Performance of Neural Network Inverse-Model-Based Control (NN-IMBC) Strategy Versus Conventional Dual Mode Control (DMC) Strategy in Batch Reactors

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Abstract

Neural Network Inverse-Model-Based Control (NN-IMBC) and Dual-Mode Control (DMC) strategies are used to track the optimal reactor temperature profiles and their performance is evaluated through a few robustness tests. A complex exothermic batch reaction scheme is used as a case study. The optimal reactor temperature profiles are obtained by solving optimal control problems off-line using Control Vector Parameterisation (CVP) and Successive Quadratic Programming (SQP) techniques. Both strategies are evaluated in tracking both the constant and dynamic optimal set points. Neural Network estimator is embedded to the strategy as the on-line estimator to estimate the amount of heat released by the chemical reaction. Both NN-IMBC and DMC are found to be well performed in tracking both constant and dynamic set points. However NN-IMBC is more practical and easier to be implemented in term of tuned parameters needed compared to DMC. No tuned parameter is needed in NN-IMBC while in DMC seven tuned parameters are needed. NN-IMBC also promises robust controller if it is trained with a wide range of the reactor temperature covering all possible conditions of the process.

Introduction

Batch reactor is the common type of industrial reactor especially used for production of small volume and expensive products. It is suitable to cater the fluctuations of market condition of various products due to its flexibility in operation. However it is an inherently unsteady-state process, where composition and temperature change with time. Therefore modelling of such reactor results to a system of Differential Algebraic Equations (DAEs). A batch reactor can be controlled in terms of either the reactor temperature or coolant flow or jacket temperature (Cott and Macchietto, 1989). The optimal control profiles can be generated by formulating and solving a dynamic optimisation problem (Aziz and Mujtaba., 2002; Luus and Okongwu, 1999). However,

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designing controllers to implement and track the optimal control profiles or the set points is an important area of research especially for inherently dynamic batch processes.

The Neural Network based controllers were applied by previous researchers in controlling the batch reactor temperature (Galvan et al., 1992; Dirion et al., 1996 and Galvan and Zaldivar, 1998, Aziz et al., 2000). However, there is no effort has been made to compare the performance of Neural Network Inverse-Model-Based Control (NN-IMBC) strategy with the dual-mode control (DMC) strategy in batch reactors.

In this work, both control strategies i.e. NN-IMBC and DMC are implemented to track the optimal temperature profiles of exothermic batch reaction and their performances are evaluated and compared. To further investigate the robustness of both control strategies, a few robustness tests are carried out. The on-line neural network based estimator is also embedded in this NN-IMBC strategy to estimate the heat release, Q at any given period of time. Throughout the work, the multi-layered feed forward neural network has been used.

A complex exothermic batch reaction is considered in this work. NN-IMBC and DMC strategies are applied to track the optimal reactor temperature which maximise the conversion to the desired product in fixed batch time. The optimal temperature profiles are obtained by solving a maximum conversion problem (optimal control problem) which become the set points (both constant and dynamic set points) to be tracked by the controllers (Aziz et al., 2000). Control Vector Parameterisation (CVP) technique is used to pose the optimal control as Non-linear Programming Problem (NLP) which is solved using a Successive Quadratic Programming (SQP) based optimisation technique.

Dual-Mode Control (DMC) Strategy

Dual-mode control (DMC) strategy is commonly used strategy in batch reactors that have initial heat-up (i.e. for exothermic reaction). DMC strategy is combination of on-off and conventional control type strategy. First, maximum heating (on) is applied until the reactor temperature is within a specified degree of the set point and then maximum cooling (off) is applied when the temperature has reached its final desired set point. At this point, standard feedback controllers are switched on and used to maintain the temperature (constant or dynamic set points). In the standard DMC strategy, the PID controller is normally used.

The DM control strategy consists of a sequence of control actions, each one carried out after the reactor has reached a certain condition. The sequence of operations is as follows:

1. Full heating is applied until the reactor temperature is within a certain percent (E_m) of its set point temperature.

2. Full cooling is then applied for a certain period of time (TD-1).

3. The jacket set point temperature (T_{Jsp}) of controller is then set to the pre-load temperature (PL) for a certain period of time (TD-2).

