

**ADAPTIVE CONTROL USING A HYBRID-NEURAL MODEL:
APPLICATION TO A POLYMERIZATION REACTOR**

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ABSTRACT

This work presents the use of a hybrid-neural model for predictive control of a plug flow polymerization reactor. The model type was the so-called "Hybrid-neural Model" (HNM), which is based on fundamental conservation laws associated with a neural network (NN) used to model the uncertain parameters. By simulations, the performance of this approach was studied considering a peroxide initiated styrene tubular reactor. The HNM was synthesised considering a CSTR reactor with a Radial Basis Function neural net (RBFN) used to estimate the reaction rates recursively. The adaptive HNM was incorporated in two model predictive control strategies, a direct synthesis scheme and an optimum steady state scheme. Tests for servo and regulator control showed excellent behaviour following different setpoint variations, and rejecting perturbations. Good generalisation and training capacities of hybrid models, associated with simplicity and robustness characteristics of the MPC formulations, make an attractive combination for the control of a polymerization reactor.

Keywords: polymerization control, neural networks, hybrid-neural model.

INTRODUCTION

The use of neural networks (NN) for modelling dynamic non-linear systems, like polymerization processes, has been the subject of a great deal of recent research work. Some important features of neural network models used for process applications are their capability to act as universal approximators to non-linear functions, their applicability to multivariate modelling and their ability to assess process dynamics (Bishop,1994). Most of the efforts have been put on developing non-parametric or black box models that correlate a set of input variables with the corresponding outputs.

However, in many cases it seems to be convenient to take advantage of previous

knowledge of the non-linear system, frequently expressed as a set of ordinary or partial differential equations representing mass or energy balances. In polymeric processes, the most difficult modelling task remains the determination of some key parameters, as the reaction rates, and the extensive variation of the species properties, which are usually complex functions of the various state variables.

To cope with this problem, hybrid-neural models have been suggested (Psichogios and Ungar, 1992) which combine prior knowledge included in the phenomenological model with neural networks. This kind of model has proved to be successful for dynamic systems, with better generalisation features. In addition, they can be identified with a more reduced set of data than the black-box equivalent model (Psichogios and Ungar, 1992). Thompson and Kramer (1994) classified these hybrid models into two main types: series models bringing intermediate values (parameters or variables) to be used by the phenomenological model and parallel models compensating the bias of the parametric model. Van Can et al. (1996) demonstrated that the series approach results in more accurate models, with better dimensional and range extrapolation properties than the other approaches.

Taking the mentioned advantages, different forms of neural network models have been considered as non-linear models for advanced control algorithms. The ability to approximate almost any non-linear multivariable function, its robustness in stochastic environment and its simpler construction have encouraged the extensive use of neural networks, both in academic and industrial domains (Ungar et al,1996).

Specifically, Model Based Controllers (MBC) with non-linear dynamic models based on neural networks have been studied by Hernández and Arkun (1990); Nahas et al. (1992), Psychogios and Ungar (1991), with promissory results. Even though they are generally successful, process models based on neural networks need a great number of adjustable parameters (network weights) resulting in two main problems: a big computational load to train the network (weight adaptation) and the possibility of over-fitting, with a lose of generalisation capacity when a reduced numbers of data pairs are available for training (excess of degrees of freedom).

Those two problems can be minimised if some prior knowledge is used in the model construction, such as HNM. Since HNM's neural net has fewer parameters than a pure *black box* NN model, an on-line training method may be used in order to obtain adaptive HNM. For on-line adaptation, several neural network structures and training algorithms have been informed, one of them, the Radial Basis Function Nets (RBFN) has outputs linearly combined which allows the use of RLS type algorithms for the estimation of the network weight.

In this paper, we used an HNM with a RBFN neural network to control a simulated polymerization reactor using two model predictive control schemes. Initially, the basis of hybrid-neural models and RBFN neural nets are presented, followed by process description and HNM synthesis. Finally, the control algorithms, implementation and results are showed and discussed.

