Proceedings of the 17th World Congress
The International Federation of Automatic Control
Seoul, Korea, July 6-11, 2008

Reliable Multi-Objective On-line Re-Optimisation Control of Batch Processes Based on Bootstrap Aggregated Neural Networks

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Abstract: The paper presents a reliable multi-objective re-optimisation control strategy for batch processes based on bootstrap aggregated neural networks. Bootstrap aggregated neural networks not only give better generalisation performance than single neural networks but also provide model prediction confidence bounds. In order to overcome the problem of unknown disturbances, on-line re-optimisation is carried out to amend the control policy for the remaining batch duration. In addition to the process operation objectives, the reliability of model prediction is incorporated in multi-objective optimisation in order to improve the reliability of the obtained optimal control policy. The standard error of the individual neural network predictions is taken as the indication of model prediction reliability. The proposed method is demonstrated on a simulated fed-batch process.

1. INTRODUCTION

Batch or semi-batch processes are suitable for the responsive manufacturing of high value added products (Bonvin, 1998). In the operation of batch processes, it is usually desirable to meet a number of objectives concerning product quality and economics of plant operations. These objectives are usually conflicting to each other and their relative importance usually changes with market conditions. Multi-objective optimisation control can be utilised to maximise the profit from batch process manufacturing.

The effectiveness of multi-objective optimisation depends on the accuracy of the process model. Developing detailed mechanistic models is usually very time consuming and may not be feasible for agile responsive manufacturing. Data based empirical models, such as neural network models (Ahmad and Zhang, 2006) and nonlinear partial least square models (Qin and McAvoy, 1992; Li et al., 2005; Zhao et al., 2006), and hybrid models (Tian et al., 2001) have to be utilised. Bootstrap aggregated neural networks have been shown to possess better generalisation capability than single neural networks (Sridhar et al., 1996; Zhang et al., 1997) and are used in this paper to model batch processes. An additional feature of stacked neural networks is that they can also provide prediction confidence bounds indicating the reliability of the corresponding model predictions (Zhang, 1999). Due to model-plant mismatches, the "optimal" control policy calculated from a neural network model may not be optimal when applied to the actual process (Zhang, 2004). Thus it is import that the calculated optimal control policy should be reliable. Zhang (2004) proposes a reliable optimal control approach for batch processes through incorporating model prediction confidence into the optimisation objective function in a single objective optimisation framework. However, single objective optimisation may not be efficient in handling multiple process operating objectives. Mukherjee and Zhang (2006) present a reliable off-line multi-objective optimisation control method where model prediction reliability is incorporated as additional objectives in the multi-objective optimisation framework.

An important concern for the optimisation of fed-batch processes is the presence of unmeasured disturbances and model plant mismatches which tend to degrade the performance of off-line computed optimal control profile. The computed optimal profile is not "optimal" when it is applied to the actual process. The most common disturbances are due to the variation in raw materials, reactive impurities, and reactor fouling etc. The lack of availability of robust on-line sensors for monitoring the progress of the batch quality variables further complicates the problem. The quality variables are only accessible via delayed off-line laboratory analysis and are often measured at the end of a batch. The open loop operations of batch reactors thus provide a degraded "optimal" performance. Two important strategies that have been reported are the mid-course correction policy (Yabuki and MacGregor, 1997) and a variation of it, the repeated on-line re-optimisation control strategy (Xiong and Zhang, 2005). The concept is to build data based empirical models which can predict the end point quality value and execute mid course control adjustments designed at reducing the predicted deviations of the final product quality variables from their respective target values. The on-line re-optimisation policy is implemented using sampled system state values during the early stage of a batch to re-calculate the control profile for the remaining batch stage.

This paper presents a reliable multi-objective on-line re-optimisation control technique for batch processes. The batch length is divided into three process operation stages, the initial batch stage, the re-optimisation control profile calculation stage and, finally, the implementation stage for the on-line re-optimised control profile. In the initial batch

stage, system state values are recorded via off-line laboratory analysis at predetermined sample times. The second stage, usually lasting for a single sampling interval, allows the calculation of the on-line re-optimisation profile based on previous sampled system state values and future off-line computed control profiles.

Bootstrap aggregated neural network models are built to predict the relevant batch end point quality variables with inputs to the model being the sampled system state values during the initial stage and control profiles for the remaining batch stage. The neural network models are then used for the computation of the reliable on-line optimal control profile using multi-objective optimisation principles.

