

## Real-Time Optimization Systems Based On Grey-Box Neural Models

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### Abstract

This paper investigate the feasibility using of grey-box neural type models (GNM) for design and operation of model based Real Time Optimization (RTO) systems operating in a dynamical fashion. The GNM is based on fundamental conservation laws associated with neural networks (NN) used to model uncertain parameters. The proposed approach is applied to the simulated Williams-Otto reactor, considering three GNM process approximations. Obtained results demonstrate the feasibility of the use of the GNM models in the RTO technology in a dynamic fashion.

### 1. Introduction

The online optimization of chemical plants has enjoyed considerable industrial interest because of its capacity to achieve competitive advantages in the marketplace. Numerous successful applications of the real-time optimization in industrial practice have been reported (Nath and Alzein, 2000). The economic performance of an RTO system is measured by the expected profit achieved, which is strongly influenced by the quality of the model used (Loeblein and Perkins, 1998). The RTO systems reduce the plant/model mismatch by updating the model using actual and historical plant data sets (Yip and Marlin, 2002). Because the RTO execution is time consuming, simple phenomenological steady state models are currently used. In practical situations, however, it is difficult to reach the steady state among each RTO execution period, leaving the plant in a permanent state of slow dynamic changes. Under this condition model is not entirely consistent and an inefficient update process could reduce the economic performance of the plant. The key to solve this problem is the use of phenomenological dynamical plant models, that have the disadvantages of being difficult to obtain and difficult to update in real time.

An alternative way of solving this difficulty is the use of dynamical models, based on combinations of first principles and neural networks (NN), called grey-box neural models (GNM). A GNM normally consists of a phenomenological part (heat and/or mass balances differential equations) and an empirical part (a neural network in this work). Due to the inherent flexibility of NN, models based on this structure are well suited to represent complex functions such as those encountered in chemical reaction processes. This work proposes incorporate in the RTO system a dynamical GNM of the

plant based on phenomenological principles and neural networks. The model update is equivalent to the network training. But, the main reason for the use of this approach is the fact that a steady state equivalent model may be easily derived from the dynamical GNM and used efficiently in the optimization step.

## 2. Grey-box neural models (GNM)

Neural networks are non-parametric, massively connected models that perform quite well for approximating nonlinear, multivariable functions. This unique property has allowed using them successfully in predictive control of nonlinear processes. Grey-box Neural Models combine a phenomenological model of the system with neural networks, which estimate the uncertain parameters of the process. This technique enables the synthesis of simpler mathematical models than purely phenomenological ones, with more robust generalization properties than purely NN models. These two properties make the GNM especially attractive in tasks associated with Process Identification, Process Control and Optimization, (Cubillos and Lima, 1998; Xion and Jutan, 2002). The GNM technique consists on formulating a process model, formed by equations derived from phenomenological principles - such as mass, energy and momentum balances - and neural networks, dedicated to estimate those parameters difficult to model or uncertain. This form of representation is an attempt to add prior knowledge to black-box neural models, in order to reduce its complexity and improve their adaptive and predictive properties (Psichogios and Ungar, 1992). Thompson and Kramer (1994) classified these grey-box models into two main types: NN bringing intermediate values (parameters or variables) to be used by the phenomenological model (*series grey-box models*) or NN in parallel with the dynamic model compensating the plant/model mismatch (*parallel grey-box models*). Figure 1 shows the series scheme for a Grey-box model as used in this work.

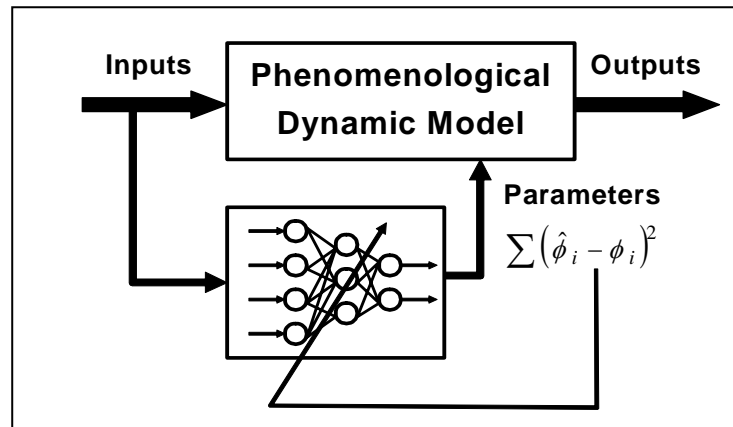


Figure 1 : The GNM approach

### 3. Process descriptions

In this work we applied the proposed approach to the simulated CSTR reactor from the Otto-Williams benchmark plant modified by Forbes and Marlin (1996) that may be described by elementary kinetics. The reaction sequences are:



Instantaneous profits can be expressed as a function of the feed and product flowrates as (Forbest et al.,1994)

$$P = 1143.38 * X(P) * Fr + 25.92 X(E) * Fr - 76.23 * Fa - 114.34 * Fb \quad (2)$$

The ideal CSTR had no reactor temperature dynamic, and the manipulated variables to optimize where  $Tr$  and flowrate of B component ( $Fb$ ).  $Fa$  and  $M$  were set to [ 2 Kg/s, 10220 Kgs].

#### GNM synthesis

To study the feasibility of the use of the GNM type models in the RTO technology, three different modelling schemes were selected as described in Fobest et al. (1994):

- i) Single reaction approximation (M1): [  $A + 2B \rightarrow P + E$  ]
- ii) Two reactions approximation (M2): [  $A + 2B \rightarrow P + E$  ;  $A + B + P \rightarrow G$  ]
- iii) Complete three reactions system (M3) as described in (1).

Each GNM was synthesized considering the non stationary mass balance for each species. Feedforward neural networks were added to estimate the hypothetical reaction rates with unknown kinetics. Target reaction rates were calculated directly from discretized mass balances. For example, for a single reaction model (M1), P component balance may be used to estimate unique reaction rate given by:

$$R_k = (Fr * X(P)/M)_{k+1} - (X(P)_k - X(P)_{k-1}) / To \quad (3)$$

In order to obtain adequate data estimation for the reaction rates, PRBS input sequences in  $Fb$  and  $Tr$  were introduced, using a sample time of 1000 sec. Operation conditions and outlet concentrations were register to train the neural networks. The model update that consists of the NN adaptation was carried out using a second order recursive algorithm. The best NN structures were found by a systematic training procedure, considering outlet concentrations of A and B components and the reactor temperature as the inputs to the networks. Finally, networks with one hidden layer with four nodes and sigmoidal activation functions were selected.

Based on the updated dynamic GNM it was possible to derive an equivalent steady state model able to be used for optimization purposes.

To illustrate the approach, considering the two model approximation (M2), the model has to estimate two reaction rates (R1 and R2) using a neural networks. In the steady state the model equations are:

$$\begin{aligned}
 &F_a - (F_a+F_b)*X(A) - R_1*M - R_2*M = 0 \\
 &F_b - (F_a+F_b)*X(B) - 2*R_1*M - R_2*M = 0 \\
 &-(F_a+F_b)*X(P) + R_1*M - R_2*M = 0 \\
 &-(F_a+F_b)*X(E) + 2*R_1*M = 0 \\
 &-(F_a+F_b)*X(G) + 3*R_2*M = 0
 \end{aligned} \tag{4}$$

A similarly approach was used to derive the other GNM models, where the NN' were used to estimate the respective reaction rates. Figure 2 shows the prediction of the outlet concentration for E product using M2 model. Similarly results are found for the M1 and M3 models showing that the GNM scheme is able to adequately track the process dynamic.

#### 4. RTO results

The GNM approach with the three alternative adapted models were tested in the RTO scheme considering similar operation conditions as used by Forbes and Marlin (1996), with feed flow rate and reactor temperature as the optimization variables. The optimization problem is to maximize the profit, as indicated in Equation 2, constrained by the corresponding dynamical GNM models. A dynamical test applied considering the reactor operating in a non optimum point. At a pre-established time, the RTO is connected to the plant, running each sample time, in order to position the process at the optimum. Current reactor states were using as initial guess to the next optimization step. Figure 3 shows the behavior of the RTO system for the three GNM models and the true model over a time horizon of 22000sec (21 RTO executions).

Results indicate that all GNM models were able to find an optimally set of inputs close to the true optimum and maintained this conditions over the time. It can be observed that the deviations respects to the nominal optimum are more severe when more inexact is the process model using in the RTO. Other issue observed is the sensitive of the RTO/GNM system to the initial conditions in the optimizer. In order to compare the performance of each model considered in this work, a dynamic performance index, defined as the total profit obtained over the time window was calculated and shown in Table 1. Results show that a more exact model brings best performance, specifically the three reaction model.

