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NEURAL NETWORK MODEL PREDICTIVE CONTROL APPLIED TO A FED-BATCH SUGAR CRYSTALLIZATION

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Abstract: This paper is focused on a comprehensive study of neural network (NN) model based predictive control (MPC), as an operation strategy for a fed-batch sugar crystallizer. The process is divided into four subsequent control loops and for each of them an individual NN-based MPC is designed. The operation is tested for a number of scenarios and is compared with alternative (linear and batch nonlinear MPC) control solutions. The results demonstrate that the NN-MPC is a promising alternative of the traditionally applied linear controllers when the process is strongly nonlinear and input-output data is the only process information available.

Keywords: Model predictive control, sugar crystallization, neural network model, nonlinear process identification

1. INTRODUCTION

Neural Networks (NNs) became a well-established methodology as exemplified by their applications to identification and control of general nonlinear and complex systems (Haykin, 1999). Particularly, the design of robust neural controllers for nonlinear systems with uncertainties and disturbances, which guarantees stability and trajectory tracking, has received an increasing attention lately (Norgaard at al, 2000). Using NNs, control algorithms can be developed to be robust to uncertainties and modeling errors. The neural control problem can be approached in direct or indirect control design framework. Direct NN control means that the controller is a neural network, while in the indirect NN control scheme, first a NN is used to model the process to be controlled, and this model is then employed in a more conventional controller design. The implementation of the first approach is simple but the design and the tuning are rather challenging. The indirect design is very flexible, the model is typically trained in advance and the controller is designed on-line, therefore it is the chosen scheme for the present work.

The increasing use of NNs not only in modelling and control but also in various fields including pattern recognition, identification, classification, speech and vision, is in great part due to the following features (Haykin, 1999): i) NN are universal approximators. It has been proven that any continuous nonlinear function can be approximated arbitrarily well over a compact set by a multilayer NN which consists of one or more hidden layers. ii) Learning and adaptation. The intelligence of NNs comes from their generalization ability with respect to unknown data. On-line adaptation of the weights is possible. iii) Multivariable systems. NNs may have many inputs and outputs, which makes it easy to model multivariable systems.

Simultaneously with the rapid advance of the NNs, since their reborn in the early 80's of the XX century, the Model based Predictive Control (MPC) became an attractive control strategy implemented in a variety of process industries. MPC, being one of the approaches that inherently can cope with process constrains, nonlinearities and multi objectives has the potential to drive a complex process to its optimal state of profit maximization and cost minimization (Qin and Badgwell, 2003).

Based on the above considerations, the aim of this work is to study the viability of implementing the two techniques, NN models and the MPC control scheme, to fed-batch sugar crystallization. The intuition behind is to take advantage of their analytically proven features and to verify them for a real industrial case.

2. PROCESS DESCRIPTION

Typical industrial fed-batch evaporative sugar crystallization is performed in a vacuum pan crystallizer. The reactor has a cylindrical form with volume that can vary between 20-60 m^3. The feed system is usually equipped with an extra water

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input to dilute the sugar solution if necessary. The heat transfer system is a calandria type, to permit the heat interchange between steam and suspension. The vacuum pressure in the pan is generated by the contact barometric condenser and the pan is equipped with a mechanical agitator to keep the suspension homogeneous. The operation is conducted in a fed-batch mode with an average duration of a cycle about 90 minutes.

Sugar crystallization occurs through the mechanisms of nucleation, growth and agglomeration. In the course of production, the crystallization phenomenon is driven by two mechanisms (Jancic & Grootscholten, 1984): i) mass transfer from dissolved sucrose to crystal surface and ii) heat transfer in the calandria. Shortly before the grain setting and continuing during the beginning of the crystallization phase, the available crystalline surface to deposit the molecule of sucrose is much smaller than the mass of dissolved sucrose. During this period the evaporation rate is high, the crystal area/mass of crystallized sucrose rate is very low, therefore the process is driven by the mass transfer. The supersaturation tends to increase and if not controlled, it often achieves the undesirable zone of secondary crystal nucleation. Later on, when the total crystal area and the crystallization capacity increases, the crystal area/mass of crystallized sucrose rate gets high and the process is driven by the heat transfer.