HYBRID-NEURAL MODELLING

Hybrid-neural modelling technique uses a process model based on fundamental principles, associated with a neural network (NN) to estimate parameters which are uncertain or difficult to model. In this way, some previous knowledge is incorporated into the black box model, to reduce complexity and improve adaptation and prediction properties (Psichogios and Ungar, 1992). A schematic representation of this kind of model is shown in Figure 1.

----- > **Figure 1**

In 1992, Psichogios and Ungar applied this hybrid modelling scheme to a simulated bioreactor. They estimated bacterial growth parameters with a one hidden layer feedforward neural net. Results indicated an excellent prediction behaviour and good adaptation to noisy data. More recently, Thompson and Kramer (1994) have presented a general framework of model synthesis, by combining prior knowledge and neural network where HNM is classified as a serial semi-parametric approach. HNM has been also proposed as a generalized framework to model particulate drying processes (Cubillos et al., 1996).

Obviously, hybrid models have more information using explicit conservation restrictions than empirical ones, and better results should be expected. Besides, hybrid-neural modelling has two main advantages when compared to pure phenomenological modelling: a better prediction capacity of model parameters by using all influencing variables and the possibility of reducing the model complexity, and absorbing the consequent error during the neural network training procedure (Cubillos et al.1996). This results in a hybrid model that is generally simpler than the phenomenological one. Hybrid-neural model formulation methodology includes the following steps: 1) Development of mass, energy and momentum balances which, together with

thermodynamic and transport relationships, allowing the link between input and output variables with model parameters. 2) Selection of model parameters that will be estimated through NN, and determination of their dependence on input variables. 3) NN structure determination and training using existing process data.

Radial Basis Function Neural Networks.

Neural networks are non-parametric models formed by process units called nodes or neurons, ordered in layers, fully or partially interconnected. The main property is their ability to approximate non-linear functions in multidimensional space. Between many topologies associated to NN paradigm, the principal type used is the feedforward neural network (FFNN), where information travels exclusively from inputs to outputs nodes. For non-linear functional approximations, FFNNs with one hidden layer and sigmoidal type activation functions are the most popular structures because they proved to be able to approximate any continuous non-linear functions (Hornik et al,1989).

As alternative, the radial basis function neural networks (RBFN) have been used with success as dynamic models of non-linear processes (Nahas et al.,1992; Chen et al,1991). They have the great attractive that its structure is linear in the parameters, which allows to use some kind of recursive identification algorithm. The RBFN architecture is a two-layer processing structure. The first layer consists of an array of computing units. Each unit contains a parameter vector called centre, where the confluence is calculated as the Euclidean distance between the centre and the network input vector. The unit then passes the result through an activation function. The second layer is essentially a linear combination between the outputs hidden layer and their outputs weights.

The most common activation function used in RBFN is the Gaussian function:

$$\mathbf{a}_i = \exp \left(- \mathbf{n}_i^2 \right) \quad (1)$$

In this work, the goal is to develop a hybrid-neural model, where the unknown parameters (the kinetics rates) are estimated by a RBF neural network that could be trained recursively and included into a predictive-adaptive control scheme.

PROCESS DESCRIPTION AND HYBRID-NEURAL MODELLING

A polymerization reaction in solution carried out in a PFR reactor has been chosen as a simulated process. The tubular reactor has one feed stream, composed by styrene monomer, benzoyl peroxide as initiator of the reaction and toluene as solvent. The exit stream contains polymer, unreacted monomer, initiator and solvent. Feed flow rate and the reactor jacket temperature can be used as manipulated variables for controlling the quantity and quality of polymer. In this work the reactor jacket temperature is the manipulated variable and feed flow rate is used as perturbation variable to the system.

The mechanism of vinyl polymerization used is given in Table 1. It considers that the lifetime of the radical species is extremely short, therefore a quasi steady state approximation may be assumed.

Based on the previous mechanism, an approximated model of the process was developed with the following assumptions: laminar flow, physical properties variable with temperature, radial and axial distribution of the species concentration (monomer, initiator, and polymer), parabolic velocity distribution and uniform reactor temperature equal to jacket reactor temperature (Vega,1995).