The paper is organised as follows. Section 2 presents a fed-batch process used in this study. Modelling of the process using bootstrap aggregated neural networks is presented in Section 3. Section 4 presents a reliable on-line re-optimisation control strategy. Some concluding remarks are given in Section 5.

2. A FED-BATCH PROCESS

The fed-batch reactor is taken from (Terwiesch et al., 1998). The following reaction system

$$A + B \xrightarrow{k_1} C$$
$$B + B \xrightarrow{k_2} D$$

is conducted in an isothermal semi-batch reactor. The objective in operating this reactor is, through addition of reactant B, to convert as much as possible of reactant A to the desired product, C, in a specified time t_f = 120 min. It would not be optimal to add all B initially as the second order side-reaction yielding the undesired species D will be favoured at high concentration of B. To keep this undesired species low, the reactor is operated in semi-batch mode where B is added in a feed stream with concentration b_{feed} = 0.2. Based on the reaction kinetics and material balances in the reactor, the following mechanistic model can be developed.

$$\frac{d[A]}{dt} = -k_1[A][B] - \frac{[A]}{V}u \quad (1)$$

$$\frac{d[B]}{dt} = -k_1[A][B] - 2k_2[B]^2 + \frac{b_{feed} - [B]}{V}u \quad (2)$$

$$\frac{d[C]}{dt} = k_1[A][B] - \frac{[C]}{V}u \quad (3)$$

$$\frac{d[D]}{dt} = 2k_2[B]^2 - \frac{[D]}{V}u \quad (4)$$

$$\frac{dV}{dt} = u \quad (5)$$

In the above equations, $[A]$, $[B]$, $[C]$, and $[D]$ denote, respectively, the concentrations of A, B, C, and D, V is the current reaction volume, u is the reactant feed rate, and the reaction rate constants have the nominal value k_1 = 0.5 and k_2 = 0.5. At the start of reaction, the reactor contains $[A](0)$ = 0.2 moles/litre of A, no B ($[B](0)$ = 0) and is fed to 50% ($V(0)$=0.5).

3. MODELLING OF THE FED-BATCH PROCESS USING BOOTSTRAP AGGREGATED NEURAL NETWORKS

Fig. 1 shows an aggregated neural network where several networks are developed to model the same relationship and are combined together. Earlier studies show that an advantage of aggregated neural networks is that they can not only give better generalisation performance than single neural networks, but also provide model prediction confidence measures (Zhang, 1999).

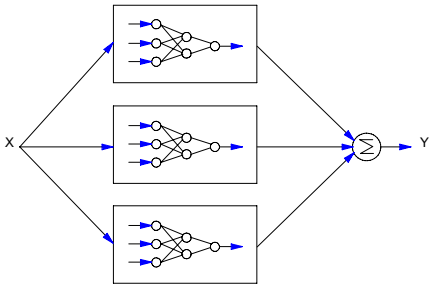

Fig. 1. A bootstrap aggregated neural network

In this study, a fixed batch time of 120 minutes is considered as in (Zhang, 2005). Since it is usually difficult to measure the product quality variables frequently during a batch, it is a general practice to measure the product quality variables only at the end of a batch. The batch duration is divided into 10 equal intervals and within each interval the reactant feed rate is kept constant. The objective in operating this process is to maximise the amount of the final product $[C](t_f)V(t_f)$ and simultaneously minimise the amount of undesired species $[D](t_f)V(t_f)$. Neural network models for the prediction of the final amounts of product $[C](t_f)V(t_f)$ and by-product $[D](t_f)V(t_f)$ at the final batch time are of the form:

$$y_1 = f_1(U) \quad (6)$$
$$y_2 = f_2(U) \quad (7)$$

where $y_1 = [C](t_f)V(t_f)$, $y_2 = [D](t_f)V(t_f)$, $U = [u_1\ u_2\ \ldots\ u_{10}]^T$ is a vector of the reactant feed rates, f_1 and f_2 are nonlinear functions represented by neural networks. The above models are used for off-line optimisation.

