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# A Combined Closed Loop Optimal Design of Experiments and Online Identification Control Approach\*

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**Abstract:** The main contribution of this paper is to propose a new approach, based on any specified continuous nonlinear model, for the combined optimal closed loop control of a process and online identification of a given model parameter. It deals with the optimal design of experiments: the idea is to twofold: first, based on a sensitivity model based predictive control, find the value of the input to apply during the experiment that allows optimizing a criteria based on the sensitivity of the process measure with respect to the unknown model parameter. Secondly, and in the meantime, based on the input/output measures collected, a process model and an observer, estimate online the model parameter. Moreover, constraints dealing with input, state and output limitations are accounted for. The main advantage of this approach is that both optimal control task and identification task are solved together online in order to get the online estimation of the unknown model parameter. This approach is applied here on a simple case in chemical engineering.

**Key Words:** Nonlinear System, Nonlinear Observer, Parametric Sensitivity, Predictive Control, Optimal Design Of Experiments, Identification.

## 1 INTRODUCTION

Identification is the task which aims to determine the numerical value of the unknown process model parameters [1, 2], based on experimental data. Unfortunately, due to the possible lack of relevant informations in the experimental data (maybe due the difficulty to get them), some of the parameters may not always be easily identified. In order to know if these data are rich enough to be used for identification, the sensitivity of the process output  $y_p$  (the measure) with respect to the unknown process parameter  $\theta$  tells us how it is possible to identify the parameter from the data. It is usually used to define the Fisher Information Matrix (FIM), whose norm is often used for this kind of study. If the sensitivity of the measured process output with respect to the unknown process parameter is small or null, this may be due to one (or more) of the following problems: 1/ the parameter does not influence this output, or 2/ the output is not well chosen, or 3/ the input signal applied on the process does not sufficiently excite the measure. This work focuses on the third problem: based on a nonlinear model, it deals with the closed-loop control problem for the optimal design of experience [3-5] coupled with the online identification of one process parameter [6, 7]. The main question is: how the input signal, to apply to get the experimental data from the plant, may be optimally tuned online such that the model parameter is estimated at the same time, based on the richest output data (in terms of the norm of the sensitivity  $\frac{\partial y_p}{\partial \theta}$ )? Moreover, some constraints have to be specified during the identification phase, in order to have a correct use of the process. In this framework, for nonlinear systems, the authors [8, 9] have presented a methodology to get an optimal design of experiments (DOE), for the parameters estimation in the field of bioreactors. Keesman and Stigter [10] have found analytic solutions for the design of the optimal input

$u$  for a parameter estimation based on a specific model. In this case, the control law was obtained explicitly from several differentiations of the optimality condition of Pontryagin  $\frac{\partial H}{\partial u} \equiv 0$  (where  $H$  is the hamiltonian formulation associated to the model and the cost function, depending on the parametric sensitivity  $\frac{\partial y_p}{\partial \theta}$ ). Stigter, Vries and Keesman [9] have presented another adaptive approach where the input design was solved online for a bioreactor. In this case, the online estimation of the sought model parameters was introduced in the control law design, which is based on the FIM. The online estimation of the parameters was obtained by a recursive estimation algorithm.

In this paper, a new control approach to be used during the identification task is presented, which is based on the optimization of the sensitivity of the process measure with respect to the sought model parameter. In the meantime, the input/output data are used for the online estimation of this parameter, and some constraints are accounted for. This approach, that couples a closed loop controller and an observer, solves at the same time the control task and the parameter estimation task. A dynamic model of parametric sensitivity (obtained explicitly from the process model) is also employed online to get the needed sensitivity of the process measure with respect to the sought model parameter. The closed loop controller is a model predictive controller (MPC), which is also based on the process model. Some constraints may be handle in the optimization task. Since it is formulated in a general framework with realistic assumptions, this method is relatively simple to use for any particular model.

This paper is organized as follow: section 2 aims to recall some basic principles of MPC. Then, in section 3, the new approach for MPC for the closed loop optimal design of experiments for online identification is given. In section 4, results are presented for a case study. In order to simplify

the notation, scalar variables are handled here (for the input, the output and the unknown model parameters), whereas the known model parameters and the state variables may be defined as vectors.