Table 1: Kinetic mechanism for styrene reaction in solution. (Vega, 1995)

Initiation	$I \xrightarrow{k_d} 2R^\bullet$ $R^\bullet + M \xrightarrow{k_i} P_i^\bullet$
Thermal initiation	$3M \xrightarrow{\Delta, k_{tr}} 2P_i^\bullet$
Propagation	$P_i + M \xrightarrow{k_{p_i}} P_{i+1}^\bullet$
Transfer for the solvent	$P_i + S \xrightarrow{k_{tr,s}} \Lambda_i + S^\bullet$ $S^\bullet + M \xrightarrow{k_{tr,s}} P_1^\bullet$
Transfer for the monomer	$P_i + M \xrightarrow{k_{tr,m}} \Lambda_i + M^\bullet$ $M^\bullet + M \xrightarrow{k_{tr,m}} P_1^\bullet$
Termination for combination	$P_i + P_j \xrightarrow{k_{tc}} \Lambda_{i+j}$

According to these assumptions, the material balance for each component in the reactor is given for the following equation:

$$\frac{\partial c_i}{\partial t} + v_z \frac{\partial c_i}{\partial z} = R_i \quad (2)$$

This model was solved numerically by spatial finite differences taking 10 segments in axial direction and 3 discrete segments in radial direction, giving 90 differential equations in total, which were integrated using a variable step RK method.

The simulation considers a pilot plant PFR reactor with 12 m in length and ¼" ID.

Detailed process conditions and parameters may be found in Vega (1995).

Hybrid-neural Model

The synthesis of an HNM for the considered process was carried out taking the considerations indicated above and based on the following assumptions:

- The process is carried out in an hypothetical CSTR type reactor.
- The kinetics of each species is unknown.
- The net reaction rate of each species (NN_{Ri}) can be estimated adequately by a RBFN neural network.

Based on these assumptions, mass balance equations for each species are described by:

$$\frac{dc_i}{dt} = \frac{F}{V} \cdot (c_{i0} - c_i) + NN_{Ri} \quad (3)$$

In order to obtain an explicit predictive model, a simple time discretization over a sample time Δt on Equation 2 gives the following equation for species concentration at an instant $k+1$:

$$c^{k+1} = c^k + \left(\frac{F}{V} \cdot (c_i - c_{i0}) + NN_{Ri}^{k+1} \right) \cdot \Delta t \quad (4)$$

NN_{Ri} indicates the net reaction rates for each species (monomer, initiator, and polymer) and they are estimated by the RBFN as a function of measured process variables as jacket temperature and exit concentrations at actual and delayed sample times.

The best topologies of the RBFN's were obtained through several off-line tests varying randomly the jacket temperature and applying the method suggested by Ungar et. al. (1996). The data set was split into a training set including 300 patterns and a test set with 200 patterns. For the training, experimental values of the reaction rates were obtained by inverting equation 4. Gaussian activation functions and an orthogonal RLS algorithm were used to obtain the basis centres and outputs connections weights. The best structure was a RBFN with 3 radial basis with both reactor jacket temperature and species concentration delayed one sample time as inputs. Figure 2 gives the complete HNM scheme.

----- > **Figure 2**

CONTROL ALGORITHMS

The design of the control algorithms used in this work was made taking the Nonlinear Model Predictive Control (NMPC) framework. In this formulation, an optimization problem must be solved in each sampling time to find a sequence of M control actions u from the current instant (k) until the instant (k+M-1). The objective function is the difference between the setpoint and the predicted output over the next P time steps. The formulation of this controller is given by (Qin & Badgwell,1997):

$$\min_{\substack{\Delta u(k) \\ \Delta u(k+M-1)}} \sum_{i=1}^P [\hat{y}(\mathbf{k+i}) - y_{set}(\mathbf{k+i})]^2 \quad (5)$$

In this scheme, the adaptive HNM model gives the prediction of the output plant. Considering the above formulation, two extreme cases were studied:

- i) A direct synthesis control scheme (DSC), with $M=1$, $P=1$. This means that the manipulated variable $u(k)$ is calculated such that the output of the process will be equal to the setpoint in the next sampling instant.
- ii) A Steady State Optimizing scheme (SSO), equivalent to use $P = \infty$, that is to find the value of $u(k)$ such that the process reaches an output steady state equal to the setpoint. This formulation makes use of the phenomenological character of the HNM model, because through equation (3) an explicit expression for the concentration at steady state may be obtained, if an appropriate prediction of the net reaction rate is available.