4. A temperature controller (PID) is cascaded to the jacket temperature controller and its set point is set to T_{sp}.

There are two steps applied in order to tune the DM control strategy. First, PID tuning parameters were tuned by performing an open-loop step response test. The Cohen and Coon method was then applied to estimate the value of the tuning parameters (K_c, τ_I and τ_D). However the tuning parameters have been fine-tuned to make the control less drastic (through a few simulation runs with small changes on the estimated tuning parameters value). Second, the remaining four constants (E_m, TD-1, TD-2 and PL) were determined by running a series of simulation runs. The details of DMC control strategy and its tuning can be found in Liptak (1986).

Neural Network Inverse-Model-Based Control (NN-IMBC) Strategy

Internal model control (IMC) strategy is one of the many control strategies that can be applied to various chemical process plants. It promises to offer better control and reliability compared to other control strategies (Hussain, 1999). In this scheme, both the forward and inverse models are used directly as elements within the feedback loop. Here we named it as NN-IMBC strategy.

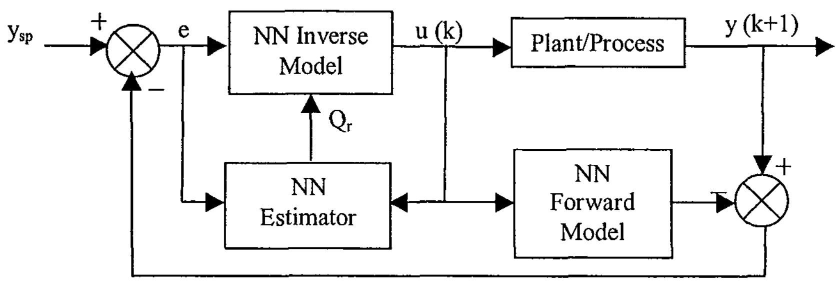

Figure 1: Neural Network Inverse-Model-Based Control (NN-IMBC) Strategy

The NN inverse model is utilised in control strategy by simply cascading it with the controlled system or plant. In this case the neural network acting as the controller, has to learn to supply at its output, the appropriate control parameters, u(k) for the desired targets, y_{sp} at its input. In addition, the forward model is placed in parallel with the plant, to cater for plant model mismatches and the error between the plant output and NN forward model is subtracted from the set point before being feedback into the inverse model. The inverse and forward models obtained a priory will be incorporated in this NN-IMBC strategy. In figure 1 the plant/process is represented by a first principle based batch reactor model.

Forward Model

In this NN-IMBC strategy, forward modelling approach is used to predict the future value of the reactor temperature, T, which is known as NN forward model. The input/output pattern for this forward model is shown in figure 2. There are two sets of data have been used for training and one set is used for validation.

	Q_r (k-1)	Q_r (k)	▩ Output
T_J (k-2)	T_J (k-1)	T_J (k)	▭ Input
	T (k-1)	T (k)	T (k+1)

Figure 2: Input/output patterns for forward model in NN-IMBC strategy

Inverse Model

Inverse model is basically the neural network structure representing the inverse of the system dynamics at the region of the training or identification. During training the network is fed with the required future or reference output together with the past inputs and past outputs to predict the current input or control action, *u(k)* (figure 3). Here, control action, *u(k)* is jacket temperature, T_J(k). This trained network represents the inverse model of the system. The assignment of the input nodes is same as that of forward model but with the prediction of *y(k+1)* replaced by the control input, *u(k)* as the network input.