## 2 MODEL PREDICTIVE CONTROL: SOME RECALLS

Even if the original idea of MPC was given by Bellman in the 1950's, this idea started to be used in the industry only in 1978 with the software IDCOM of Richalet. In 1980, the DMC approach of Cutler and Ramaker appeared. In these 2 approaches, a black-box model was used. Since that time, MPC tools were improved (QDMC, SMOC, IDCOM-M, HEICON, DMC+, RMPCT, etc.). The reader may find in [11] more historical facts about MPC, as well as more precisions about the technical and theoretical evolutions of MPC. According to the authors of this survey, MPC was concerned, in 2003, with more than 4000 applications in total in the world, without adding local solutions. The main idea of MPC is to insert in the feedback loop an element of process behavior prediction. The computer then determines, using the constrained optimization of a criterion  $J$  over the prediction horizon  $N_p$ , at the current sampled time  $k$ , the control sequence to apply over the prediction horizon. At the next sampling time, only the first component of this sequence is applied as the process input. The process measure  $y_p$  is updated and the procedure is repeated. Since this control problem is solved numerically, the continuous signals are considered at some discrete times: at the present (resp. future) time of the discretized time  $k$  (resp.  $j$ ), where  $t = k * T_s$  (resp.  $t = j * T_s$ ) and where  $T_s$  is the sampling period. The MPC aims to solve a general constrained optimization problem defined as:

$$\begin{cases} \min_{\tilde{u}} J(\tilde{u}) = \sum_{j=k+1}^{k+N_p} F(y_p(j), x_p(k), u(j-1)) \\ \tilde{u} = \{p_u(1), \dots, p_u(n_{pu})\} \\ u(j) = f_u(p_u(i), j, k) \quad i \in [1, n_{pu}] \\ u \in U \subset \mathbb{R} \\ con_i(y_p(k), x_p(k), u(j-1)) \leq 0 \\ \forall k > 0, \forall j \in [k+1, k+N_p], \forall i \in [1, n_{con}] \end{cases} \quad (1)$$

where  $F$  represents the control objective (regulation, trajectory tracking, time minimization, etc.),  $p_u(i)$  are the elements of the  $n_{pu}$  control vector parametrization of the input  $u$  over the prediction horizon  $N_p$ . The input  $u$  is constrained explicitly (magnitude, velocity) by  $U$ . There are  $n_{con}$  constraints  $con_i$  on the measured output  $y_p$  and on the process states  $x_p$ , which gives implicitly new constraints on the input. Afterwards, the process model is introduced in this formulation to predict the process behavior in the future, which helps to solve numerically the problem. An observer may also be necessary if some of the process states are not measured.

## 3 APPROACH FOR COMBINED CLOSED LOOP OPTIMAL DESIGN OF EXPERIMENTS AND ONLINE IDENTIFICATION

The sensitivity of the process measure  $y_p$  with respect to the model parameter  $\theta$  determines if this parameter may be

identified, based on the input/output data. In this work, we are interested in the case where the input signal  $u$  must be optimally tuned to get the richest experimental data fed into the online estimation tool. In this part, a new closed loop optimal control strategy for online identification of an unknown process parameter is presented. A constrained controller and an observer are used, in order to maximize online the sensitivity of the process measure  $y_p$  with respect to the model parameter  $\theta$ , while handling some specified constraints. This approach is based on a (general) continuous (dynamic) nonlinear model of the process, described by ordinary differential equations (ODEs) or by partial differential equations (PDEs). The sensitivity model is explicitly derived from the original process model, and is used in the control law. The optimal input and the parameter estimation are both obtained online, and the parameter estimation is fed back into the control law, as an estimated input disturbance. The various elements of this new control structure are now presented: the initial control problem, a process model, a process observer, the sensitivity model and the final formulation of the constrained optimal problem for identification based on the model.

