR) is a typical chemical reactor system with complex nonlinear dynamic characteristics. There has been considerable interest in its real time control based on the mathematical modeling. However, the lack of understanding of the dynamics of the process, the highly sensitive and nonlinear behavior of the reactor, has made difficult to develop the precise mathematical modeling of the system. An efficient control of the product concentration in CSTR can be achieved only through accurate model. Developing mathematical models of nonlinear systems is a central topic in many disciplines of engineering. Models can be used for simulations, analysis of the system's behavior, better understanding of the underlying mechanisms in the system, design of new processes and design of controllers. In a control system the plant displaying nonlinearities has to be described accurately in order to design an effective controller. In obtaining the mathematical model, the designer follows two methods. The first one is to formulate the model from first principles using the laws governing the system. This is generally referred to as mathematical modeling. The second approach requires the experimental data obtained by exciting the plant and measuring its response. This is called system identification and is preferred in the cases where the plant or process involves extremely complex physical phenomena or exhibits strong nonlinearities.

Obtaining a mathematical model for a complex system is complex and time consuming as it often requires some assumptions such as defining an operating point and doing linearization about that point and ignoring some system parameters.

Section I describes the introduction, section II explains the mathematical modeling, section III describes the CSTR system description, section IV explains the simulation results and discussion, section V explains the conclusion and section VI gives the references.

II. MATHEMATICAL MODELLING

A mathematical model is a description of a system using mathematical concepts and language. The process of developing a mathematical model is termed mathematical modeling. A model may help to explain a system and to study the effects of different components, and to make predictions about behavior. Mathematical modeling is the method of translating the problems from real-life systems into conformable and manageable mathematical expressions whose analytical consideration determines an insight and orientation for solving a problem and provides us with a technique for better development of the system. Using the high-level mathematical modelling methods is a powerful way of predicting and decision-making in financial markets.

Mathematical modeling is the art of translating problems from an application area into tractable mathematical formulations whose theoretical and numerical analysis provides insight, answers, and guidance useful for the originating application. Learning about mathematical modeling is an important step from a theoretical mathematical training to an application-oriented mathematical expertise, and makes the student fit for mastering the challenges of our modern technological culture.

There is a large element of compromise in mathematical modelling. The majority of interacting systems in the real world are far too complicated to model in their entirety. Hence the first level of compromise is to identify the most important parts of the system. These will be included in the model, the rest will be excluded. The second level of compromise concerns the amount of mathematical manipulation which is worthwhile. Although mathematics has the potential to prove general results, these results depend critically on the form of equations used. Small changes in the structure of equations may require enormous changes in the mathematical methods. Using computers to handle the model equations may never lead to elegant results, but it is much more robust against alterations. Mathematical modeling can be used for a number of different reasons. How well any particular objective is achieved depends on both the state of knowledge about a system and how well the modeling is done. This course – Mathematical Modeling - is meant to teach us how to transfer scientific, physical and mechanical problems into mathematical formulation using parameters to represent events.

III. CSTR SYSTEM DESCRIPTION

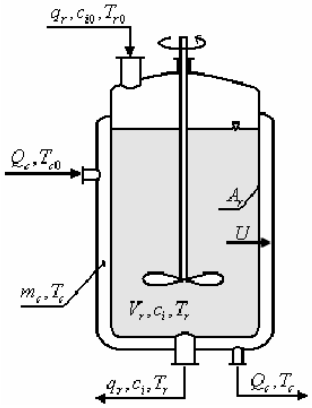

Fig.1 Schematic Diagram of the CSTR

Chemical reactors are generally the most important unit operations in a chemical plant. The CSTR is often used in dynamic modeling studies, because it can be modeled as a lumped parameter system. Consider a CSTR which is operating at a constant temperature (it is isothermal). The volume is also assumed constant. The reaction scheme consists of the following irreversible reactions. The feed stream contains only component A. The examined system is represented by Continuous stirred Tank Reactor (CSTR) which is widely used in the process industries. The Schematic diagram of CSTR is given in the figure no.1. The Continuous Stirred Tank Reactor is taken for nonlinearity identification process. It consists of a CSTR with a cooling jacket carrying out the Vander Vusse reaction scheme described by the following reactions:

$$A \xrightarrow{k1} B \xrightarrow{k2} C \text{----------(1)}$$

$$2A \xrightarrow{k3} D \text{----------(2)}$$

Here B is the desired product,
C and D are the undesired byproducts
k_1, k_2 and k_3 are the reaction rate constants.
In this reactor, a product A is to be converted to the desired product B, in an exothermic CSTR, but the product B is degraded to product C. In addition to this consecutive reaction, a high order parallel reaction occurs and A is converted to by product D. The mathematical model of this reactor is described by the set of four Ordinary Differential Equations (ODE) which come from material and heat balances inside the reactor.

$$\frac{dC_A}{dt} = \frac{q_r}{V_r}(C_{A0} - C_A) - k_1 C_A - k_3 C_A^2 \text{----------(3)}$$

$$\frac{dC_B}{dt} = -\frac{q_r}{V_r} C_B + k_1 C_A - k_2 C_B \text{----------(4)}$$

$$\frac{dT_r}{dt} = \frac{q_r}{V_r}(T_{r0} - T_r) - \frac{h_r}{\rho_r c_{pr}} + \frac{A_r U}{V_r \rho_r c_{pr}}(T_c - T_r) \text{----------(5)}$$

$$\frac{dT_c}{dt} = \frac{1}{m_c c_{pc}}(Q_c + A_r U(T_r - T_c)) \text{----------(6)}$$

Where $C_A \geq 0$, $C_B \geq 0$
In the set of equations t is the time, c are concentrations, T represents temperatures, c_p is used for specific heat capacities, q represents volumetric flow rate, Q_c is heat removal, V are volumes, ρ represents densities, A_r is the heat exchange surface and U is the heat transfer coefficient. Indexes $(.)_A$ and $(.)_B$ belongs to compounds A and B, $(.)_r$ denotes the reactant mixture, $(.)_c$ cooling liquid and $(.)_0$ are feed (inlet) values. The concentrations C_A and C_B, reactor temperature T and the coolant temperature T_c constitute the four states of the plant.
The model of the reactor belongs to the class of lumped parameter nonlinear systems. Nonlinearity can be found in reaction rates (k_j) which are described via Arrhenius law:

$$k_j(T_r) = k_{0j} \cdot \exp\left(\frac{-E_j}{RT_r}\right), for\ j = 1,2,3 \text{----------(7)}$$

Where k_0 represent pre-exponential factors and E are activation energies.
The reaction heat (h_r) in the equation (2) is expressed as:

$$h_r = h_1 k_1 c_A + h_2 k_2 c_B + h_3 k_3 c_A^2 \text{----------(8)}$$

Where h_j means reaction enthalpies.

Rate of flow of energy in / out.

This is given by mass flow * specific heat (C_P) * Temperature difference. If the mass flow rate and the specific heat are constant the datum temperature will disappear in the energy balance expression.

Heat of reaction.

This is the difference in energy required to break the bonds in the reactants when compared to the energy required to break the bonds in the products. The heat of reaction (ΔH) is negative for an exothermic reaction and positive for an endothermic reaction. In other words, if a reaction is exothermic then heat is given out and if it is endothermic then heat is taken from the system.

Rate of change of energy (E).

When deriving a model that is to be used to study process dynamics as well as the implementation and testing of process control strategies, the energy balance is generally posed in terms of "rate of change of temperature with respect to time".

Arrhenius temperature dependence.

The effect of temperature on the reaction rate k is usually found to be exponential,
$k = k_0 e^{-E/RT}$
where k_o a pre-exponential (or Arrhenius) factor, E the activation energy, T is the reaction temperature and R the gas law constant.