In this study, simulated process operational data from 50 batch runs were generated with the reactant feed rate randomly distributed in the range [0, 0.01]. Of the 50 batches of data, 40 batches were used to develop neural network models and the remaining 10 batches were used as unseen testing data. Gaussian noise with zero mean and a variance of 2.5×10^{-4} was added to the reactant feed rate to simulate the effect of measurement noise.

Two bootstrap aggregated neural networks each containing 20 neural networks were developed for predicting $[C](t_f)V(t_f)$ and $[D](t_f)V(t_f)$. Each individual neural network has a single hidden layer with 10 hidden neurons. Hidden neurons use the sigmoid activation function whereas the output layer neuron

uses the linear activation function. The Levenberg-Marquardt training algorithm with "early stopping" was used in this study to train the networks. For training each network, bootstrap re-sampling with replacement (Efron, 1982) was used to generate a replication of the 40 batches of process data. Half of the replication was used as training data while the other half was used as the validation data.

For on-line re-optimisation, the batch length is divided into three process operation stages. The initial batch sampling stage lasting for 48 minutes, allows the recording of concentrations of [*C*] and [*D*] via off-line laboratory analysis with each sampling interval being 12 minutes. Corresponding future off-line calculated control inputs are also recorded for being used as neural network model inputs. The fifth sampling interval lasting from 48 minutes to 60 minutes is used for performing on-line re-optimisation. The re-optimised control profile is implemented from time 60 minutes onwards to the final batch time of 120 minutes. The control action is constant during each sampling interval and thus is a piecewise continuous function.

The neural network models for the prediction of concentration variables $[C](t_f)V(t_f)$ and $[D](t_f)V(t_f)$ at the final batch time used in on-line re-optimisation are of the form:

$$y_1 = f_3(U_1) \tag{8}$$

$$y_2 = f_4(U_1) \tag{9}$$

where $y_1 = [C](t_f)V(t_f)$, $y_2 = [D](t_f)V(t_f)$, $U_1 = [C_1\ C_2\ C_3\ C_4\ u_6 \cdots\ u_{10}]^T$, C_1 to C_4 are the sampled concentration values in [0 min, 48 min], u_6 to u_{10} are the reactant feed rates for the remaining batch period [60 min, 120 min], f_3 and f_4 are nonlinear functions represented by neural networks.

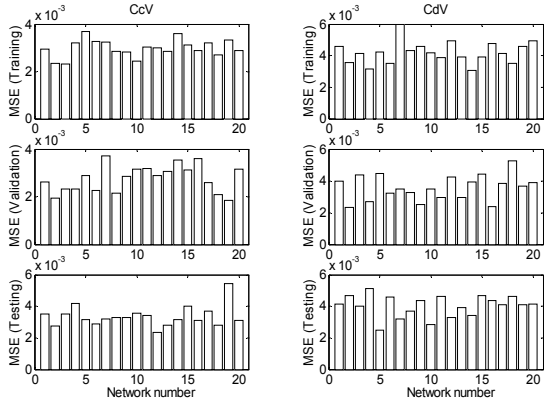

Fig. 2. Model errors of individual networks for the fed batch reactor

Table 1. Bootstrap aggregated neural network prediction accuracy on the testing data

$[C](t_f)V(t_f)$		$[D](t_f)V(t_f)$	
MSE	Standard Prediction Error	MSE	Standard Prediction Error
0.0034	0.0020	0.0040	0.0028

Two bootstrap aggregated neural networks each containing 20 neural networks were developed for representing Eq(8) and Eq(9). Fig. 2 shows the mean squared errors (MSE) for the individual networks on training, validation, and testing data sets for the two neural network models. It can be observed from Fig. 2 that the individual neural network errors on the training, validation and testing data sets are inconsistent in that networks giving small errors on the training data may not give small errors on the testing data. Table 1 shows the MSE of the bootstrap aggregated neural network models and the standard error from the individual network predictions on the testing data.