### 3.1 Initial formulation of the MPC problem

The initial question is: how to tune online the process input  $u(t)$  such that the process measure  $y_p(t)$  is the richest (in term of sensitivity) for its use in the online estimation tool? This may be formulated as a MPC problem, where the sensitivity of the process measure  $y_p$  with respect to the model parameter  $\theta$  must be maximized. In the meantime, during the use of the process for the identification task, some constraints must be satisfied, in order to maintain the process behavior inside a prescribed region:

- first, due to the physical constraints, the input found by the optimization task must be physically acceptable. Indeed, any actuator is limited in magnitude. Velocity limitations may also be present:

$$\begin{cases} u_{min} \leq u(t) \leq u_{max}, \quad \forall t > 0 \\ \Delta u_{min} \leq \frac{du(t)}{dt} \leq \Delta u_{max}, \quad \forall t > 0 \end{cases} \quad (2)$$

- the output and state variables must be kept inside a prescribed zone. It deals with safety, stability, or production specifications. These  $n_c$  constraints, which depend on the process output and the process state, may be formulated as:

$$\begin{aligned} c_i(y_p(t), x_p(t), \alpha, \theta, u(t)) &\leq 0, \quad \forall t > 0 \dots \\ \dots \forall i \in I^{n_c} &= \{1, \dots, n_c\} \end{aligned} \quad (3)$$

**Remark 1**  $\alpha$  and  $\theta$  are both model parameters, but  $\alpha$  is the vector of model parameter with known values, whereas  $\theta$  is the sought model parameter with unknown value.

Therefore, the initial constrained optimization problem for identification ( $COP_I$ ) may be formulated as:

$$(COPI_I) \left\{ \begin{array}{l} \max_{\tilde{u}} J(\tilde{u}) = \sum_{j=k+1}^{k+N_p} \left( \frac{\partial y_p}{\partial \theta}(j) \right)^2 \\ \tilde{u} = \{p_u(1), \dots, p_u(n_{pu})\} \\ u(j) = f_u(p_u(i), j, k) \quad i \in [1, n_{pu}] \\ \forall k > 0, \forall j \in [k, k + N_p - 1] : \\ u_{min} \leq u(j) \leq u_{max} \\ \Delta u_{min} \leq \frac{u(j) - u(j-1)}{T_s} \leq \Delta u_{max} \\ \forall k > 0, \forall j \in [k + 1, k + N_p], \dots \\ \dots \forall i \in I^{n_c + n_{co}} = \{1, \dots, n_c + n_{co}\} : \\ c_i(y_p(j), x_p(j), \alpha, \theta, u(j-1)) \leq 0 \end{array} \right. \quad (4)$$

The main problem in this formulation (4) is that, at each present time  $k$ , it can not be solved. Indeed, it is based on signals into the future  $j$ : the sensitivity of the process measure  $y_p$  with respect to the model parameter  $\theta$ , the process measure  $y_p$ , the parameter  $\theta$  and the process state  $x_p$ . These future values are not known at the present time  $k$ , whereas the process input  $u$  and the process measure  $y_p$  are the only data available at the present time  $k$ . In order to get an optimization problem that is numerically solvable, the idea is to approximate these signals based on the available data and estimations updated at each time  $k$ , and on the use of the process model at different steps in an internal model control structure. The elements required for this approximation are presented in the following parts.

### 3.2 Process model

In this approach, a model of the process is used. It is assumed that it may be represented by a set of nonlinear differential equations:

$$(M) \left\{ \begin{array}{l} \dot{x}(t) = f(x(t), \alpha, \theta, u(t)), \quad t > t_i \\ y(t) = h(x(t), \alpha, \theta, u(t)), \quad t > t_i \\ x(t_i) = x^{t_i}, \quad t = t_i \end{array} \right. \quad (5)$$

where  $x \in \mathbb{R}^n$ ,  $u \in U \subset \mathbb{R}$  and  $y \in \mathbb{R}$  are respectively the state vector, the input and the output.  $f$  and  $g$  are nonlinear functions.

**Assumption 1** In the system (5),  $f$  et  $h$  are  $C^1$ .

### 3.3 Process observer

One of the use of the observers [6, 7] is dealing with the online parameter estimation problem: indeed, the parameter to estimate may be considered as a new state variable and is combined to the model state to get an augmented state for which an observer has to be designed.