The process objectives are to maximize the speed of crystal growth, keeping high the produced sugar quality and minimizing the costs and losses. These objectives must be fulfilled without occurrence of secondary nucleation or agglomeration. The sugar quality is evaluated by the particle size distribution (PSD) at the end of the process which is quantified by two parameters - the final average (in mass) particle size (MA) and the final coefficient of particle variation (CV). The main challenge of the sugar production is the large batch to batch variation of the final PSD. This lack of process repeatability is caused mainly by improper control policy and results in product recycling and loss increase. The sugar production is heuristically operated, and while the traditionally applied PI(D) controllers are still the preferred solutions they usually lead to energy and material loss that can easily be reduced if an optimized operation policy is implemented. These problems constitute the main motivation for the operation strategy formulated in the next section.

3. OPERATION STRATEGY

Sugar production is characterized by strongly non-linear and non-stationary dynamics and goes naturally through a sequence of relatively independent stages: charging, concentration, seeding, setting the grain, crystallization (the main phase), tightening and discharge ((Georgieva et al., 2003). Therefore the operation strategy is formulated as a cascade of individual control loops for each of the stages (Fig.1). The feedback control policy is based on measurements of the flowrate, the temperature, the pressure, the stirrer power and the supersaturation (by a refractometer). Measurements of these variables are usually available for a conventional crystallizer. In the present study, the control actions are performed by manipulating the valves of the liquor/syrup feed flowrates (F_f) and the steam flowrate (F_s), while the volume of massecuite (V_m), the supersaturation (S) and the current of the agitator (IA) are the controlled variables. This choice is completely inspired by the industrial practice in several refineries.

Charging (stage 1): During the first stage the crystallizer is fed with liquor until it covers approximately 40 *%* of the vessel height. The process starts with vacuum pressure of around 1 *bar* (equal to the atmospheric pressure) and reduces it up to 0.23 *bar*. When the vacuum pressure reaches 0.5 *bar*, the feed valve is completely open such that the feed flowrate is kept at its maximum value. When the liquor covers 40 *%* of the vessel height, the feed valve is closed and the vacuum pressure needs some time to stabilize around the value of 0.23 *bar* before the concentration stage starts.

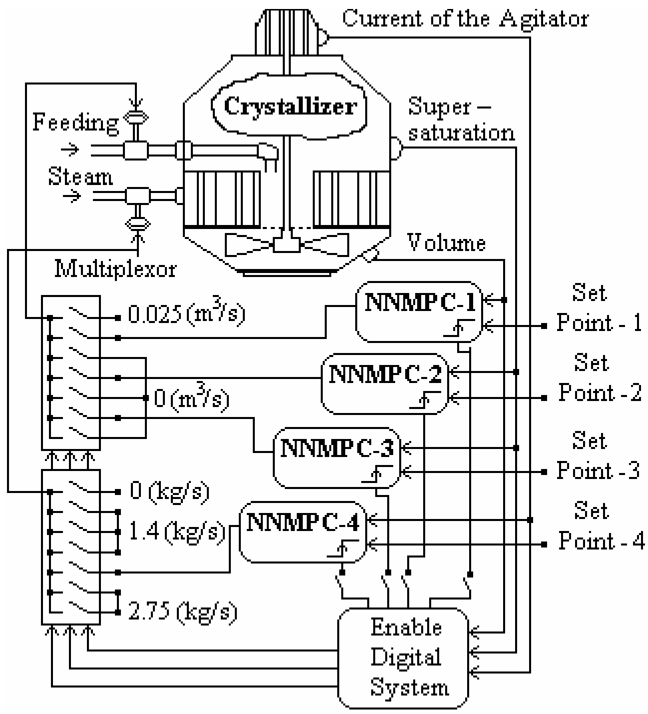

Fig. 1. Cascade NNMPC control strategy

Concentration (stage 2): Once the vacuum pressure stabilizes, the stirrer is switched on and the concentration begins. In order to guarantee unperturbed operation of the barometric condenser and the steam production boiler, the steam flowrate must increase slowly (from 0 to 2 *kg/s*, in two minutes approximately). The concentration of the dissolved sucrose by evaporation under vacuum results in volume reduction. However, for technological reasons, the minimum suspension level of the pan must be above the calandria. Therefore a feed flowrate action is required to control the level (the volume) of the pan and this constitutes the *first control loop*. In this stage, the supersaturation increases rapidly (at about a rate of 0.025 per *min*.). When it reaches a value of 1.06, the feeding is stopped and the steam flowrate is reduced slowly to 1.4 *kg/s*, with the same speed as it was increased. The concentration stage is over when the supersaturation reaches the value of 1.11.