Table 1: Cumulative profit

MODEL	True	GNM/M1	GNM/M2	GNM/M3
Total Profit (\$)	8663	8237	8537	8576

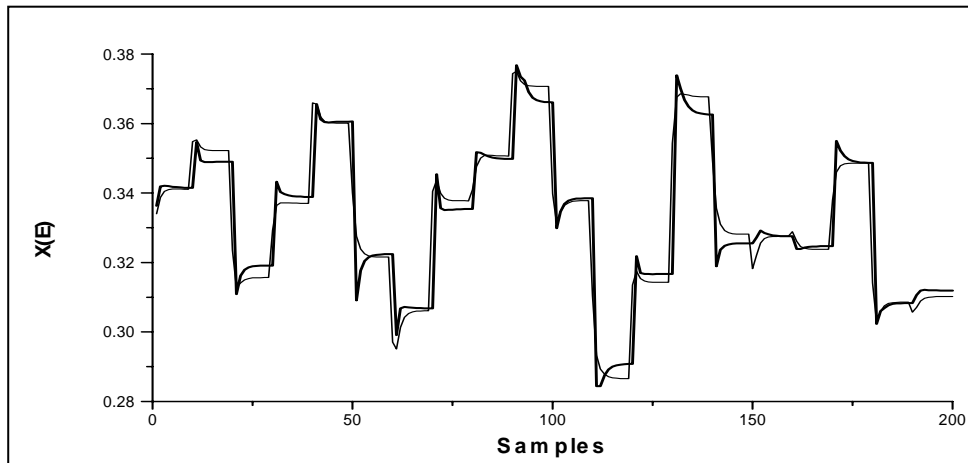


Figure 2: Actual (cont) and prediction (dash) E concentration by GNM/M2 model

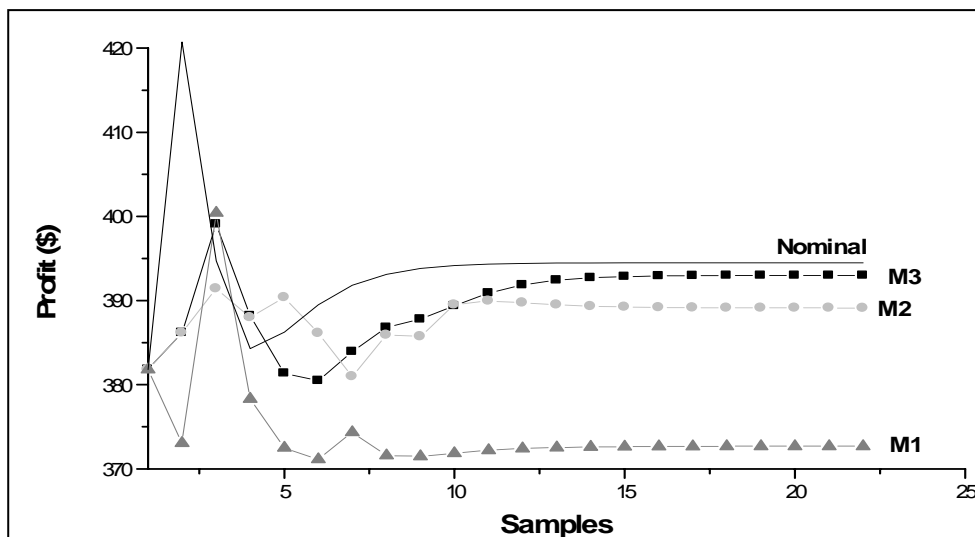


Figure 3: Instantaneous profits

## 5. Conclusions

The obtained results demonstrate the feasibility of the use of the GNM models in the RTO technology in a dynamic fashion. We considered that this approach introduces improvements in the RTO technology, allowing extension to highly non linear plants, feasibility of on-line adaptation using dynamical information and the integration among MPC – RTO systems by using current plants models. However, issues as models adequacy to optimization task should be analyzed in depth.

### Notation

F<sub>a</sub>,F<sub>b</sub> = Inlet flow rates  
F<sub>r</sub> = Outlet flow rate  
M = Reactor Mass holdup  
P = Economic objective function  
R = Reaction rate (in mass)  
T<sub>o</sub> = Sample time  
T<sub>r</sub> = Reactor temperature  
X(i)= composition of component i in mass fraction

### Subscripts

i = component i  
k= Sample instant

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