**Assumption 2** The state  $x_o$  of the observer ( $O$ ), constituted of the estimated process state  $\hat{x}_p$  augmented with the estimated parameter  $\hat{\theta}$ ,  $x_o = [\hat{x}_p \ \hat{\theta}]$ , is observable. Moreover, any input  $u$  render the system uniformly observable.

Many factors must be accounted for during the design of such a nonlinear observer: the model class, the observability of the states, the value of the process input and the sensitivity of the measure with respect to the state. Consequently, the synthesis of such an observer is strongly connected to

the structure of the model ( $M$ ) and to the control applied at the process input. Based on the assumption 2 and on the theory of nonlinear system observers, an observer is designed, based on ( $M$ ), in order to estimate online the process state variables  $\hat{x}_p(k)$  and the unknown model parameter  $\hat{\theta}$ . This parameter is therefore estimated at each sampling period by this observer, and its value is introduced in the predictive controller in order to improve the closed loop performances.

### 3.4 Sensitivity model

Let us now define the sensitivity model ( $M_\theta$ ) which describes the dynamic of the state vector  $x_\theta = \frac{\partial x}{\partial \theta} \in \mathbb{R}^n$  and the output  $y_\theta = \frac{\partial y}{\partial \theta} \in \mathbb{R}$ : they are respectively the sensitivity of the state of the model ( $M$ ) with respect to the parameter  $\theta$  and the sensitivity of the output of the model ( $M$ ) with respect to the parameter  $\theta$ .

$$(M_\theta) \left\{ \begin{array}{l} \dot{x}_\theta(t) = \frac{\partial}{\partial t} \frac{\partial f}{\partial x} \frac{\partial x}{\partial \theta}(t) = \dots \\ \dots f_\theta(x_\theta(t), x(t), \alpha, \hat{\theta}(t), u(t)), \quad t > t_i \\ y_\theta(t) = \frac{\partial h}{\partial x} \frac{\partial x}{\partial \theta}(t) = \dots \\ \dots h_\theta(x_\theta(t), x(t), \alpha, \hat{\theta}(t), u(t)), \quad t > t_i \\ x_\theta(t) = x_\theta^{t_i}, \quad t = t_i \end{array} \right. \quad (6)$$

### 3.5 Final Formulation

The previously described models ( $M$ ), ( $M_\theta$ ) and the observer ( $O$ ) are used to predict, in a future time  $j$  over the prediction horizon, the value of real signals, based on the actual errors available (at  $k$ ) between the process and the model. This error is classically assumed constant over the horizon, and is updated at each time  $k$ . Therefore, the signals used in the ( $COPI_I$ ) may be approximated at each time  $k$  into future time  $j$ :

$$\left\{ \begin{array}{l} \forall k > 0, \forall j \in [k + 1, k + N_p] : \\ x_p(j) = x_m(j) + (\hat{x}_p(k) - x_m(k)) \\ y_p(j) = y_m(j) + (y_p(k) - y_m(k)) \\ \frac{\partial y_p}{\partial \theta}(j) = \frac{\partial y_m}{\partial \theta}(j) + \left( \frac{\partial y_p}{\partial \theta}(k) - \frac{\partial y_m}{\partial \theta}(k) \right), \\ \forall k > 0 : \\ \theta = \hat{\theta}(k), \end{array} \right. \quad (7)$$

where all the following signals are used in the control law:

- $x_m(j)$  is the model state obtained at the time future  $j$ , computed at time  $k$ , by the resolution of the model ( $M$ ) over the prediction horizon  $N_p$  with the current input sequence  $\tilde{u}$ , with the initial state  $x_m(k)$  and with the estimated parameter  $\hat{\theta}(k)$ .
- $\hat{x}_p(k)$  is the process state estimated at time  $k - 1$  by the observer ( $O$ ), with the best previous input  $u(k - 1)$ , with the initial conditions  $[\hat{x}_p(k - 1) \ \hat{\theta}(k - 1)]^T$ . At time  $k = 0$ ,  $\hat{x}_p(k)$  must be initialized.
- $x_m(k)$  is the model state obtained at time  $k - 1$  by the resolution of the model ( $M$ ) from  $k - 1$  to  $k$ , with the best previous input  $u(k - 1)$ , with the initial conditions  $\hat{x}_p(k - 1)$  and with the estimated parameter  $\hat{\theta}(k - 1)$ . At time  $k = 0$ ,  $x_m(k)$  must be initialized.
- $y_m(j)$  is the model output given by  $x_m(j)$  in ( $M$ ).
- $y_p(k)$  is the measure available at time  $k$ .