Table 1: PARAMETERS OF THE REACTOR

$k_{01} = 2.145 \cdot 10^{10}$ min^{-1}	$k_{02} = 2.145 \cdot 10^{10}$ min^{-1}	$k_{03} = 1.5072 \cdot 10^{8}$ min^{-1}mol^{-1}
$E_1/R = 9758.3$ K	$E_2/R = 9758.3$ K	$E_3/R = 8560$ K
$h_1 = -4200$ kJ.kmol^{-1}	$h_2 = 11000$ kJ.kmol^{-1}	$h_3 = 41850$ kJ.kmol^{-1}
$V_r = 0.01$ m^3	$\rho_r = 934.2$ kg.m^{-3}	$c_{pr} = 3.01$ kJ.kg^{-1}.K^{-1}
$U = 67.2$ kJ.min^{-1}m^{-2}K^{-1}	$c_{pc} = 2.0$ kJ.kg^{-1}.K^{-1}	$A_r = 0.215$ m^2
$c_{A0} = 5.1$ kmol.m^{-3}	$T_{r0} = 387.05$ K	$U = 67.2$ kJ.min^{-1}m^{-2}K^{-1}
$m_c = 5$ kg	$c_{B0} = 0$ kmol.m^{-3}	

This reaction describes the chemical conversion, under ideal conditions, of an inflow of substance A to a product B. For controlling the heat inside the reactor, a heat exchanger with a coolant flow is used. To simplify the problem the following assumptions are taken:

- The liquid in the reactor is ideally mixed.
- The density and the physical properties are constant.
- The liquid level h in the tank is constant, implying that the input and output flows is equal: Q1 = Q2.
- The reaction is first order with a temperature relation according to the Arrhenius law.
- The shaft work can be neglected.
- The temperature increase of the coolant over the coil can be neglected.

It suffices to know that within the CSTR two chemicals are mixed and react to produce a product compound A at a concentration $C_A(t)$, with the temperature of the mixture being T(t). The reaction is exothermic and producing heat which slows down the reaction. By introducing a coolant flow-rate $Q_c(t)$, the temperature can be varied and hence the product concentration controlled. C_A is the inlet feed concentration, Q is the process flow-rate, T and T_C are the inlet feed and coolant temperatures, respectively, all of which are assumed constant at nominal values. The reaction is exothermic. The reactant is solvated in an organic solvent. The reacting mixture properties can be approximated to be that of the solvent. The heat of reaction, fluid mixture density and heat capacity can be considered to be temperature invariant and constant. The CSTR has been designed such that a heat exchanger maintains the feed temperature to a design temperature (To) irrespective of seasonal variation of temperature which may result in changes in the storage tank temperature (To'). It can be considered that the inlet concentration can change with time. However, the volume of liquid in the reactor and the inlet volumetric flow rate to the reactor can be considered to be constant.

Modeling the rate of heat transfer through a cooling coil / jacket

Equation models the rate of heat removal through a cooling coil or jacket as 'Q (J / s)'. Adjusting 'Q' (via manipulation of the coolant flow) will regulate temperature in a CSTR. Therefore to develop a more realistic model of the system Q must be related to the flow rate through the coil or jacket. To develop the model a number of assumptions are made:

- Density and specific heat of the coolant are constant.
- Coolant dynamics are be ignored (they are assumed fast when compared to the temperature dynamics of the liquid in the CSTR).
- The area of the coil multiplied by the overall heat transfer coefficient is approximated.
- The logarithmic mean temperature difference is approximated using an arithmetic mean.