IMPLEMENTATIONS AND RESULTS

Based on the above considerations, a complete simulation shell was implemented using the Simulink dynamic simulation environment including the simulated process, the HNM model with the RBFN trained on-line, and the two NMPC control strategies. In this adaptive control scheme, the centres of the RBFN, obtained from off-line training, are maintained constant whereas the outputs weights of the RBFN are re-estimated on-line using a RLS algorithm with constant forgetting factor.

The variables were suitable scaled between -1 and 1 for RBFN training and for the solution of the optimization problem. The sampling time was 0.5 min and a SQP routine was used to solve the optimization problem at each sampling time. Additional bounded limits for the manipulated variable were included. The monomer concentration C_m was selected as controlled variable.

Different tests were carried out considering changes in setpoint and perturbation. Some data were corrupted with white noise. As comparison, an equivalent DSC controller using a black-box type neural network model was included. In all these tests was

necessary to carry out an initial sequence of adaptation before operating the system in closed loop. It was observed that the HNM model converges more quickly and it is more stable than the black box model. The figures 3 and 4 show results for setpoint tracking obtained for DSC and SSO controllers, without noise and corrupted with +/- 10% of the concentration measurement, respectively. Figure 5 illustrates the capacity of the DSC formulation (HNM and black box) to eliminate a series of perturbations in the feed flow rate.

-----> **Figures 3,4,5**

DISCUSSIONS AND CONCLUSIONS

Based on the results of this work, it is possible to assure that the hybrid-neural model is suitable to be used in NMPC type controller, in an adaptive fashion. Using RBFN to describe the kinetic rates into the HNM, on-line re-estimation was available. Results from different control tests show that the adaptation capacity of HNM is higher than a black box type neural model, both in the previous initialization as well as in rejecting perturbations. This is due to the fact that HNM has less parameters to estimate than the black box model, and also, the equations of the hybrid model are hard bounded, limiting the model outputs and improving the prediction.

Regarding the tests of setpoint tracking, (Figure 3), DSC with HNM and the black box model exhibit similar results, with cumulative squares errors (ISE) of 0.11 and 0.12 respectively. Also, it is observed that the SSO formulation followed the setpoint with an asymptotic behaviour, but with a worse dynamics (ISE=0.23). The same tendency is observed when the controlled variable is corrupted with white noise (Figure 4) confirming the property of noise cancellation of neural networks.

In general, we can conclude that the studied formulations are adequate for the control of time-varying non-linear systems such as polymerization processes, where high interference and variations in their parameters justify an on-line adaptive adjustment. In particular, the inclusion of a HNM model improves the auto-adjustment capacity and prediction notably. It is also possible to assure that the steady state optimizing formulation (SSO) can be used as a suitable model for real time optimization, with more ambitious indexes such as economics or environmental, but with poorer dynamic efficiency.

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NOTATION

a_i	Output of node i of the layer RBF neural network.
c_i	Concentration of i specie
c_{i0}	Initial concentration of specie i
F	Volumetric Flowrate
I	Initiator concentration
$k_d, k_i, k_{IT}, k_{Pi}, k_{tr,s}, k_{tr,m}$	Kinetic parameters.
y_{set}	Setpoint
M	Control horizon
M	Monomer concentration
n_i	Confluence function of node i
NN_{Ri}	Net reaction rate of specie i estimated by HNM.
P	Prediction Horizon
P	Polymer concentration
R	Radical concentration
R_i	Net reaction rate of specie i
S	Solvent concentration
t	Time
u	Manipulated variable
V	Reactor volume
v_z	Axial velocity
y	Controlled variable
z	Axial position