Seeding (stage 3): At this moment seed crystals are introduced into the pan to provoke crystallization. This stage is rather unstable and to prevent seed crystals from dissolution in the liquor, the feed valve must be closed and the steam flowrate kept at its minimum for a short period (about 2 *min*.). Keeping these conditions unchanged contributes to the formation of the grain and is also important for the final crystal size distribution. The supersaturation continues naturally to increase but usually no control action is required.

Crystallization with liquor (stage 4): During this stage the supersaturation is first controlled by a proper feeding to be around a set point of 1.15. This constitutes the *second control loop*. At the beginning of this stage, the mass transfer is the driving crystallization force, the crystallization rate increases and the controller usually reduces the feed flowrate to maintain the reference value of the supersaturation. When all liquor quantity is introduced, the feeding is stopped and the supersaturation is now kept at the same set point of 1.15 by the steam flowrate as the manipulated variable. This constitutes the *third control loop*. The heat transfer is now the driving crystallization force. A typical problem of this control loop is that at the end of this stage the steam flowrate achieves its maximum value of 2.75 *kg/s* but it is not sufficient to keep the supersaturation at the same reference value therefore a reduction of the set point is required. The stage is over when the stirrer power reaches the value 20.5 *A.*

Crystallization with syrup (stage 5): A stirrer power of 20.5*A* corresponds to a volume fraction of crystals equal to 0.4. At this moment the feed valve is reopened, but now a juice with less purity (termed syrup) is introduced into the pan until the maximum volume (30 m^3) is reached. The control objective is to maintain the volume fraction of crystals around the set point of 0.45 by a proper syrup feeding. This constitutes the *fourth control loop*.

Tightening (stage 3): Once the pan is full the feeding is closed. The tightening stage consists principally in waiting until the suspension reaches the reference consistency, which corresponds to a volume fraction of crystals equal to 0.5. The supersaturation is not a controlled variable at this stage because due to the current conditions in the crystallizer, the crystallization rate is high and it prevents the supersaturation of going out of the metastable zone. The stage is over when the stirrer power reaches the maximum value of 50 *A*. The steam valve is closed, the water pump of the barometric condenser and the stirrer are turned off. Now the suspension is ready to be unloaded and centrifuged.

4. NEURAL NETWORK PROCESS MODEL

The need for neural networks arises when dealing with non-linear systems for which the linear controllers and models do not satisfy. Two main achievements contributed to the increasing popularity of the NNs. The proof of their universal approximation properties and the development of suitable algorithms for NN training as the backpropagation and the adaptation of the Levenberg-Marquard algorithm for NN optimization. The most used NN structures are Feedforward networks (FFNN) and Recurrent (RNN) ones. The RNNs offer a better suited tool for nonlinear system modeling and is implemented in this work (Fig.2). The Levenberg-Marquard (LM) algorithm was preferred as the training method due to its advantages in terms of execution time and robustness. Since the LM algorithm requires a lot of memory, a powerful (in terms of memory) computer is the main condition for successful training. In order to solve the problem of several local minima, that is typical for all derivative based optimization algorithms (including the LM method), we have repeated several time the optimization specifying different starting points.

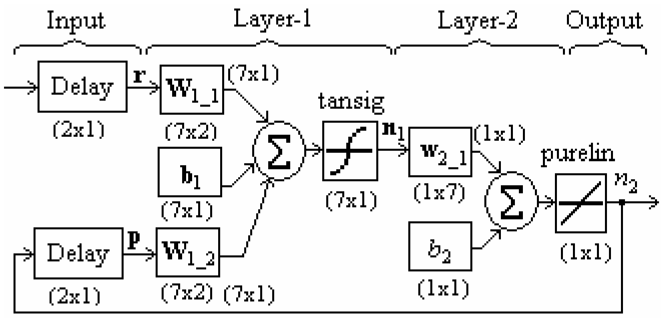

Fig. 2. NN architecture

The individual stages of the crystallization process are approximated by different RNNs of the type shown in Fig. 2. Tangent sigmoid hyperbolic activation functions are the hidden computational nodes (Layer 1) and a linear function is located at the output (Layer 2). Each NN has two vector inputs (r and p) formed by past values of the process input and the NN output respectively. The architecture of the NN models trained to represent different process stages, is summarized as follows