4. RELIABLE ON-LINE RE-OPTIMISATION CONTROL

The optimal control scheme involves satisfying conflicting objectives, i.e. maximise the amount of the final desired product $[C](t_f)V(t_f)$ and simultaneously minimise the amount of the final undesired species $[D](t_f)V(t_f)$. In order to obtain a reliable control policy from the aggregated neural network model, minimisation of the standard error of individual network predictions are introduced as additional objectives in the optimisation method. This may be formulated in terms of a multi-objective optimisation problem which is solved using the goal attainment method (Gembicki, 1974).

$$F(U) = \begin{bmatrix} -[C](t_f)V(t_f) \\ [D](t_f)V(t_f) \\ \sigma_{e,C_c}(t_f) \\ \sigma_{e,C_d}(t_f) \end{bmatrix} \tag{10}$$

$$\min_{U,\gamma} \gamma \tag{11}$$

subject to $F_i(U) - W_i\gamma \le F_i^*$

$$0 \le u_j \le 0.01 \quad j = 1,2,\cdots,10$$

$$V(t_f) \le 1.00$$

where γ is a scalar variable, W_i are the weighting parameters, F_i^* are design goal values, U is the sequence of the reactant feed rates into the reactor, V is the reaction volume obtained by integrating the reactant feed rate, $\sigma_{e,C_c}(t_f)$ and $\sigma_{e,C_d}(t_f)$ denote the individual standard prediction errors from the two bootstrap aggregated neural network models. For off-line optimisation, $U = [u_1 \cdots\ u_{10}]^T$ and the model used is given by Eq(6) and Eq(7). For on-line re-optimisation, $U = [u_6 \cdots\ u_{10}]^T$ and the model used is given by Eq(8) and Eq(9).

Off-line optimisation is first performed and the first half of the control profile, u_1 to u_5, is implemented. Then on-line re-optimisation is performed to re-calculate the control profile for the remaining batch period, i.e. u_6 to u_{10}.

The presented objective function in Eq(10), $F(U)$, maximises the amount of product, $[C](t_f)V(t_f)$, and minimises the amount

of by-product, $[D](t_f)V(t_f)$. Simultaneously it also minimises the standard prediction errors from the aggregated neural network models for these two quality variables. The neural network model prediction under the optimal control policy obtained by solving the multi-objective optimisation has a narrow model prediction confidence bound and thus the computed on-line optimal control policy is reliable.

The principle of on-line re-optimisation control has been applied to the following two cases:

Case I: $F^* = [-0.065 \quad 0.015 \quad 0.001 \quad 0.001]$

Case II: $F^* = [-0.075 \quad 0.030 \quad 0.001 \quad 0.001]$

The weights in the goal attainment optimisation algorithm for the maximisation of $[C]$, minimisation of $[D]$ and the minimisation of the standard prediction errors of the two neural network models, $\sigma_{e,C_c}(t_f)$ and $\sigma_{e,C_d}(t_f)$, have the same values which were used for the calculation of the offline 'optimal' control profile. In order to demonstrate the advantage of the proposed technique, 50 solutions of the optimal control problem were computed by varying the weights on $[C](t_f)V(t_f)$ and $[D](t_f)V(t_f)$, W_1 and W_2 respectively, randomly and uniformly within [0, 1]. Model plant mismatch is simulated by taking k_1 and k_2 as normally distributed random variables with a mean of 0.50 and a standard deviation of 0.05.

Table 2. Comparison between off-line and on-line optimisation

Cases		Off-line optimisation	On-line re-optimisation
I	$[C](t_f)V(t_f)$	0.06324	0.06277
	$[D](t_f)V(t_f)$	0.02804	0.02665
II	$[C](t_f)V(t_f)$	0.06327	0.06299
	$[D](t_f)V(t_f)$	0.02807	0.02713