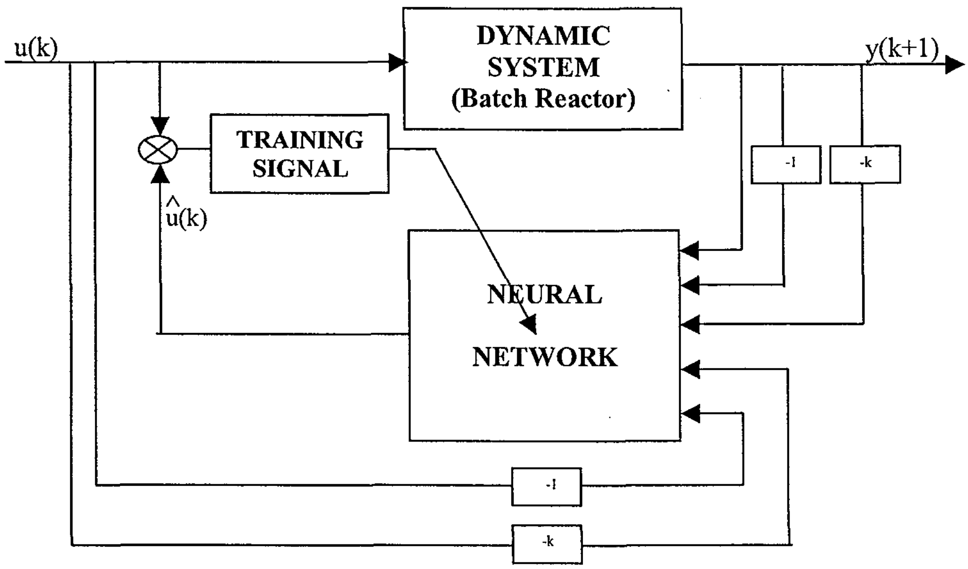

Figure 3: Method for the training of the inverse model for control

The input/output pattern for this inverse model (for the batch reactor under consideration) is shown in figure 4. It is to be noted that at any k, T_{sp} (k+1) and T_{sp} (k+2) are also known in advance. There are two sets of data have been used for training and one set is used for validation.

T_J (k-2)	T_J (k-1)	T_J (k)		
	Q_r (k-1)	Q_r (k)		
	T (k-1)	T (k)		
		T_{sp} (k)	T_{sp} (k+1)	T_{sp} (k+2)

▩ Output

□ Input

Figure 4: Input/output patterns for inverse model

Case Study

Figure 5 shows the jacketed batch reactor of our interest. Here the reaction scheme is the same as that used by Cott and Macchietto (1989), which is:

$$A + B \rightarrow C$$
$$A + C \rightarrow D$$

where A, B are raw materials, C is the desired product and D is the waste product.

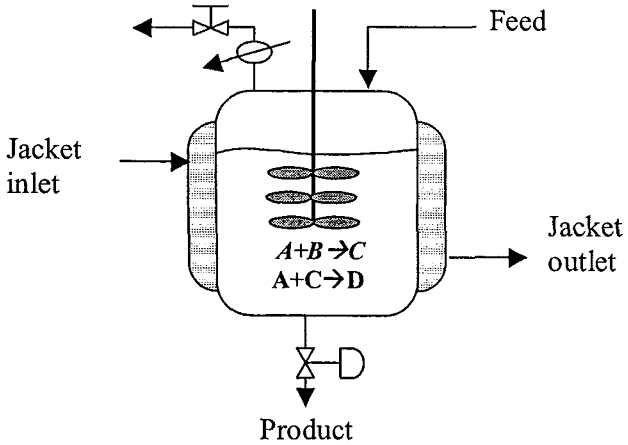

Figure 5: Jacketed batch reactor system

Model Equations

The model equations for the batch reactor can be written as:

$$\frac{dM_A}{dt} = -R_1 - R_2 \tag{1}$$

$$\frac{dM_B}{dt} = -R_1 \tag{2}$$

$$\frac{dM_C}{dt} = +R_1 - R_2 \tag{3}$$

$$\frac{dM_D}{dt} = +R_2 \tag{4}$$

$$\frac{dT_r}{dt} = \frac{(Q_r + Q_j)}{M\ C_{pr}} \tag{5}$$

$$\frac{dT_j}{dt} = \frac{(T_{jsp} - T_j)}{\tau_j} - \frac{Q_j}{V_j \rho_j C_{pj}} \tag{6}$$

$$R_1 = k_1 M_A M_B \tag{7}$$

$$R_2 = k_2 M_A M_C \tag{8}$$

$$k_1 = \exp\left(k_1^1 - \frac{k_1^2}{(T_r + 273.15)} \right) \tag{9}$$

$$k_2 = \exp\left(k_2^1 - \frac{k_2^2}{(T_r + 273.15)} \right) \tag{10}$$

$$Q_r = -\Delta H_1 R_1 - \Delta H_2 R_2 \tag{11}$$

$$M_r = M_A + M_B + M_C + M_D \tag{12}$$

$$C_{pr} = \frac{C_{PA} M_A + C_{PB} M_B + C_{PC} M_C + C_{PD} M_D}{M_r} \tag{13}$$

$$Q_j = UA(T_j - T_r) \tag{14}$$

All the parameter and constant values used in the model and control equation are given in Table 1.