$$u_{NN} = [r, p] = [u_c(k-1), u_c(k-2), y_{NN}(k-1), y_{NN}(k-2)] \quad (1)$$

$$x = W_{11}r + W_{12}p + b_1 \quad (2)$$

$$n_1 = \left(e^x - e^{-x}\right)/\left(e^x + e^{-x}\right) \quad (3)$$

$$n_2 = w_{21}n_1 + b_2 \quad (4)$$

where $W_{11} \in R^{m\times 2}$, $W_{12} \in R^{m\times 2}$, $w_{21} \in R^{1\times m}$, $b_1 \in R^{m\times 1}$, $b_2 \in R$ are the network weights (in matrix form) to be adjusted during the NN training, m is the number of nodes in the hidden layer.

Since the objective is to study the influence of the NNs on the controller performance, a number of NN models is considered based on different training data sheets.

Case 1 (Generated data): Randomly generated bounded inputs (u_i) are introduced to a simulator of a general evaporative sugar crystallization process introduced in Georgieva et al. 2003. It is a system of nonlinear differential equations for the mass and energy balances with the operation parameters computed based on empirical relations (for nonstationary parameters) or keeping constant values (for stationary parameters). The simulator responses are recorded

(y_i) and the respective mean values are computed ($u_{i,\mathrm{mean}}$, $y_{i,\mathrm{mean}}$). Then the NN is trained supplying as inputs $u_i - u_{i,\mathrm{mean}}$ and as target outputs $y_i - y_{i,\mathrm{mean}}$.

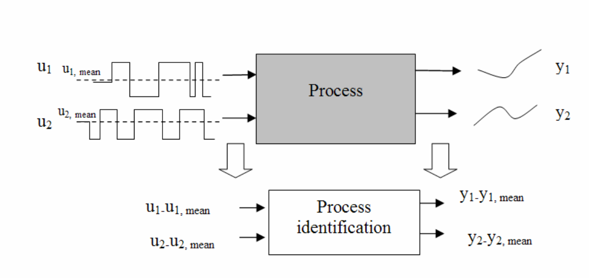

Fig. 3 Case1: NN data generation

Case 2: Industrial data: The NN is trained with real industrial data. In order to extract the underlying nonlinear process dynamics a prepossessing of the initial industrial data was performed. From the complete time series corresponding to the input signal of one stage only the portion that really excites the process output of the same stage is extracted. Hence, long periods of constant (steady-state) behavior are discarded. Since, the steady-state periods for normal operation are usually preceded by transient intervals, the data base constructed consists (in average) of 60-70% of transient period data. A number of sub cases are considered.

Case 2.1: Industrial data of two batches is used for NN training.

Case 2.2: Industrial data of four batches is used for NN training.

Case 2.3: Industrial data of six batches is used for NN training.

5. MPC – PROBLEM FORMULATION

The term model-based predictive control (MPC) does not refer to a particular control method, instead it corresponds to a general control approach (Morari, 1994, Rossiter, 2003). The main difference between MPC configurations is the model used to predict the future behavior of the process and the optimization procedure. Nonlinear model predictive control (NMPC) is an optimisation-based multivariable constrained control technique that uses a nonlinear dynamic model for the prediction of the process outputs (Qin and Badgwell, 2003). At each sampling time *k* the model predicts future process responses to potential control signals over the prediction horizon (H_p). The predictions are supplied to an optimization procedure, to determine the values of the control action over a specified control horizon (H_c) that minimize the following performance index

$$\min_{u_{\min}\le[u_c(k),u_c(k+1),\dots,u_c(H_c)]\le u_{\max}} J=\lambda\sum_{k=1}^{H_p}\left(y_r(k)-y_{NN}(k)\right)^2-\rho\sum_{k=1}^{H_c}\left(u_c(k-1)-u_c(k-2)\right)^2 \quad (5)$$

subject to the following constrains

$$u_{\min}\le u_c\le u_{\max}, \quad (6)$$

$$\Delta u_{\min}\le \Delta u\le \Delta u_{\max} \quad (7)$$

$$y_{\min}\le y_p\le y_{\max}, \quad (8)$$

where $u_{\min}$ and $u_{\max}$ are the limits of the control inputs, $\Delta u_{\min}$ and $\Delta u_{\max}$ are the minimum and the maximum values of the rate-of-change of the inputs and $y_{\min}$ and $y_{\max}$ are the minimum and maximum values of the process outputs.

