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Application of Model Predictive Control suitable for closed-loop re-identification to a polymerization reactor



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ABSTRACT

Recently, a linear Model Predictive Control (MPC) suitable for closed-loop re-identification was proposed, which solves the potential conflict between the persistent excitation of the system (necessary to perform a suitable identification) and the control, and guarantees recursive feasibility and attractivity of an invariant region of the closed-loop. This approach, however, needs to be extended to account for a proper robustness to moderate-to-severe model mismatches, given that re-identifications are necessary when the system is not close to the operating point where the current linear model was identified. In this work, new results on robustness are presented, and an exhaustive application of the new MPC suitable for closed-loop re-identification to a nonlinear polymerization reactor simulator is made to explore the difficulties arising from a real life identification. Furthermore, several closed-loop re-identification are performed in order to clearly show that the proposed controller provides uncorrelated input–output data sets, which together with the guaranteed stability, constitute the main controller benefit.

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1. Introduction

Multivariable model-based control techniques, which use a prediction model to optimize systems performance, are control strategies widely used in industry. In particular, linear Model Predictive Control (MPC) has shown to be extremely useful in this context, since it bases its formulation on a simplified linear model of the plant, explicitly considers constraints on the variables, handles the complete process with many manipulated and controlled variables as a whole, and it optimizes the process performance [3,27].

One of the key point of an MPC formulation is the model used for prediction. This point, however, is not so simple to analyze/understand, given that in most applications, good performances are obtained by using only a simplified linear model of the complex nonlinear system under control. First, the fact – usually disregarded by the industrial practitioners – that a crucial part of the model employed by an MPC strategy is the knowledge of the

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constraints on the variables, should be emphasized. Second, the other fundamental aspect to be taken into account in an MPC formulation, is the accuracy of the linear model parameters (mainly the gain, to perform a suitable economic optimization). In this context, it becomes clear that an updating of the model should be done every time the process is moved to an operating point far from the one used to identify the model currently used by the controller. And more important, it would be desirable to perform this updating in closed-loop, since disconnecting the controller any time an identification is needed, is not a practical solution [20,24,30,16,7,15].

The general topic of system identification is a vast area of research, which involves the problem of handling the collected data from real process, and how to extract the valuable information from these data [28,20]. Although the focus of this article is not put on the identification itself, but on the design of a controller formulation that permits an easy closed-loop identification, a brief discussion on the literature related to the closed-loop identification method is necessary. Roughly speaking, identification methods can be characterized into the following main groups [20,28]: (i) The direct approach ignores the feedback law and identifies the open-loop system using measurements of the input and the output. (ii) The indirect approach identifies the closed-loop transfer function and determines the open-loop parameters subtracting the controller dynamic. To do that, the controller dynamic must be linear and known. (iii) The joint input–output approach takes the input and

output, jointly, as the output of a system produced by some extra input or setpoint signal. Since the last two methods need the exact knowledge of a linear controller, they are not directly applicable for closed-loops under constrained MPC.

If now the classification is circumscribed to the closed-loop reidentification under MPC controllers, then the following approaches should be mentioned. Genceli and Nikolaou [9] proposed a controller named Model Predictive Control and Identification (MPCI) where a persistent excitation condition is added by means of an additional constraint in the optimization problem. This strategy, which has been explored later in [2], turns the MPC optimization problem non-convex, and so, most of the well-known properties of the MPC formulation cannot be established. Zacekova et al. [29] presented a two-step controller approach: the first stage is devoted to optimize the control trajectory - as usual in MPC - while the second stage is devoted to generate the persistent excitation (PE) input signal by maximizing the minimal eigenvalue of the information matrix (a matrix describing the input variability). The link between these two stages is the optimal cost of the first one, which is used as constraint of the second one. The second optimization problem, however, is nonlinear and difficult to solve. Potts et al. [26] made a study of several MPC re-identification methods, focusing on the socalled MPC Relevant Identification (MRI). This method does not only take into account the identified model accuracy, but also the model aptitude for predictions, i.e., the model aptitude from the controller point of view. Marafioti [22] presents a new MPC-type formulation, defined as Persistently Exciting Model Predictive Control (PE-MPC). This formulation incorporates the persistent excitation (PE) signal by including a constraint into the MPC optimization problem, as it was made in [9]. The main difference between these two works is that the former allows the constraint to be inactive in the transient regime, and so, the MPC controller is not forced to obtain identification results at each sampling time. An enhanced formulation is presented in [23]. Similar results are presented in [18], where the time domain constraints are fulfilled while the identification criterion is taken into account. Heirung et al. [13] proposed the inclusion of an additional term in the MPC cost, and the use of a recursive (and modified) least square algorithm to obtain the online closed-loop identification. This way, the persistent excitation condition is no longer necessary, given that the excitation level is increased according to the estimated model parameters. Finally, [25] proposed to generate a PE signal by means of the maximization (instead of the minimization) of the MPC cost function. This way, the variance (variability) of the signal is maximized while the process variables fulfill the constraints. Neither the external excitation signal nor the dither signal are required in this approach. Also, the excitation signal depends - through the output noise - on the feedback signal, which means that the so obtained input and output signals will be highly correlated.

