System Identification Using Predictive Controller Case Study: Continuous Stirred Tank Reactor

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ABSTRACT

In the last decades, a substantial amount of research has been carried out on identification of nonlinear processes. Dynamical systems can be better represented by nonlinear models, which illustrate the global behavior of the nonlinear process reactor over the entire range. CSTR is highly nonlinear chemical reactor. A compact and resourceful model which approximates both linear and nonlinear component of the process is of highly demand. Process modeling is an essential constituent in the growth of sophisticated model-based process control systems. Driven by the contemporary economical needs, developments in process design point out that deliberate operation requires better models. The neural network predictive controller is very efficient to identify complex nonlinear systems with no complete model information. Closed loop method is preferred because it is sensitive to disturbances, no need identify the transfer function model of an unstable system. In this paper identification nonlinearities for a nonlinear process reactor CSTR is approached using neural network predictive controller.

Keywords: Continuous Stirred Tank Reactor, Multi Input Multi Output, Neural Networks, Chebyshev Neural Networks, Predictive Controller.

INTRODUCTION

Several information exists for explaining the nonlinear performance of processes such as CSTRs, distillation columns, evaporators and biotechnological processes. Nonlinearity behavior in the process control reactor occurs from various parameters such as temperature dependence of reaction rates [1]. It may also result from process limitations such as valve limits, leading to input saturation (i.e., flow rate manipulation) or from physical constraints on output variables (e.g., mole fractions of chemical species) [2], [3]. Optimization and control of process systems usually requires a precise process model [4]. Essential first principles models can be difficult to build up if the original process is not well understood [5]. The resulting fundamental models have numerous unknown parameters and severe complexity. As contemporary chemical processes are constantly faced with the requirements of becoming safer, more reliable, and more economical in operation, the need for a rigorous, yet practical, approach for the design of effective chemical process control systems that can meet these demands becomes increasingly apparent [8]. However, the control design problem is highly non trivial because most chemical processes are essentially Multi-Input Multi-Output (MIMO) and nonlinear, and the use of controllers only designed on the basis of the approximate linearized process can direct to traditional, besides reduced, control performances. In addition, the unavoidable presences of physical constraints on the process variables and in the capacity of control actuators not only limit the nominal performance of the controlled system, but also can influence the stability of the overall system [10]. Process nonlinearity is one of the most important factors in system identification problems that plays significant role in identifying a model for a system from measured input/output data, without necessarily knowing anything about the physical laws controlling the system [11].

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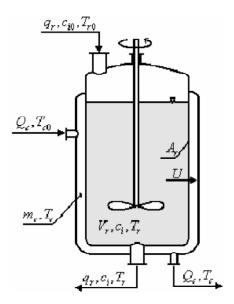## CSTR SYSTEM DESCRIPTION

Figure 1: Schematic Diagram of the CSTR

The Continuous stirred Tank Reactor (CSTR) is widely used in the process industries. The Schematic diagram of CSTR is given in the figure 1. The nonlinear process control reactor (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:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \tag{1}$$

$$2A \xrightarrow{k_3} D \tag{2}$$

Here B is the required 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 transformed to the desired product B, in an exothermic CSTR, but the product B is degraded to product C. In addition to this successive 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) is derived from material and heat balances inside the reactor.

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

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

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

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

Where $C_A \geq 0$, $C_B \geq 0$

In the differential equations, t represents time, c represents 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:

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

Where k_0 represent pre-exponential factors and E are activation energies.

The reaction heat (h_r) in the equation (2) is expressed as:

$$h_r = h_1 k_1 c_A + h_2 k_2 c_B + h_3 k_3 c_A^2 \tag{8}$$

Where h_j means reaction enthalpies.

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.

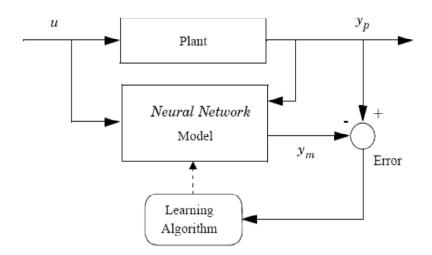## SYSTEM IDENTIFICATION

Figure 2: System Identification Block Diagram

System identification is mostly used in engineering and non-engineering areas. The block diagram of the system identification is given in figure 2. According to different classification methods they can be divided into non-parametric model identification and parametric model identification or online identification and offline identification. There are three principles of identification: least square method, the gradient correction method and the maximum likelihood method. The identification system described in this paper is the least square offline parametric identification system. Due to the complexity and diversity of the real system, the actual modeling problem from data acquisition to model establishment is difficult to complete by manual because it need repeatedly questing and the amount of calculation is quite huge. The System Identification Toolbox of MATLAB can simplify the computation process and improve the efficiency of identification.