- $y_m(k)$  is the model output given by  $x_m(k)$  in  $(M)$ .
- $\frac{\partial y_m}{\partial \theta}(j)$  is the modeled sensitivity of the model output  $y_m$  with respect to the parameter  $\theta$  at time  $j$ , computed at time  $k$ , with the resolution of the sensitivity model  $(M_\theta)$  over the prediction horizon  $N_p$ , with the current input sequence  $\tilde{u}$ , with the estimated parameter  $\hat{\theta}(k-1)$ , coupled with the resolution of the model  $(M)$  from the initial conditions  $\frac{\partial x_m}{\partial \theta}(k)$ .
- $\frac{\partial y_p}{\partial \theta}(k)$  is the modeled sensitivity of the process output  $y_p$  with respect to the parameter  $\theta$ , computed at time  $k-1$ , by the resolution of the sensitivity model  $(M_\theta)$  from  $k-1$  to  $k$ , with the best input  $u(k-1)$ , with the estimated parameter  $\hat{\theta}(k-1)$ , with the estimated process state  $\hat{x}_p(k-1)$  from the initial conditions  $\frac{\partial x_p}{\partial \theta}(k-1)$ . At time  $k=0$ ,  $\frac{\partial x_p}{\partial \theta}(k)$  must be initialized.
- $\frac{\partial y_m}{\partial \theta}(k)$  is the modeled sensitivity of the model output  $y_m$  with respect to the parameter  $\theta$ , computed at time  $k-1$ , by the resolution of the sensitivity model  $(M_\theta)$  from  $k-1$  to  $k$ , with the best input  $u(k-1)$ , with the estimated parameter  $\hat{\theta}(k-1)$ , coupled with the resolution of the model  $(M)$  from the initial conditions  $\frac{\partial x_m}{\partial \theta}(k-1)$ . At time  $k=0$ ,  $\frac{\partial x_m}{\partial \theta}(k)$  must be initialized.
- $\hat{\theta}(k)$  is the estimated parameter at time  $k$ , computed at time  $k-1$  by the observer, with the best previous input  $u(k-1)$  and the initial conditions  $[\hat{x}_p(k-1) \hat{\theta}(k-1)]^T$ . At time  $k=0$ ,  $\hat{\theta}(k)$  must be initialized.

Based on these approximations, the initial constrained optimization problem for identification ( $COPI_I$ ) is reformulated as ( $COPI_{NL}$ ), based on the considered nonlinear model of the process  $(M)$ .

$$\left\{ \begin{array}{l} \max_{\tilde{u}} J(\tilde{u}) \\ J(\tilde{u}) = \sum_{j=k+1}^{k+N_p} \left( \frac{\partial y_m}{\partial \theta}(j) + \left( \frac{\partial y_p}{\partial \theta}(k) - \frac{\partial y_m}{\partial \theta}(k) \right) \right)^2 \\ \tilde{u} = \{p_u(1), \dots, p_u(n_{pu})\} \\ u(j) = f_u(p_u(i), j, k) \quad i \in [1, n_{pu}] \\ \text{under the input constraints, } (\forall k > 0) : \\ \left\{ \begin{array}{l} u_{min} \leq u(j) \leq u_{max} \\ \Delta u_{min} \leq \frac{u(j) - u(j-1)}{T_s} \leq \Delta u_{max} \\ \forall j \in [k, k + N_p - 1] \end{array} \right. \\ \text{under the state/output constraints, } (\forall k > 0) : \\ \left\{ \begin{array}{l} c_i(y_m(j) + (y_p(k) - y_m(k)), \dots \\ \dots x_m(j) + (\hat{x}_p(k) - x_m(k)), \dots \\ \dots \alpha, \hat{\theta}(k), u(j)) \leq 0, \\ \dots \forall j \in [k+1, k+N_p], \quad \forall i \in \mathbb{I}^{n_c+n_{co}} \end{array} \right. \\ \text{based on the online resolution of the models} \\ (M), (M_\theta), \text{ on the process measure and on the observer.} \end{array} \right. \quad (8)$$

This constrained optimization problem allows determining online both the optimal input to apply during the experiment and the value of the unknown parameter: it is an optimal design of experiments for online parameter identification.