H_p is the number of time steps over which the prediction errors are minimized and the control horizon H_c is the number of time steps over which the control increments are minimized, y_r is the desired response (the reference) and y_{NN} is the predicted process output (Diehl et al., 2002). $u_c(k), u_c(k+1), u_c(H_c)$ are tentative future values of the control input, which are parameterized as peace wise constant. The length of the prediction horizon is crucial for achieving tracking and stability. For small values of H_p the tracking deteriorates but for high H_p values the bang-bang behavior of the process input may be a real problem. The MPC controller requires a significant amount of on-line computation, since the optimization (5) is performed at each sample time to compute the optimal control input. At each step only the first control action is implemented to the process, the prediction horizon is shifted or shrunk by usually one sampling time into the future, and the previous steps are repeated. See (Rossiter, 2003) for more details. λ and ρ are the output and the input weights respectively, which determine the contribution of each of the components (the output error and the control increments) of the performance index (5). Their choice depends on the particular problem, but in most of the cases it is a trial and error procedure. However, in this work, the following empirical formula is deduced and applied for the choice of ρ

$$(u_{\max}-u_{\min})^2\cdot\rho=e_{p\max}\cdot P/100, \quad (9)$$

where P defines the desired contribution of the second term in (5) ($0\% \le P \ge 100\%$) and

$$e_{p\max}=\max\left((y_r-y_{\max})^2,(y_r-y_{\min})^2\right) \quad (10)$$

The intuition behind (9-10) is to make the terms of (5) compatible when they are not previously normalized and to overcome the problem of different numerical ranges of the two terms.

Process constrains

The key for a successful MPC control is not only to find a reliable predictive model, but also the adequate formulation of the process constrains. For the case in hand, the constrains are really a big challenge. They are divided in two groups.

The technological (*hard*) constrains are related to the limited capacity and efficiency of the installed equipment. The maximum steam flowrate, which corresponds to the upper bound of (6), is limited by the evaporation capacity of the crystallizer the condensation capacity of the barometric condenser and by the steam availability in the factory. The minimum steam flowrate, the lower bound of (6), is confined by the capacity of the agitator to maintain the suspension homogeneity. The rate of variation of the steam flowrate (7) and the vacuum pressure (7) is also constrained in order to keep not perturbed the pressure in the crystallizer. In the presence of disturbances, the control system of the vacuum pressure often operates in a low efficiency regime. Therefore it appears more reasonably to keep constant the vacuum pressure and manipulate slowly the steam flowrate (7).

The process (*soft*) constrains are usually due to economical and security reasons. For example, restrictions on the amount of liquor or syrup used in the production, correspond to constrain (8). During the first part of the process high purity-low brix juice is fed in the pan, termed liquor. At the second half of the batch, for economical reasons, the crystallization continues with other low purity-high brix juice, termed syrup, until it reaches the maximum volume of the pan.

6. NN-MPC CONTROL TESTS

The operation strategy discussed in section 3 (Fig. 1) and the NN-based MPC (NN-MPC) procedure introduced in section 4 and 5 are tested numerically in MatLab environment. The general architecture and the software modules developed are schematically represented in Fig. 3. The module *process* is the simulator of a detailed phenomenological model (Georgieva et al. 2003). The output predictions are computed by individual NN models corresponding to each control loop. The control and the prediction horizons are set at H_c=2 and H_p=5, respectively. The following scenarios are considered:

Test 1: The process simulator is the same as the one used for generating data for the NN training in Case 1.

Test2: All industrial measurements corresponding to a normal batch (not used for NN training in Case 2) are introduced in the process simulator. These are: the vacuum pressure, brix and temperature of the feed flow, pressure and temperature of the steam. The data used is the original, without any preprocessing and is the main source of process disturbances.