Here, an off-line dynamic optimisation problem is solved to find the optimum temperature profile that will maximise the product "C" and minimise the by-product "D". Two runs were carried out; RUN1 uses one control interval (time) and RUN2 uses three fixed control intervals. The batch time is 120 minutes and the initial values of [M_A, M_B, M_C, M_D, T_r, T_j] are [12.0, 12.0, 0.0, 0.0, 20.0, 20.0] respectively. The reactor temperature is used as the controlled variable and is bounded between 20 and 100°C. The manipulated variable, T_j is bounded between 20 and 120°C.

The results (optimal temperature profiles) for both runs are then used as the set points to be tracked by NN-IMBC and DMC. The results are summarised in Table 2.

Table 1: The constant parameter values of the model and control equation

$C = 167.3$ kJ/kmol°C	$C = 1.8828$ kJ/kg°C	$V = 0.6921\ m^3$	$k^1 = 20.9057$
$C_{PC} = 217.6$ kJ/kmol°C	$C_{Pj} = 1.8828$ kJ/kg°C	$A = 6.24\ m^2$	$k_1^2 = 10000$
$C_{PD} = 334.7$ kJ/kmol°C	$U = 40.84$ kJ/min.m^2.°C	$\Delta t = 0.2$ min	$k_2^1 = 38.9057$
$\Delta H = -41840.0$ kJ/kmol	$\rho = 1000.0$ kg/m^3	$\tau = 3.0$ min	$k_2^2 = 17000$
$\Delta H = -25104.0$ kJ/kmol		$W_r = 1560.0$ kg	

Results and Discussion

Table 2: Summary of the results

Run	Off-line Optimum Temperature Profile	Off-line product
1	Temperature,°C: 92.46 Switching time,min: t = 0, 120.0	6.5126
2	Temperature,°C: 92.83, 91.17, 93.41 Switching time, min: t = 0, 40.0, 80.0, 120.0	6.5171
	DMC Tuning Parameters	
$E_m = 5.0\%$ PL = 46 °C TD-1 = 2.8 min TD-2 = 2.4 min	$K_c = 26.54$ min $\tau_I = 2.87$ min $\tau_D = 0.43$ min	

In Table 2, it can be seen that by using three control intervals, the amount of product achieved is slightly higher than that obtained using one control interval. The responses of the NN-IMBC and DMC for RUN1 and RUN2 are shown in figure 6 and 7 respectively. It can be seen that both the NN-IMBC and DMC were able to track the constant and dynamic set points very well. This fact was supported by the small amount of offset produced by both controllers and the amount of desired product obtained on-line (after implementing NN-IMBC and DMC). For both runs, the products were within 3% of that obtained by off-line dynamic optimisation (amount of product is about 6.34 for both runs). However in tracking the dynamic set points, the NN-IMBC was less sluggish in control action as compared to the DMC. Despite of less sluggish in control action, the NN-IMBC shows a bit drastic changes in the controller action. This is due to the use of piecewise constant (constant over a time interval) value of T_J in the training of NN-IMBC. T_J values were obtained by solving the following optimisation problem:

$$\min_{T_J} \quad \sum_{j=1}^{N} (T_r - T_{rsp})_j$$

Subject to: constraints (model equations etc.)

N is the number of intervals within the batch time of interest.

The drastic changes in control action can be overcome if smaller time intervals for calculating T_J are used. Despite this shortcoming, implementation of the NN-IMBC is still practical and easy because it does not require any tuned parameters compared to DMC which need seven tuning parameters.

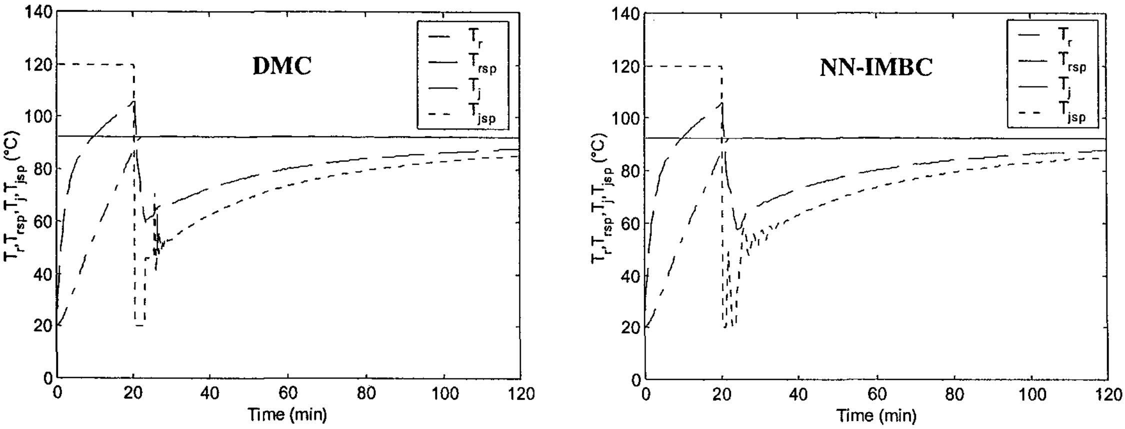

Figure 6: DMC and NN-IMBC responses for constant set point (RUN1)