In general, none of these works pay attention to the formal feasibility and attractivity/stability of the MPC formulated for reidentifying the system. Recently, [10] has proposed a novel MPC suitable for re-identification that ensures feasibility and stability, and performs a safe closed-loop re-identification. The main idea in this paper is to extend the concept of equilibrium-point-stability to the invariant-set-stability, and to propose an MPC that drives the system into that invariant set, when outside, and persistently excites the system, when inside. This way, the method avoids the potential conflict between persistent excitation and control.¹ The MPC problem formulation is based on the concept of generalized distance from a point (the state and input trajectory) to a set (target invariant set and input excitation set). So, it guarantees the attractivity/stability of the target invariant set and also the feasible persistent excitation of the system, since both tasks are developed separately in the state space.

The method proposed in [10], however, involves some theoretical definitions which are model-dependent: invariant sets and distance functions to the invariant set. Then, two issues arise: (1) if the method could be adapted to reach a sufficient degree of robustness to properly account for moderate-to-severe model mismatches and changes of the operating points, and (2) if the model identification performed with the data obtained in closed-loop gives accurate models in every desired scenario. The first question is of interest since the invariant set used as a target by the MPC may be invariant in a region of the nonlinear system (precisely, in the proximity of the equilibrium where the current linear model was obtained) but not in other ones (when the nonlinear system may be steered, by a disturbance or by a change of operating conditions, far from the original equilibrium). The second question, on the other hand, is related to the quality of the collected data for identification, which in turn depends on the degree of correlation between inputs and outputs (noise) that the controller produces.

The objective of this work is then to extend the MPC suitable for re-identification to properly account for the robustness to moderate-to-severe plant-model mismatches. In this regard, the controller is applied to a nonlinear styrene polymerization reactor simulator, and several closed-loop re-identifications are performed to test both, the robustness and identification abilities of the proposed strategy. By means of the simulations it is shown that in most of the cases it is possible to compute proper robust invariant sets (according to new theoretic results) – and hence, it is possible to design a proper MPC for re-identification. Also, it is shown how to practically compute the invariant sets according to the regions of the nonlinear state space, where frequent re-identifications are needed. Finally, several identifications are performed to show that the collected input-output noise data are not correlated by the controller. This means that good identifications could be made under the proposed robust scheme.

The paper is organized as follows. After an Introduction in Section 1, Section 2 presents the problem statement and the MPC controller formulations suitable for closed-loop re-identification. Then, in Section 3, new results related to MPC robustness are given. In Section 4, a description of the styrene polymerization reactor is presented, while Section 5 describes the linear models for predictions and the constraint sets involved in the problem. Section 6 presents a detailed description of the simulation results, showing the pros and cons of the MPC in different scenarios. Finally, Section 7 provides some conclusions of the work.

2. Problem statement and controller formulation

2.1. Model and constraints assumptions

Consider a system described by a linear time-invariant discretetime model

$$x^+ = Ax + Bu, \quad y = Cx \tag{1}$$

where $x \in \mathbb{R}^n$ is the system state, x^* is the successor state, $u \in \mathbb{R}^m$ is the current control, and $y \in \mathbb{R}^p$ is the system output. The system is subject to hard constraints on state and input, $x(k) \in \mathcal{X} \subset \mathbb{R}^n$ and $u(k) \in \mathcal{U} \subset \mathbb{R}^m$, for all $k \ge 0$. Furthermore, it admits soft output constraints in the form of output zones, $y(k) \in \mathcal{Y}$, where \mathcal{Y} is intended as an output set of appropriated dimension to perform a system identification. It is assumed, for simplicity, that matrix *A* has all its eigenvalues strictly inside the unit circle, the pair (*A*, *B*) is controllable, the set \mathcal{X} is convex and closed, the sets \mathcal{U} and \mathcal{Y} are convex and

¹ It should be remarked that this kind of natural duality of the control task was first highlighted in [5].

compact and all sets, \mathcal{X}, \mathcal{U} and \mathcal{Y} , contain the origin in their interior. Furthermore, it is also assumed that $A\mathcal{X} \subseteq \lambda\mathcal{X}$, with $\lambda \in [0, 1)$.