In Figures 5-7 are depicted the results of Test 1, corresponding to the input and the output time trajectories of the sequence of NN-MPC control loops (1,2,3,4) . In order to improve the visibility of the plots not all of the cases are shown on the same figure. Since case 2.1 is the worst one, it was excluded from the final version of the paper. The NN models trained only with data from two batches are not enough representative for the real process stages and predictions based on these NN models are highly unreliable. Therefore the controllers are unable to keep the process outputs around their predefined set points. See that there is also a significant difference between the performance of cases 2.2 and 2.3. Predictions based on data of four batches lead also to considerable deterioration of the tracking performance. Since case 1 is based on a generated (by a simulator) data and then the same simulator imitates the process (Test 1) it can be considered as a nominal case. Note that case 2.3 exhibits similar to case 1 behavior, which confirms the expected improvement of the model quality when more data are available. In fact, the control inputs of case 2.3 have smother time curves when compared with case 1.

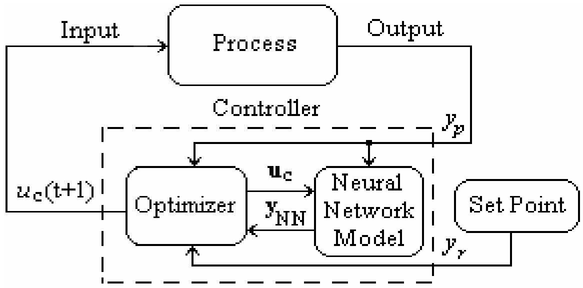

Fig. 4. NN-MPC general structure

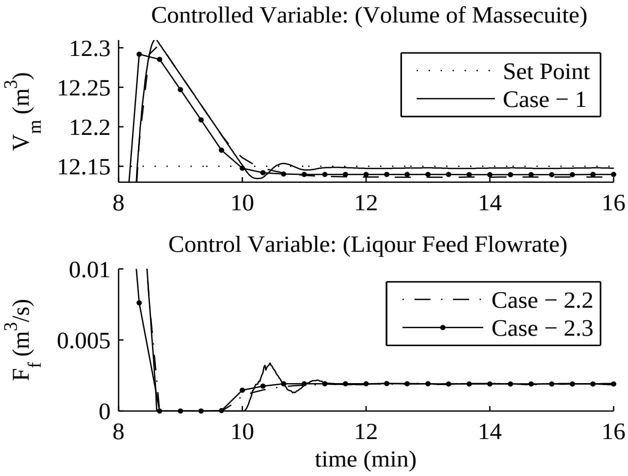

Fig. 5. Test 1: Input-output process behavior (NN-MPC control loop 1)

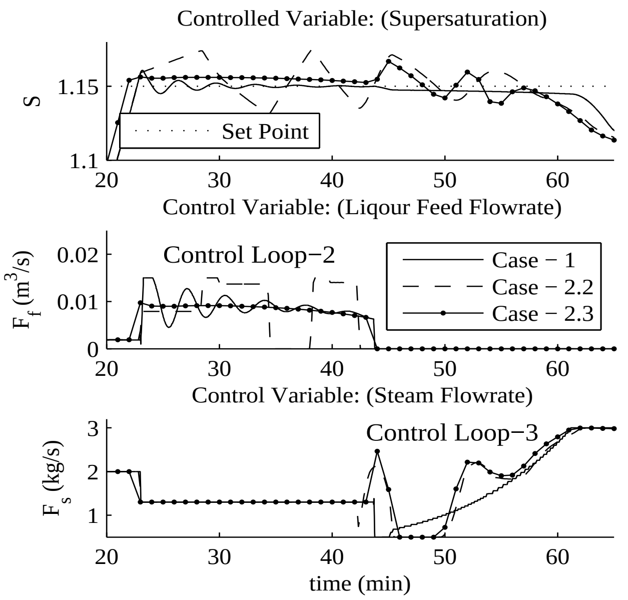

Fig. 6. Test 1: Input-output process behavior (NN-MPC control loop 2 and 3)