CSTR	Continuos Stirred Tank Reactor
DSC	Direct Synthesis Controller
HNM	Hybrid-neural Model
ISE	Integral of the Square Error
MBC	Model Based Controller
NN	Neural Network
OSS	Optimizing Steady State Controller
NMPC	Nonlinear Model Predictive Control
PFR	Plug Flow Reactor
RBFN	Radial Basis Function Network
RK	Runge Kutta Integration Method
RLS	Recursive Least Square
SQP	Sequential Quadratic Programming

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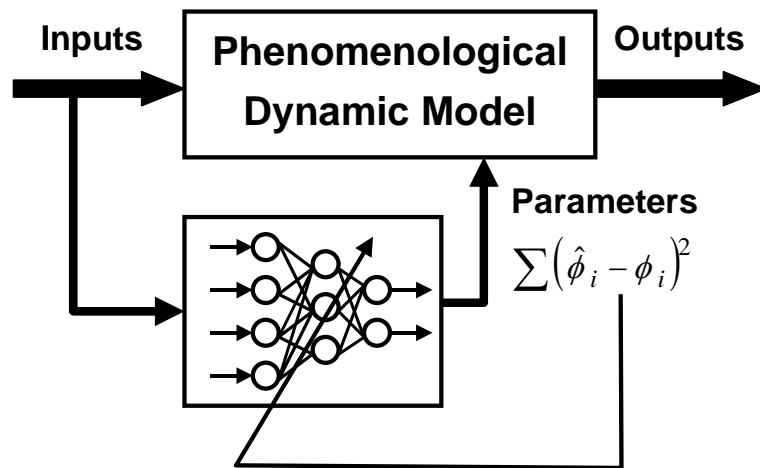