IV. SIMULATION RESULTS AND DISCUSSION

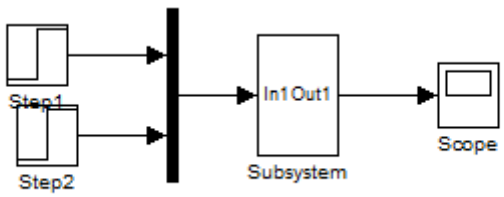

Fig.2 Simulation Setup for Steady state analysis of CSTR

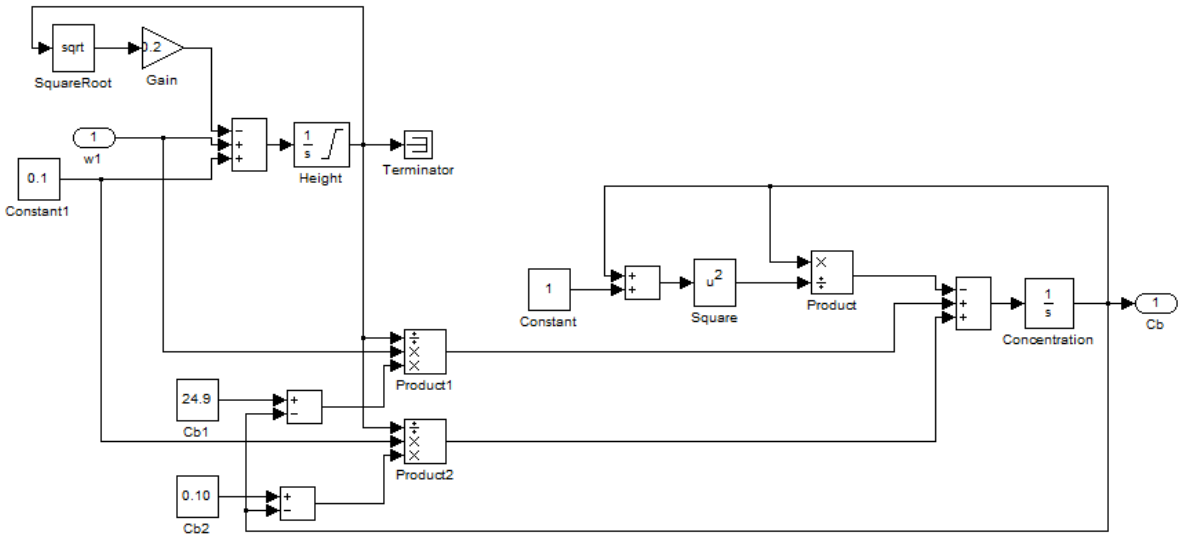

Fig.3 Simulation Set up of Modeling of CSTR

The simulation results present the step response of the non linear process reactor – Continuous Stirred Tank Reactor. The simulation work was carried out in MATLAB software. The variation in the output shows the system performance affected by nonlinearities. The concentration of product A and B are the two output parameters and volumetric flow rate q & heat removal rate Q are the two input parameters. The simulation results presents the two output results.