It may now be solved by any algorithm available for this kind of problem formulation<sup>1</sup>.

#### 4 CASE STUDY: SAPONIFICATION

We are now interested in the evaluation of this new optimal control approach for the online identification of a model parameter in a simple case. Saponification is the basic reaction of a base with a fat to produce soap. In this example, the continuous stirred tank reactor contains ethyl acetate (fat) and sodium hydroxide (base) and is assumed to be isothermal. To simplify the study, it is assumed that both concentrations initially inside the reactor and at the reactor input are equals, and that their feed flow rate are identical and constant. A model constituted of one nonlinear ordinary differential equation is written as:

$$\begin{cases} \dot{C}_a(t) = -k_v C_a^2(t) + \frac{D(t)}{V} (C_{ain} - C_a(t)), & t > 0 \\ C_a(0) = C_{a0}, & t = 0 \end{cases} \quad (9)$$

where the concentration of ethyl acetate  $C_a(t)$  inside the reactor (in  $[\text{mol.l}^{-1}]$ ) is both the state  $x$  and the measured output  $y$  of the process  $y_p$ .  $D(t)$  is the input flow rate of sodium hydroxide (in  $[\text{mol.min}^{-1}]$ ) to manipulate (i.e., this is the control variable  $u$ ). In term of parameters, the value of the constant volume of the reactor  $V$  (in  $[\text{l}]$ ) and the value of the concentration of ethyl acetate  $C_{ain}$  (in  $[\text{mol.l}^{-1}]$ ) at the reactor inlet are known. They are respectively  $\alpha_1$  and  $\alpha_2$ , as defined in the remark 1. The reaction rate  $\theta_1 = k_v$  (in  $[\text{l.mol}^{-1}.\text{min}^{-1}]$ ), assumed to be constant but unknown, has to be determined by this approach. The model (9) may then be reformulated in a more general form following  $(M_x)$  in (5), where the state  $x = x_1$ :

$$(M) \begin{cases} \dot{x}_1(t) = -\theta_1 x_1^2(t) + \frac{u(t)}{\alpha_1} (\alpha_2 - x_1(t)), & t > 0 \\ y(t) = x_1(t), & t > 0 \\ x_1(t) = x_1^0(t), & t = 0 \end{cases} \quad (10)$$

Based on this model, an observer ( $O$ ) (see the assumption 2) may be designed [12] to estimate  $[x_{p1} \theta_1]^T$  (with  $t > 0$ ):

$$(O) \begin{cases} \dot{x}_o(t) = A_o(y_p(t))x_o(t) + \dots \\ \dots B_o(u(t)) - S_o^{-1}C^T(Cx_o(t) - y_p(t)), & t > 0 \\ \dot{S}_o(t) = -\theta_o S_o(t) + A_o^T(y_p(t))S_o(t) - \dots \\ \dots S_o(t)A_o(y_p(t)) + C^T C, & t > 0 \end{cases} \quad (11)$$

where  $\theta_o$  is the observer tuning parameter and (with  $t > 0$ ):

$$\begin{cases} A_o(y_p(t)) = \begin{pmatrix} 0 & -y_p^2(t) \\ 0 & 0 \end{pmatrix} \\ B_o(u(t)) = \begin{pmatrix} \frac{u(t)}{\alpha_1} (\alpha_2 - y_p(t)) \\ 0 \end{pmatrix} \\ C = [1 \ 0] \end{cases} \quad (12)$$

The model  $(M_\theta)$  is written as:

$$(M_\theta) \begin{cases} \dot{x}_{\theta 1}(t) = -(2x_1(t)x_{\theta 2}(t) + \frac{u(t)}{\alpha_1})x_{\theta 1}(t) \dots \\ \dots - x_1^2(t), & t > 0 \\ y_\theta(t) = y_{\theta 1}(t) = x_{\theta 1}(t), & t > 0 \\ x_{\theta 1}(t) = 0, & t = 0 \end{cases} \quad (13)$$

<sup>1</sup>This algorithm is implemented on the ODOE4OPE software: <http://ODOE4OPE.univ-lyon1.fr> Please contact the author for its use.