Figure 1 : The hybrid-Neural modelling approach

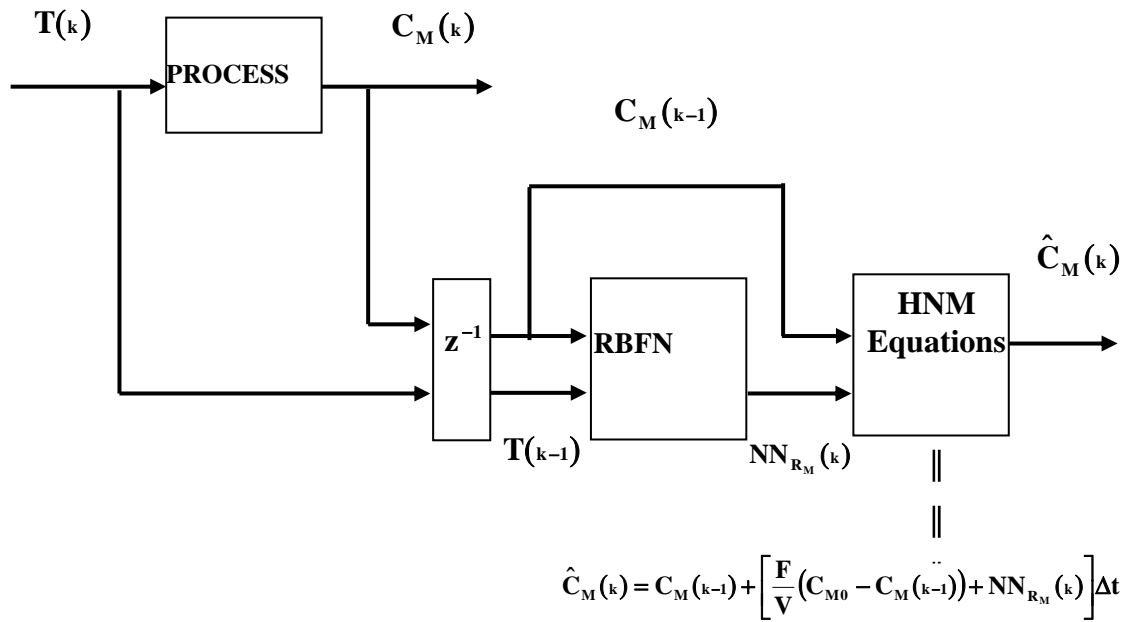


Figure 2 : The HNM for the polymerization reactor

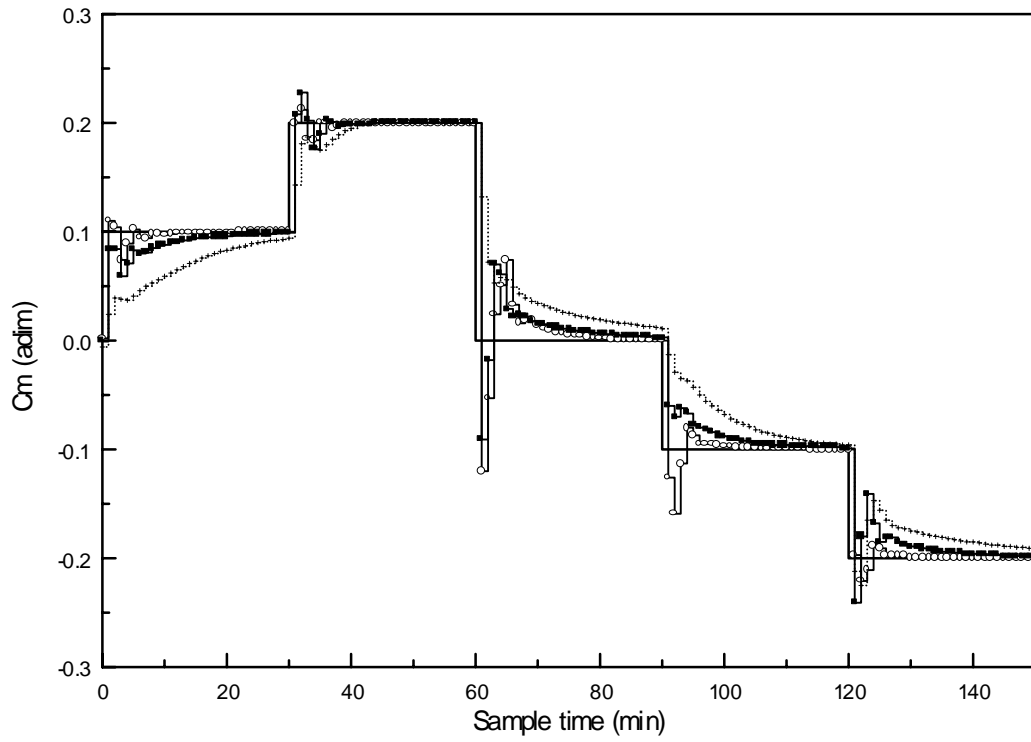


Figure 3: Results for setpoint tracking. (SSO + ; DSC Black-Box O, DSC-MNM v)