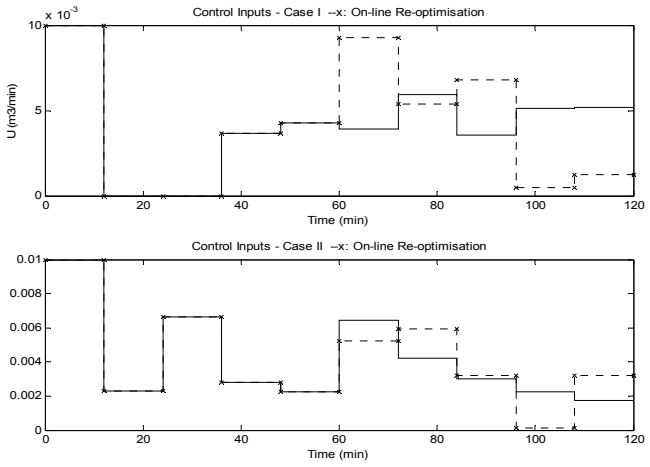

Fig. 3. Optimal control profile for fed-batch reactor

Fig. 3 shows one of the computed on-line re-optimisation control profiles for Case I and Case II respectively. Similar profiles are obtained for all the 50 different Pareto solutions generated. The corresponding trajectories for the system states for the two investigated cases are shown in Fig. 4 and Fig. 5 respectively. The optimisation and simulation results for the same sample solution are presented in Table 2. The values of the mechanistic model calculated (i.e. the actual process) system states for the off-line and on-line re-optimised optimal control profile are presented for the considered sample solution. The mechanistic model calculated output signifies the end point quality values when the calculated 'optimal' control profile is applied to the actual process (i.e. the simulation on the mechanistic model).

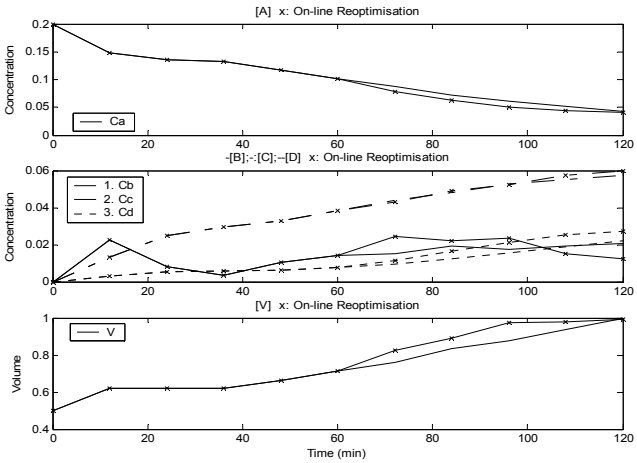

Fig. 4. Optimal system state profile for fed-batch reactor: Case I

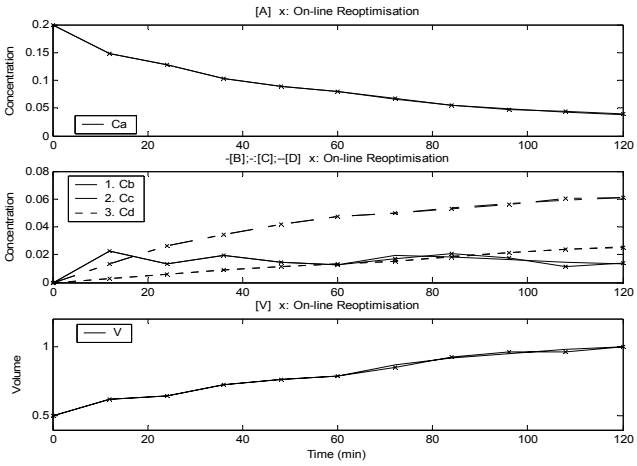

Fig. 5. Optimal system state profile for fed-batch reactor: Case 2

The values shown in Table 2 signify the effect of the principle of on-line re-optimisation control scheme. For Case I, though $[C](t_f)V(t_f)$ under the off-line computed optimal control profile is 0.743 % better than that under the on-line re-optimised control profile, the corresponding value of $[D](t_f)V(t_f)$ is 4.96 % better if the on-line re-optimisation control scheme is put in action. Similarly, for the study in Case II, though $[C](t_f)V(t_f)$ under the off-line computed optimal control profile is 0.442% better than that under the on-line re-optimised control profile, the corresponding value of $[D](t_f)V(t_f)$ is 3.35% better if the on-line re-optimisation control scheme is utilised. Since this is a multi-objective

optimisation problem, the on-line re-optimisation control scheme improves the overall process operation.

Fig. 6 shows the relative errors of the bootstrap aggregated neural network model predictions under the two different optimal control profiles: considering confidence bounds (o) and not considering confidence bounds (*). It can be seen from Fig. 6 that the neural network predictions under the control profiles calculated by considering the model prediction confidence bounds are generally more accurate than those under the control profiles calculated without considering the model prediction confidence bounds. Thus, the optimisation results incorporating the model prediction confidence bounds are more reliable than those without incorporating the model prediction confidence bounds.