The constrained optimization problem for online optimization is here to find the optimal profile of input flow-rate  $D(t)$  that maximizes the sensitivity  $\frac{\partial C_a}{\partial k_v}(t)$  of the concentration ethyl acetate  $C_a(t)$  with respect to the rate of reaction  $k_v$ . The problem ( $COP_{I_1}$ ) given in (4) is written as (assuming that the control action is parametrized with a control horizon of 1):

$$\begin{cases} \max_{\tilde{D}} J(\tilde{D}) = \sum_{j=k+1}^{k+N_p} \left( \frac{\partial C_a}{\partial k_v}(j) \right)^2 \\ \tilde{D} = D(k) \end{cases} \quad (14)$$

where the control is always constrained in magnitude and velocity:

$$\begin{cases} 0 \text{ mol.min}^{-1} \leq D(k) \leq 0.3 \text{ mol.min}^{-1} \\ -0.03 \text{ mol.min}^{-2} \leq \frac{D(k) - D(k-1)}{T_s} \leq +0.03 \text{ mol.min}^{-2} \end{cases} \quad (15)$$

Moreover, the concentration of ethyl acetate inside the reactor may be limited in some cases:

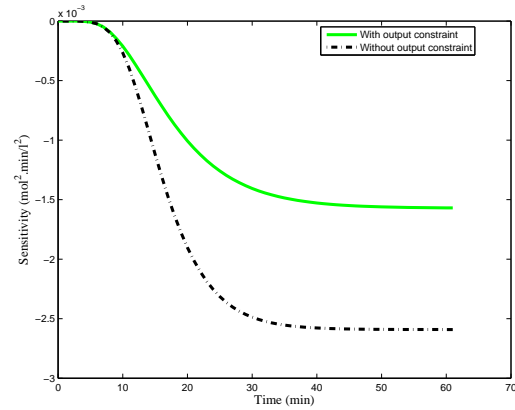
$$C_a(.) \leq C_a^{max} = 0.015 \text{ mol.l}^{-1} \quad (16)$$

Indeed, in order to see the influence of this output constraint (i.e., dealing with the possibility given to use the process) over the identification task, two cases are simulated:

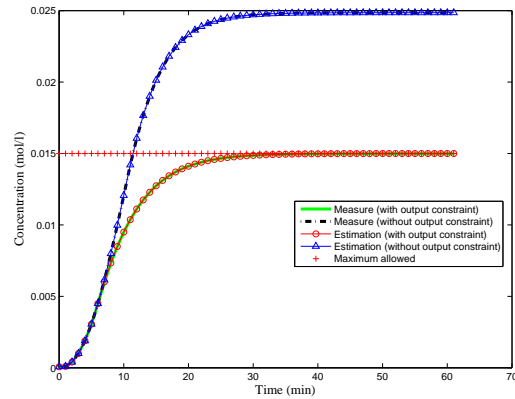
- Case 1: the optimization of the sensitivity (14) is constrained by (15), and the process output behavior is free;
- Case 2: the optimization of the sensitivity (14) is also constrained by (15), but the process output is also constrained, by (16).