The first stage of predictive control is to train a neural network to represent the forward dynamics of the plant. The neural network plant model uses previous inputs and previous plant outputs to predict future values of the plant output. The structure of the neural network plant model is given in the following figure.3. This network can be trained offline in batch mode, using data collected from the operation of the plant. System identification based on MATLAB is highly resourceful. Primarily, a second-order system is built with System Simulation Toolbox of SIMULINK, and then the parameters of the system are identified by use of System Identification Toolbox. The computation process is very straightforward and the identification system is direct-viewing and easy to adapt.
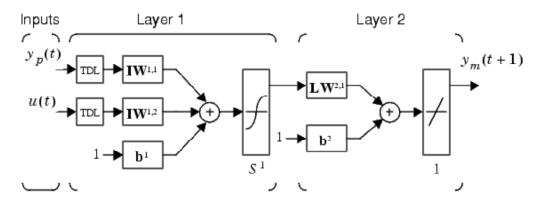

Figure 3: Structure of Neural Network Plant Model

In nonlinear predictive control, there usually exist two components, a nonlinear model to predict the behavior of the system, and an optimization algorithm to generate the control command to minimize the performance function (which is highly influenced by current and predicted errors). If artificial neural networks are used as nonlinear model; the controller is called "neuro-predictive". In neuro-predictive control, second-order derivative-based optimization methods, particularly, Levenberg-Marquardt methods are employed to achieve a better performance. Using such optimization methods, rather than steepest descent (first order ones), leads to better performance of control system; although, they need much more computation in comparison to first-order methods, as an important drawback.

NEURAL NETWORK PREDICTIVE CONTROL

Neural networks have been applied very effectively in the identification and control of dynamic systems. The neural network predictive controller that is implemented in the Neural Network Toolbox uses a neural network model of a nonlinear plant to predict future plant performance. The controller then calculates the control input that will optimize plant performance over a specified future time horizon. The first step in model predictive control is to determine the neural network plant model (system identification). In feedback control, as the most common type of control, the control command is generated using the error which has already occurred, whereas, in predictive control the predicted error is utilized to generate control command to avoid the error before appearing to do so a model (for predict the system's response) and a control algorithm (to generate the control command) are needed.

SIMULATION RESULT

The Proposed neural network predictive controller based nonlinearity identification on the Nonlinear Chemical Reactor CSTR was carried out. The Simulation results shows that the NN identification is the best approach for successful nonlinearity identification of CSTRs, because obtained model has good capability to predict the step response of the process. In the architecture of the NN Plant model 7 hidden layers have been constructed. 8000 training samples with the sampling interval of 0.2 was carried in the NN Training stage with control weighting factor ρ as 0.05 and Search Parameter α as 0.001

The Simulation results of Plant Input and Plant Output of CSTR is given in the figure 4 and 5, Validation performance result is given in the figure.6, Training State Result is given in the figure 7, Training data for NN Predictive Control is given in figure 8, Validation data for NN Predictive Control is given in figure 9 and system response is given in the figure 10 were presented in this paper.

Algorithm progressed

Training Function   =   Levenberg Marquardt (trainlm)

Performance   =   Mean Square Error (mse)

Data Division Specified (divideind)

Progress

No of Epochs   :   7 iterations

Time taken for the Progress   :   0:00:00

Gradient   :   0.000961

Mu   :   0.000100

Validation checks   :   6

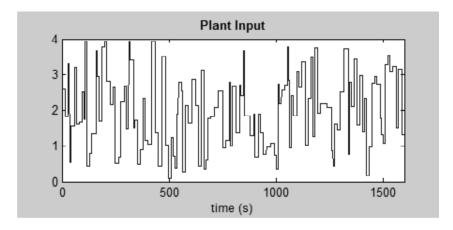## Simulation results of Plant Input and Plant Output of CSTR
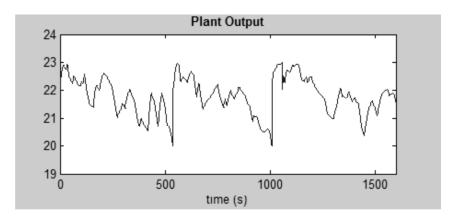
Figure 4: CSTR Plant Input