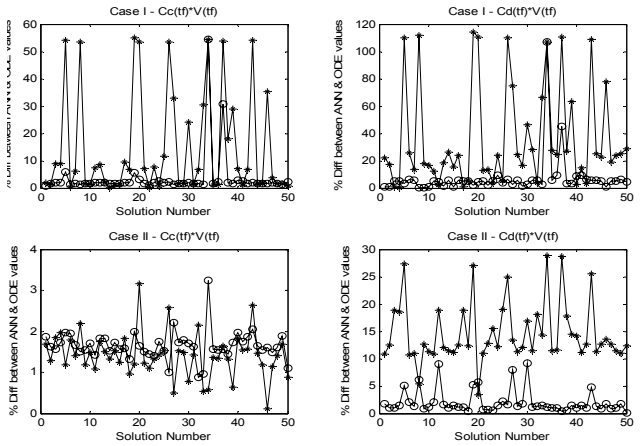

Fig. 6. Bootstrap aggregated neural network model prediction accuracy for fed-batch reactor, o - with model prediction confidence bounds, * - without model prediction confidence bounds

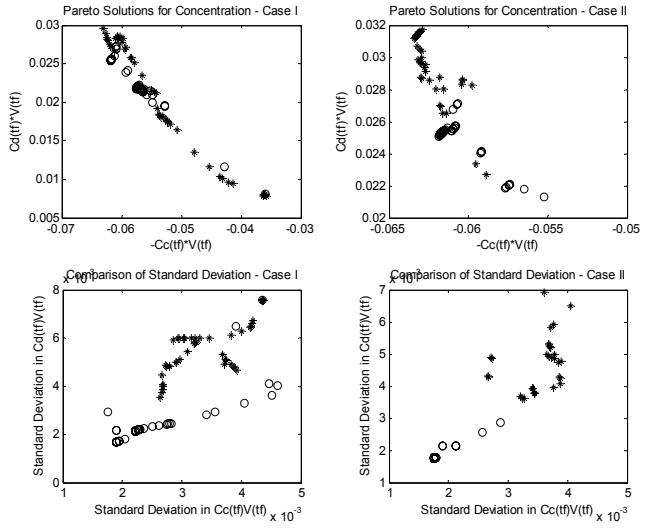

Fig. 7. Comparison of Pareto solutions for fed-batch reactor (O: with confidence bound; *: without confidence bound)

Fig. 7 shows the Pareto solutions obtained for the optimisation results with and without model prediction confidence bounds. The standard prediction errors of the individual neural network models are also given in Fig. 7. It can be concluded from Fig. 7 that the resulting end point quality variable values are better when the minimisation of the standard prediction errors is incorporated as an additional optimisation objective.

Fig. 8 illustrates the percentage improvement in the quality variables due to use of on-line re-optimised control profile. It may be concluded from the diagram that there is a consequent improvement in the end point quality variables since most of the obtained solutions show a positive improvement in either of the concentration values. The number count of the improvements in the solutions is presented in Table 3. It can be seen from Table 3 that the proposed reliable on-line re-optimisation technique overall improves the process operation. Out of the 50 solutions considered, there are no simultaneous deteriorations in $[C](t_f)V(t_f)$ and $[D](t_f)V(t_f)$.

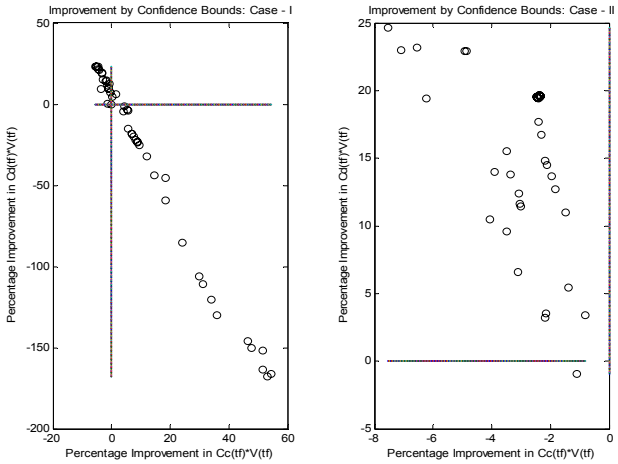

Fig. 8. Improvement by on-line re-optimisation incorporating model prediction confidence bound