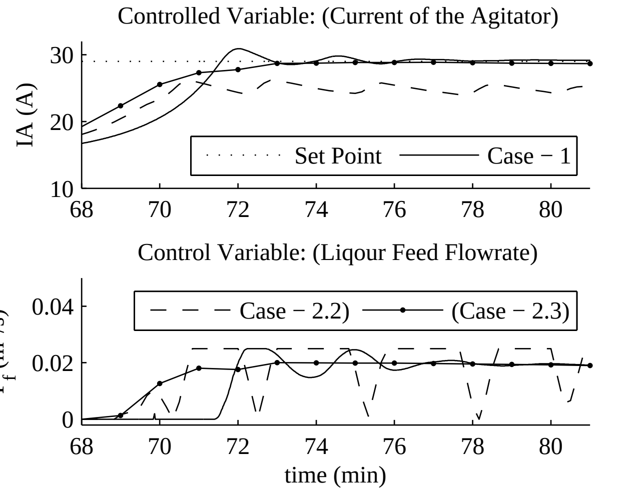

Fig. 7 Test 1: Input-output process behavior (NN-MPC control loop 4)

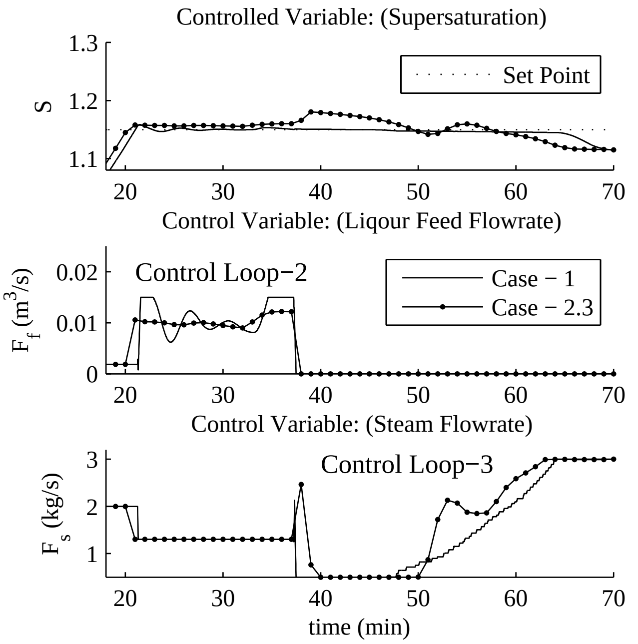

Fig. 8. Test 2: Input-output process behavior (NN-MPC control loop 2 and 3)

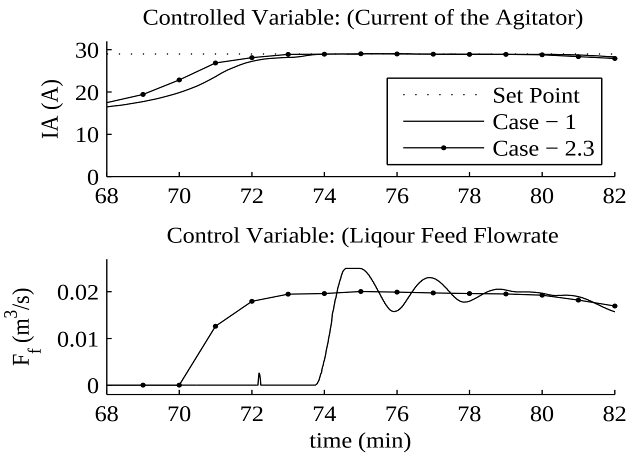

Fig. 9. Test 2: Input-output process behavior (NN-MPC control loop 4)

In Figures 8-9 are depicted the results of Test 2, where the input-output trajectories of Case 1 (generated data) are compared with the most realistic and well designed Case 2.3 (6 batches of industrial data for NN training). The objective, to keep the level of the pan constant, during the concentration stage, is easily achieved even by a simpler controller, therefore the results for the first control loop are not depicted in Figures 8-9. From control point of view, the main challenge starts at the moment of seeding. After that, phenomena like crystal growth, agglomeration, secondary nucleation and aggregation take place and make the process rather complex and nonlinear. The combination Test2-Case1 (bold line in Figs.8-9) is somehow academic and not quite realistic because the NNs are trained with generated by a simulator data. In practice, if we have already a reliable simulator, the NN model can be unnecessary. From other side, the combination Test2-Case 2 corresponds to the situations where NNs really make sense. Based only on input-output process data, a NN model is obtained and if the model is trained with enough representative data as is the Case 2.3 (bold line+dots in Figs.8-9), the cascade MPC succeed to follow the set-points. See that the performance of the two cases is similar, however, the control actions of Case 2.3 are smother than the control actions of Case 1. The same conclusion was obtained for Test 1 (Figs. 5-7). Though these results go beyond what can be theoretically proven we believe that the generalization properties of the NNs trained by scenario Case 1 are worse than the NNs corresponding to Case2.3. All this due to the not completely overlapping space of the input output data in the two cases. In summary, the networks are trained to map different data ranges and apparently Case 2.3 covers better the normal operation regime of the process.