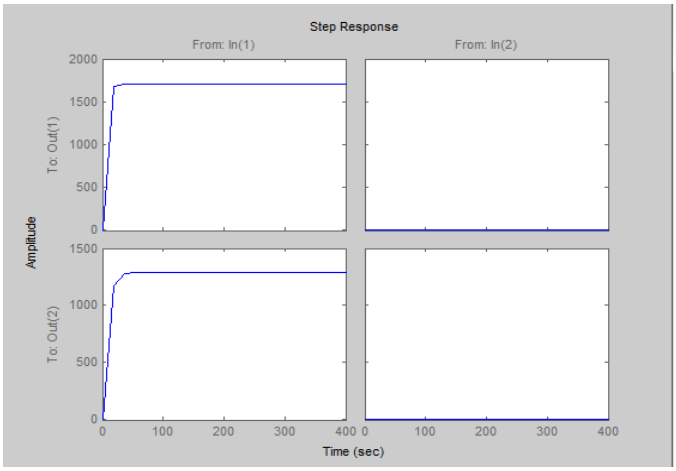

Fig 4. Simulation result of CSTR using MATLAB Software

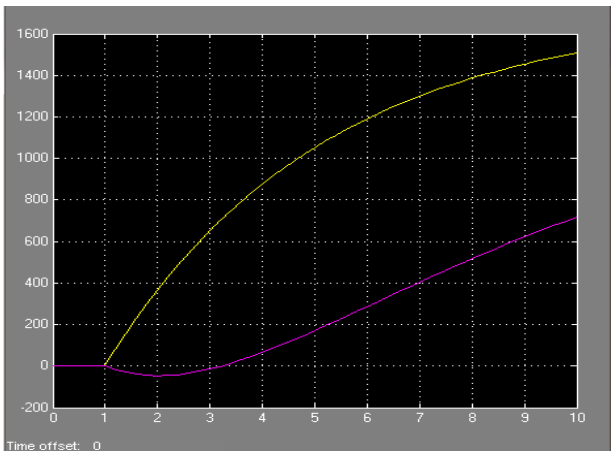

Fig 5. Simulation result of CSTR using MATLAB Simulink Software

V. CONCLUSION

If a reliable model is not available, it is quite difficult to design a controller producing desired outputs. When the data set does not represent the whole operating range adequately, the model to be obtained will not be as robust. Traditional modeling techniques are rather complex and time consuming when we incorporate entire dynamics of the process. In the present work, modeling of CSTR was carried out with mass balance and energy balance equations. The models formulated capture the nonlinearity present in the CSTR. The models thus developed can be used in de signing model based control schemes which offers robust controller performance. A modified dynamic structure model was developed in this work. This model takes into account the presence of acid and bases in the reaction with ions which depend on chemical reactions of acid and bases concentrations feeds. In addition, the concentrations effect of acid and bases on the system were included. Model simulations indicate that it is capable of predicating reactor performance indicators as well as calculating the changes of ions through chemical of the reaction. The model presented in this work was compared with two previously available models and results of the proposed model were compared with experimental data of neutralization process. From its observed accuracy, we can conveniently use this model as a predictive tool to study the effects of operating, kinetic and hydrodynamics parameters on the reactor performance. The model developed here will also be used in model based prediction control to control the reactor which is part of our future work.

REFERENCES

[1]. Srinivas Palanki, Soumitri Kolavennu, (2003), Simulation of Control of a CSTR Process, Int. J. Engng Ed. Vol. 19, No. 3, pp. 398±402.
[2]. Ivan Zelinka, Jiri Vojtesek and Zuzana Oplatkova, (2006), Simulation study of the CSTR reactor for control Purposes, Proceedings of 20th European Conference on modeling and Simulation.
[3]. Suja Malar.R.M, Thyagarajan.T (2009), Modeling of Continuous Stirred Tank Reactor using Artificial Intelligence Techniques, International Journal of simulation model.
[4]. Balaji.V, Vasudevan.N, Maheswari.E(2008), MATLAB simulation for Continuous Stirred Tank Reactor, The Pacific Journal of Science and Technology, Vol. 9, no. 1.
[5]. Bequette, B.W. (2003). Process Control: Modeling, Design and Simulation, Prentice Hall, Upper Saddle River**.**
[6]. Sukanya R.warier, Sivanandamvenkatesh "Design of controller based on MPC for a conical tank system",(ICAESM-2012).
[7]. Tuan. T. Q., Minh. Phan Xuan. Adaptive Fuzzy Model predictive control for non-minimum phase and uncertain dynamical nonlinear systems, Journal of Computers, vol. 7, no. 4, 2012, pp. 1014 to 1024.
[8]. Qiao Ji-Hong, Wang Hong-Yan. Backstepping Control with Nonlinear Disturbance Observer for Tank Gun Control System, Control and Decision Conference (CCDC), 2011 Chinese, 2011, pp. 251 to 254.
[9]. Hong Man, Cheng Shao. Nonlinear model predictive control based on LS-SVM Hammersteinwiener model, Journal of Computational Information Systems, vol. 8, no. 4, 2012, pp. 1373 to 1381.

AUTHORS

M. Shyamalagowri received the B.E degree in Electrical and Electronics Engineering from KSR College of Technology, Thiruchengode in 2001 and M.E., Control Systems from PSG College of Technology, Coimbatore in 2006. She is currently working for Ph.D degree in the area of Control Systems at Anna University of Technology, Coimbatore. Her area of interest is Control Systems, Process Control. She is working as an Assistant Professor in EEE Department in the Erode Sengunthar Engineering College having the experience of 10 years 8 months.

R. Rajeswari received the B.E. (EEE) Degree from TCE, MK University in the year 1995 and M.E. (Power System Engineering) from TCE, MK University in the year 1998. She has completed the Doctoral Degree from Anna University, Chennai in the area of Power System Protection in the year 2009. Her area of interest is Power System Engineering. Presently she is working as Asst Prof (Senior) / EEE at Government College of Technology, Coimbatore.