Table 3. Improvement in solutions by using on-line re-optimisation control

Criteria considered	Number of cases	
	Case I	Case II
Improvement in $[C](t_f)V(t_f)$	10	15
Improvement in $[D](t_f)V(t_f)$	38	35
Simultaneous Improvement in $[C](t_f)V(t_f)$ & $[D](t_f)V(t_f)$	0	2
Simultaneous deterioration in $[C](t_f)V(t_f)$ & $[D](t_f)V(t_f)$	0	0

5. CONCLUSIONS

A reliable on-line re-optimisation control strategy for batch processes based on bootstrap aggregated neural network models is proposed. In addition to process operation objectives, model prediction reliability offered by bootstrap aggregated neural networks is incorporated as additional optimisation objectives. In order to overcome the effect of

unknown disturbances and model plant mismatches, on-line re-optimisation is carried out at the middle of a batch. Optimal control actions for the remaining batch period are re-calculated based on the updated predictions of final product quality. The effectiveness of the proposed technique is demonstrated by application to a simulated fed batch process.

REFERENCES

Ahmad, Z. and J. Zhang (2006). Combination of multiple neural networks using data fusion techniques for enhanced nonlinear process modelling. *Computers & Chemical Engineering*, **30** (2), 295-308.

Bonvin, D. (1998). Optimal operation of batch reactors--a personal view. *Journal of Process Control*, **8**(5-6), 355-368.

Efron, B. (1982). *The Jackknife, the Bootstrap and Other Resampling Plans*. Society for Industrial and Applied Mathematics: Philadelphia.

Gembicki, F. W. (1974). Vector Optimisation for Control with Performance and Parameter Sensitivity Indices, PhD Thesis, Case Western Reserve University, Cleveland, USA.

Li, C. H. Ye, G. Wang, and J. Zhang (2005). A recursive nonlinear PLS algorithm for adaptive nonlinear process modelling, *Chemical Engineering and Technology*, **28**(2) 141-152.

Mukherjee A. and J. Zhang (2006). Reliable multi-objective optimal control of batch processes based on stacked neural network models", in (Eds) W. Marquardt and C. Pantelides, *Computer-Aided Chemical Engineering 21*, *16th European Symposium on Computer Aided Process Engineering and 9th International Symposium on Process Systems Engineering*, 1407-1412.

Qin, S. J. and T. J. McAvoy (1992). Nonlinear PLS modeling using neural network. *Comput. Chem. Eng.* **16**(4), 379-391.

Sridhar, D. V., R. C. Seagrave, and E. B. Bartlett (1996). Process modelling using stacked neural networks. *AIChE Journal*, **42**, 2529-2539.

Terwiesch, P., D. Ravemark, B. Schenker, and D. W. T. Rippin (1998). Semi-batch process optimization under uncertainty: theory and experiments, *Computers & Chemical Engineering*, **22**, 201-213.

Tian, Y., J. Zhang, and A. J. Morris (2001). Modeling and optimal control of a batch polymerization reactor using a hybrid stacked recurrent neural network model, *Ind. Eng. Chem. Res*., **40**(21), 4525-4535.

Xiong, Z. and J. Zhang (2005). Neural network model-based on-line re-optimisation control of fed-batch processes using a modified iterative dynamic programming algorithm, *Chemical Engineering and Processing*, **44**, 477 – 484.

Yabuki, Y. and J. F. MacGregor (1997). Product quality control in semibatch reactors using midcourse correction policies. *Ind. Eng. Chem. Res*., **36**(4), 1268-1275.

Zhang, J., A. J. Morris, E. B. Martin, and C. Kiparissides (1997). Inferential estimation of polymer quality using stacked neural networks. *Computers & Chemical Engineering*, **21**, s1025-s1030.

Zhang, J. (1999). Developing robust non-linear models through bootstrap aggregated neural networks. *Neurocomputing*, **25**, 93-113.

Zhang, J. (2004). A reliable neural network model based optimal control strategy for a batch polymerization reactor. *Ind. Eng. Chem. Res*., **43**(4), 1030-1038.

Zhang, J. (2005). Modelling and optimal control of batch processes using recurrent neuro-fuzzy networks. *IEEE Transactions on Fuzzy Systems*, **13**(4), 417-427.

Zhao, S. J., J. Zhang, Y. M. Xu, and Z. Xiong (2006). A nonlinear projection to latent structures method and its applications, *Ind. Eng. Chem. Res*., **45**(11), 3843-3852.