Prior to this study, alternative control solutions were subject to comprehensive investigation. In Sánchez et al., 2006, a number of SISO (single input-single output) and MIMO (multiple inputs-multiple outputs) structures of linear model predictive control (LMPC) for the same process are reported.

The linear models were extracted applying a special procedure termed double test identification. From the same sequence of controllers, only the LMPC of the supersaturation, manipulating the steam flowrate (which corresponds to the control loop 3 of this paper) was able to make feasible all conflicting control objectives and constrains summarized in section 5. Further on, in Sánchez et al., 2007 two nonlinear MPC (NMPC) control schemes were implemented to the same fed-batch sugar crystallizer - i) NMPC that does not exploit the batch nature of the process (termed as classical NMPC) and ii) the batch NMPC that takes into account the final-point control objectives explicitly formulated in the cost function (Allgöwer et. al, 2004). In the batch framework, the optimization problem has to be solved iteratively online with shrinking prediction horizon. In fact, at each moment the prediction horizon is equal to the final batch time. This means that at the beginning of the optimisation the prediction horizon is equal to the envisaged process duration and at each iteration it is reduced.

The comparison between the cases discussed in this paper and the two previous alternatives (LMPC, batch NMPC) is summarized in Table 1. Note that the case 2.3 and the batch NMPC have rather similar final CSD parameters that follow quite close the respective reference values. However, the main drawback of the batch NMPC is the high computational cost. In Fig. 10 is depicted the history of the CPU time at each iteration along the complete process duration. Obviously, the initial phase is the most demanding and it is at that period that the optimization procedure needs more computational power.

Table 1. Quality parameters at the batch end: average particle size (AM), coefficient of particle variation (CV)

	Test 1		Test 2	
	AM (mm)	CV (%)	AM (mm)	CV (%)
Case 1	0.57	32.03	0.56	32.45
Case 2.1	0.54	33.05	0.53	33.1
Case 2.2	0.56	32.18	0.54	32.6
Case 2.3	0.57	32.03	0.56	32.4
Linear MPC				
Sánchez et al., 2006	-	-	0.46-0.49	23.3
Batch NMPC				
Sánchez et al., 2007	-	-	0.56	33.9
Reference values for AM=0.55(mm), CV=33%				

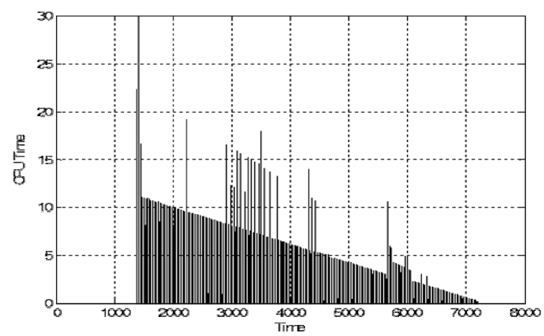

Fig.10 CPU time per iteration [s] along the process duration when applied to the batch NMPC

7. CONCLUSIONS

The main contribution of this work is the introduced neural network (NN) based MPC cascade operation strategy for a fed-batch evaporative sugar production. The overall process is divided into a sequence of stages (four control loops) and for each of the loops an individual NN-MPC is designed to satisfy a number of intermediate reference set points. NN nonlinear partial process models are associated to each of the controllers. The main conclusion is that the NN technique can produce a reliable model to be used for a model based control, based only on input-output information for a process stage. However, the main restriction is to provide sufficient data covering the usual operation regimes. The NN-MPC outperforms the linear MPC in terms of final quality measures (MA and CV) and the digital nonlinear batch MPC in terms of computational cost.

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