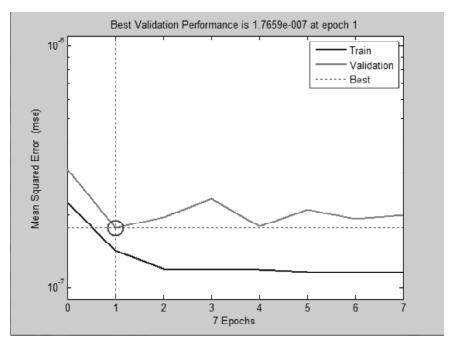**Figure 5: CSTR Plant Output**

Validation Performance Simulation Result

Figure 6: Validation Performance of NN Identifier

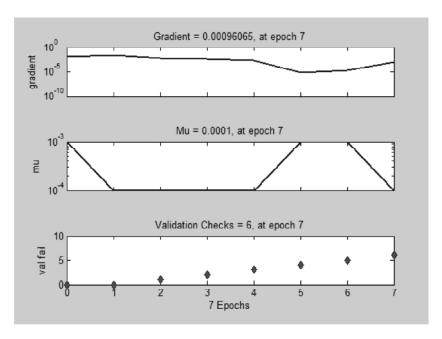## Training State Simulation Result

Figure 7: Training State of NN Identifier
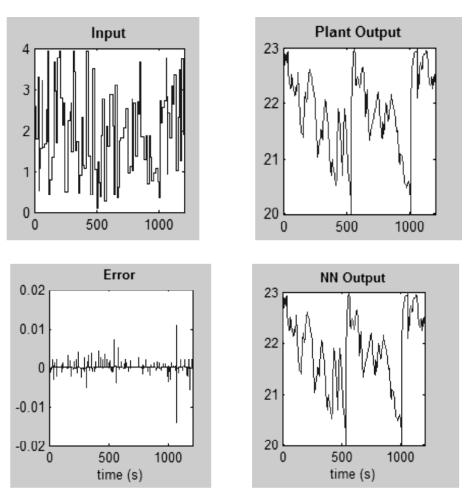
Training Data for NN Predictive Control

Figure 8: Simulation Result of Training Data of CSTR with NN Predictive Control
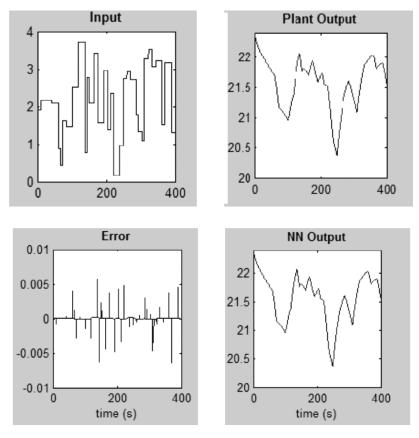
Validation Data for NN Predictive Control

Figure 9: Simulation Result of Validation Data of CSTR with NN Predictive Control
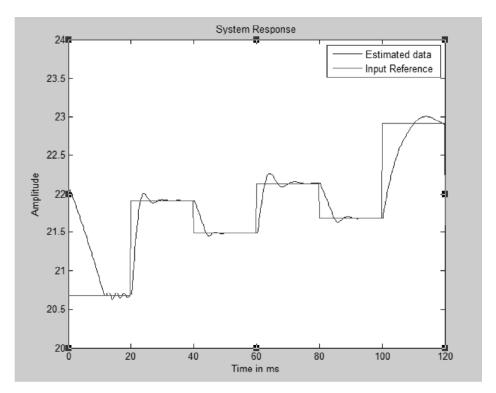
System Response

Figure 10: Nonlinearity Identification of CSTR with NN Predictive Control

CONCLUSION

In this paper, an application of a neural network based identification approach to a CSTR is presented. It is processed with NN-based identification method and nonlinear model predictive controllers with the ability of rejecting slowly varying unmeasured disturbances are applied. The need to control nonlinear multivariable processes of increasing complexity creates challenges for control engineers. One of the problems for control is the difficulty in the identification of an accurate mathematical model of the process. To address this issue, identification approaches have been getting considerable concentration in recent years. In this context, neural networks (NNs) are excellent candidates to deal with identification problems due to their functional approximation capabilities and the availability of effective learning algorithms. Use of mathematical models are fundamental for analysis of system behavior including various scientific and engineering applications like controller design, forecasting, simulation, failure detection and fault diagnosis. A large class of dynamical systems can be represented with good approximation by linear models which cannot reproduce dynamical regimes which result from system's nonlinear interactions. Nonlinear models will be required to capture these effects and this in turn leads to the complex problem associated with identifying accurate nonlinear models from plant data. This paper presents the use of chebyshev neural network models (CNN) with Levenberg Marquardt training scheme to identify the process. The performance of the proposed identification approaches is evaluated on a highly nonlinear time-varying multivariable continuous stirred tank reactor (CSTR) benchmark problem. Simulation results demonstrate the good performances of all identification approaches.

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