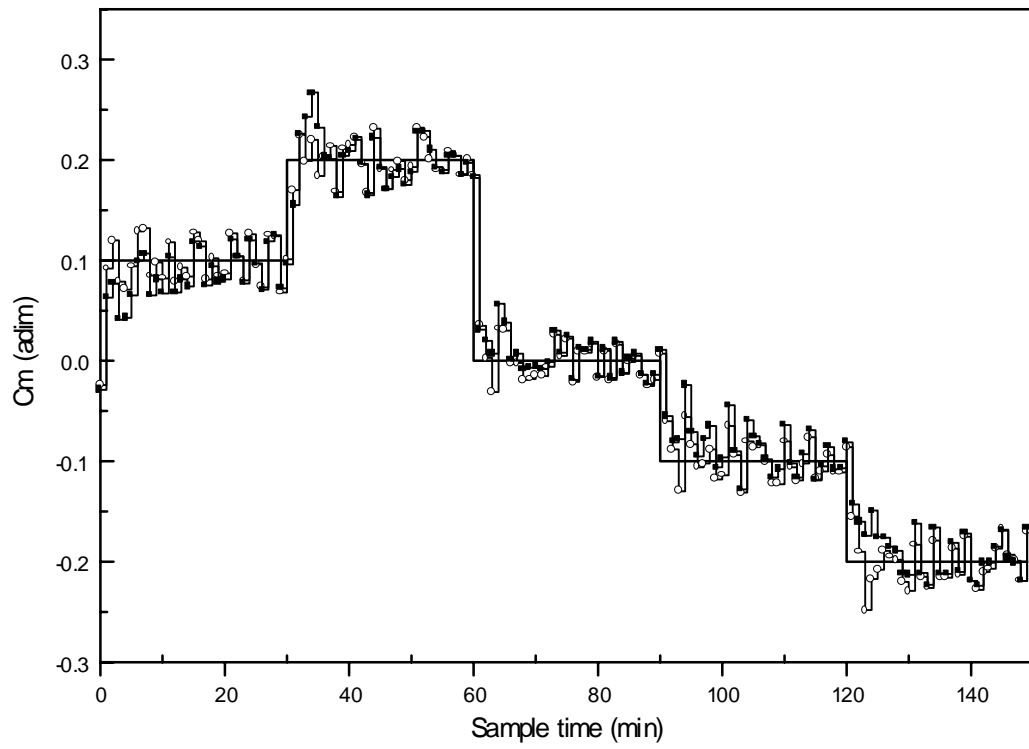


Figure 4: Results for setpoint tracking with noise environment (DSC Black-Box O, DSC-MHN v)

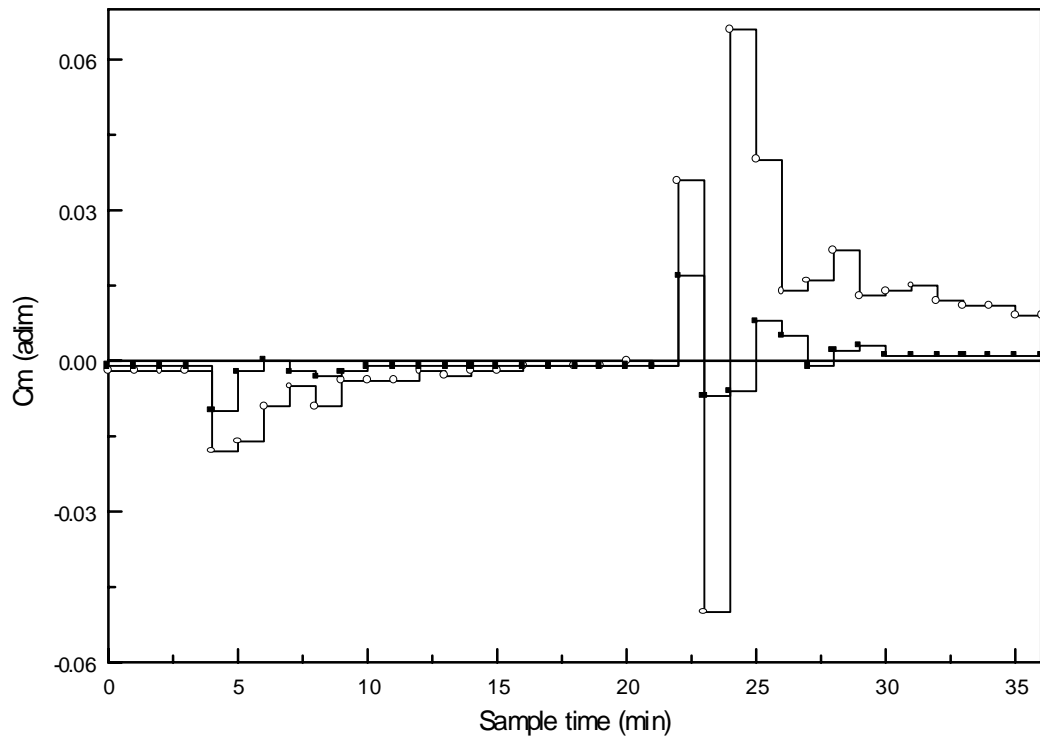


Figure 5: Results for perturbation rejection (DSC Black-Box O, DSC-MHN v)