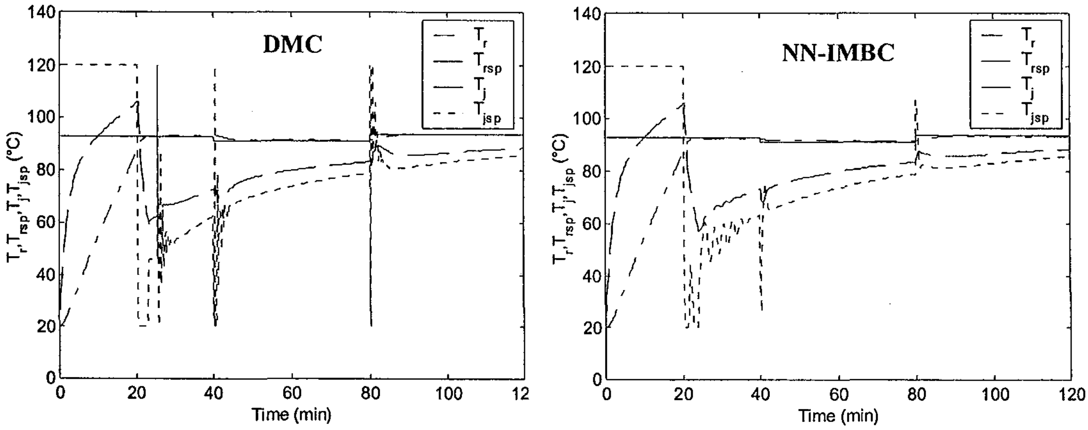

Figure 7: DMC and NN-IMBC responses for dynamic set points (RUN2)

Robustness Test

The robustness of the NN-IMBC and DMC applied in this case study has been tested. Three tests were carried out by changing the process parameters. In all tests the controllers were used to control an operation where some of the conditions have been changed from their true values. In the first test (TEST1), the heat of reactions was increased by 25%. In the second test (TEST2) the heat transfer coefficient is reduced by 40% of its original value. The third test (TEST3) involves 30% reduction in the molar (or mass) of reactants. In all tests, a constant reactor temperature set point (RUN1, Table 2) is to be tracked.

In TEST1 and TEST2, both NN-IMBC and DMC strategies were found unable to accommodate the changes (result to great overshoot response). In fact, the response of NN-IMBC is worst (greater overshoot) than the DMC. It is due to the inherent property of neural networks i.e. it is good in interpolation but not in extrapolation. The capability of the NN-IMBC is solely dependent on the range of the parameter values used for training and in this work, it was trained between the reactor temperature range of 90 and 95°C only. However in TEST3 the changes were within the limit of the training therefore the NN-IMBC performed better than DMC in accommodating the changes.

Both NN-IMBC and DMC have shown very similar responses in tracking the constant and dynamic set points. However, NN-IMBC is more practical and easier in term of tuning parameters needed. It has very high potential to be applied as a robust control strategy but must be trained very well and the training range should cover all possible conditions that can happen to the system or process.

Conclusions

Neural Network Inverse-Model-Based Control (NN-IMBC) and dual-mode control (DMC) strategy were designed and implemented to track the optimal reactor temperature profiles using a complex reaction scheme in a batch reactor. The optimal control problem has been formulated and solved to obtain the optimum temperature profiles (both constant and dynamic set points for both strategies) to maximise the amount of the desired product. The amount of the desired product obtained on-line by using the NN-IMBC and DMC is within 3% of the target values. Robustness of both strategies was tested by changing process parameters like heat transfer coefficient, heats of reactions and mass/molar rate of reactants. The NN-IMBC and DMC were found to perform well in tracking both set points. NN-IMBC promises robust controller if it is trained with a wide range of the reactor temperature covering all possible conditions of the process and is much easier to implement compared to other controllers because no tuned parameter is needed while the DMC needed seven tuned parameters.

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