In order to solve this constrained optimization problem, the `fmincon` routine of Matlab<sup>2</sup> toolbox optimization is used: it is a sequential quadratic programming. The prediction horizon  $N_p$  is tuned to 10 and the sampling period  $T_s = 1 \text{ min}$ . The volume of the reactor  $V$  is 100 l, the feed concentration  $C_{ain}$  is 1 mol.l<sup>-1</sup>. The target value for  $k_v$ , used for the process simulation, is 4.73 l.mol<sup>-1</sup>.min<sup>-1</sup>. The initial conditions used for the process is  $C_a(0) = 10^{-4} \text{ mol.l}^{-1}$ , and for the model and the observer, 30 % of initial errors are set:  $\hat{C}_a(0) = 0.7 \times 10^{-4} \text{ mol.l}^{-1}$ ,  $\hat{k}_v(0) = 3.31 \text{ l.mol}^{-1}.\text{min}^{-1}$ . The simulation results show that, in term of maximization of the sensitivity of the output with respect to the sought parameter (Fig. 1), the need to satisfy the output constraint (16) in case 2 enforces the optimizer to reduce the value of the sensitivity obtained in case 1 (Fig. 2). This maximization is underlined on (Fig. 3), where the control action is always either saturated in magnitude or in velocity (case 1). But, in case 2, after having followed the same behavior obtained in case 1 (during the 5 first minutes), the magnitude of the control action decreases to reach a constant value (ca. 0.108 mol.min<sup>-1</sup>, i.e. 36% of the full range). Indeed, the output constraint must be satisfied (Fig. 2) and is saturated after 30 minutes. At the same time, in both cases, the control applied to the simulated process and to the observer allows identifying the unknown constant parameter, in spite of the initial error of estimation of 30% (Fig. 4). The convergence with the target value is quiet similar in both

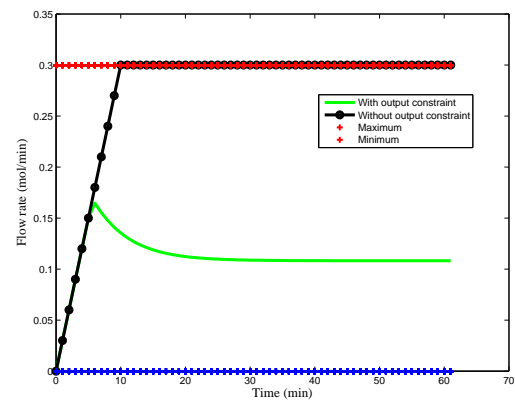
cases, whereas case 2 allows to maintain the use of the process inside an envelope specified by the prescribed output constraint.



**Fig. 1 Sensitivity of the concentration of ethyl acetate with respect to the reaction rate, in closed loop, with or without output constraint**



**Fig. 2 Concentration of ethyl acetate, in closed loop, with or without output constraint**

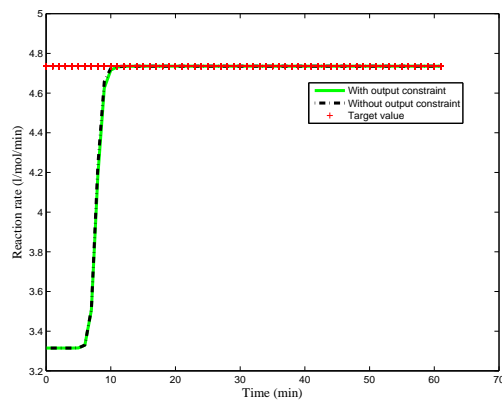


**Fig. 3 Optimal input flow-rate, in closed loop, with or without output constraint**

## 5 CONCLUSION

The main contribution of this paper was to provide a new approach for the optimal closed loop control for parameter identification, in the field of optimal design of experiments.

<sup>2</sup>www.mathworks.com



**Fig. 4 Estimation of the reaction rate, in closed loop, with or without output constraint**

The problem was to find the control to apply during the experiment that allowed optimizing a criteria which is a function of the sensitivity of the measured output with respect to the model parameter to estimate. This approach coupled a predictive controller and an observer that ensured, at the same time, both the control of the process according to the prescribed region of use and the online identification of the unknown model parameter. For the optimal control, an internal model based predictive control has been used. The online estimated parameter was fed into the control law to improve the closed loop performances. The two problems (optimal control and identification) were coupled, and solved at the same time, in a whole control problem. From the original process model, the dynamic sensitivity model was analytically defined. To keep the process behavior in a prescribed region, various constraints might be specified on the input, output and estimated states.

This approach may be applied on many cases, since it was presented in a general framework and that the main assumption dealt with the possibility to design an observer based on the model structure. There are many perspectives for this work, for example: the study and application of this approach for non uniformly observable systems, the multi variable approach, the study of the influence of output noise, the theoretical study of the stability of the closed loop approach and the theoretical study of the optimality of the solution for such controller.

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