2.2. MPC formulation suitable for sub-space re-identification

In [10] a MPC controller suitable for re-identification is presented, which is devoted to avoid the conflicts between excitation and control objectives. The main idea behind the formulation is: when the system is outside a target set – called Invariant Set for Identification (ISI set) – the target set is a *control target*; when the system is inside, the target set is a safe *identification set*, that is considered as a generalized equilibrium by the controller.

The key concept to achieve such an MPC controller is to propose an MPC cost that penalizes the distance to the target set, and it is null at every point inside the target set, in the same way as a standard MPC cost is null at the desired punctual target. This means that the controller does not make any difference between two points of the target, or, in other words, the controller leaves the system in open loop when it enters the target set. Thus, one can use any simple and robust identification methods (like subspace identification methods, [24], least square estimation, [20], etc.), avoiding the bias problems that appear when the output noise are correlated with the input signal. The complete MPC strategy suitable for re-identification has two operation modes: one that operates when no re-identification is needed, and is defined as Control Operation Mode, and another, that operates when there are reasons to suspect that a re-identification is needed, which is defined as Reidentification Operation Mode.

2.2.1. Control operation-mode

Consider a set $\mathcal{U}^t \subset \mathcal{U} \subset \mathbb{R}^m$, which is called Excitation Input Set (EIS set), and it is computed according to the necessary amplitude to perform a proper excitation. Consider also the associated Control Equilibrium Set (CES set), $\mathcal{X}_{ss}^t = (I_n - A)^{-1}B\mathcal{U}^t \subseteq \mathcal{X}$, and the Output Equilibrium Set (OES set), $\mathcal{Y}_{ss}^t = C\mathcal{X}_{ss}^t$, where $I_n \in \mathbb{R}^{n \times n}$ denotes the identity matrix. The MPC cost for the *Control operation-mode* is given by:

$$V_{N}^{CES}(x, \lambda_{ss}^{t}; \mathbf{u}, u_{ss}, x_{ss}) = \sum_{j=0}^{N-1} (\|x(j) - x_{ss}\|_{Q}^{2} + \|u(j) - u_{ss}\|_{R}^{2}) + \gamma |x_{ss}|_{\lambda^{t}}, \qquad (2)$$

where $\mathbf{u} = \{u(0), \ldots, u(N-1)\}$ is the sequence of future inputs, $\|x - y\|_M^2 \stackrel{\Delta}{=} (x - y)^T M(x - y)$, for a matrix M of appropriate dimensions, Q > 0 and $R \ge 0$ are penalization matrices, $\gamma > 0$ is a real number, $|x|_{\mathcal{X}_{ss}^t}$ is the distance function (from x to \mathcal{X}_{ss}^t) and N is the control horizon. Furthermore, u_{ss} and x_{ss} are artificial decision variables of the cost, which are only forced to be a feasible equilibrium, i.e., they must fulfill $x_{ss} = (I_n - A)^{-1} B u_{ss}$, with $u_{ss} \in \mathcal{U}$ and $x_{ss} \in \mathcal{X}_{ss} \stackrel{\Delta}{=} (I_n - A)^{-1} B \mathcal{U}$ [19].

Now, for any current state $x \in \mathcal{X}$, the optimization problem to be solved at each time step *k* reads:

$$\begin{array}{lll} \textbf{Problem} & P_{N}^{CES}(x, \mathcal{X}_{ss}^{t}) \\ & \underset{s.t.}{\min} & V_{N}^{CES}(x, \mathcal{X}_{ss}^{t}; \textbf{u}, u_{ss}, x_{ss}) \\ & x(0) = x, \\ & x(j+1) = Ax(j) + Bu(j), \quad j \in \mathbb{I}_{0:N-1} \\ & x(j) \in \mathcal{X}, u(j) \in \mathcal{U}, \qquad j \in \mathbb{I}_{0:N-1} \\ & u(j) = u_{ss}, \qquad j \in \mathbb{I}_{N-1:\infty} \\ & x_{ss} = (I_{n} - A)^{-1} Bu_{ss}. \end{array}$$

$$(3)$$

In this optimization problem, x and \mathcal{X}_{ss}^t are the parameters, while the sequence **u** and the pair (u_{ss} , x_{ss}) are the optimization variables. Notice that (x_{ss} , u_{ss}) are only forced to represent an equilibrium point, but they are free to assume any feasible equilibrium value. In such a way, this formulation derives in the so-called *zone control*, since it steers the system to any equilibrium point in \mathcal{X}_{ss}^t , no matter which point is it [6,11], and so, it steers the output *y* to the output equilibrium set $\mathcal{Y}_{ss}^t = C\mathcal{X}_{ss}^t$. The control law, derived from the application of a receding horizon policy, is given by $\kappa_N(x, \mathcal{X}_{ss}^t) = u^0(0; x)$, where $u^0(0;x)$ is the first element of the solution sequence $\mathbf{u}^0(x)$. The set \mathcal{X}_{ss}^t is an *attractive equilibrium set* for the closed-loop system:

Theorem 1. Consider that assumptions made in Section 2.1 hold, and consider a given control equilibrium set $\chi_{ss}^t = (I_n - A)^{-1} B \mathcal{U}^t \subseteq \mathcal{X}$, and the associated input set \mathcal{U}^t . Then, χ_{ss}^t is an equilibrium set for the closed-loop system $x^+ = Ax + B\kappa_N(x, \chi_{ss}^t)$. Furthermore, χ_{ss}^t is locally attractive for the closed-loop system $x^+ = Ax + B\kappa_N(x, \chi_{ss}^t)$, with a domain of attraction given by \mathcal{X} .

Proof. The proof can be found in [6,11]. \Box

What Theorem 1 states is that the control equilibrium set \mathcal{X}_{ss}^t is both, an equilibrium, and even more an attractive equilibrium set for the closed-loop system. The fact that the system is steered to a complete equilibrium set (not only to a point), and once the system is inside it, the controller does not apply any control action, allows us to think that this set could also be used as a set where the system can be excited (for identification purposes), to spatially separate the conflicting tasks of controlling and re-identifying. However, it should be noticed that it is not possible to perform an excitation procedure entirely inside a control equilibrium set, because in general, it is not possible to move from one equilibrium point to another without leaving the equilibrium set first. So, an extension to a generalization of the equilibrium set (an invariant set), that also include the transient system trajectories, is needed.

2.2.2. Re-identification Operation Mode

The idea here is to track and reach a set that not only includes equilibrium states, but also transient states, and then, once the system is inside this set, performing a persistent excitation and an identification.

To do that, consider an Invariant Set for Identification (ISI set) $\mathcal{X}^t \subset \mathcal{X} \subset \mathbb{R}^n$ for the system defined in Section 2.1, and the associated Excitation Input Set (EIS set) \mathcal{U}^t (the relationship between EIS and ISI sets will be described later on). Also consider a *Generalized distance stage cost function*, $d_{\mathcal{X}}(x)$, as the one defined in [10]. This function has to be convex and continuous, for all $x \in \mathcal{X}$, and it has to be null for all $x \in \mathcal{X}^t$ and positive for all² $x \in \mathcal{X} \setminus \mathcal{X}^t$. Finally, consider a fix input sequence of appropriated length, $\mathbf{u}_{PE} = \{u_{PE}(0), u_{PE}(1), \ldots, u_{PE}(T)\}$, with enough variability and amplitude to *Persistently Excite* the system (for the concept of persistent excitation, see [12]). Then, the MPC cost for the *Re-identification operation-mode* is given by:

$$V_N^{EXC}(x, \mathcal{X}^t, \mathbf{u}_{PE}, k; \mathbf{u}) = (1 - \rho(x))V_N^{ISI}(x, \mathcal{X}^t; \mathbf{u})$$
(4)

$$+\rho(x)\|u(0) - u_{PE}(k)\|,$$
 (5)

where $\rho(x)=1$ if $x \in \mathcal{X}^t$, and $\rho(x)=0$, otherwise. Furthermore, $V_N^{ISI}(x, \mathcal{X}^t; \mathbf{u})$ is given by:

$$V_N^{ISI}(x, \mathcal{X}^t; \mathbf{u}) = \sum_{j=0}^{N-1} (\alpha d_{\mathcal{X}^t}(x(j)) + \beta d_{\mathcal{U}^t}(u(j)))$$
(6)

$$+d_{\lambda^{\ell}}^{ter}(x(N)). \tag{7}$$

² Given two sets $\mathcal{X} \subseteq \mathbb{R}^n$ and $\mathcal{X}^t \subseteq \mathbb{R}^n$, $\mathcal{X} \setminus \mathcal{X}^t = \{x : x \in \mathcal{X} \land x \notin \mathcal{X}^t\}$.

where α and β are positive real numbers, $d_{\chi}(x)$ is a generalized distance from point x to set \mathcal{X} and $d_{\mathcal{X}^t}^{ter}(\cdot)$ is a terminal cost function defined on \mathcal{X}^{ter} , which is the *terminal set* where the terminal state x(N) is forced to belong to.³ Now, for any initial state x in the Nstep controllable set to χ^{ter} ($\chi_N(\chi^{ter})$), at a given time step k, the optimization problem to be solved at each time instant k, is given by:

Problem
$$P_N^{EXC}(x, \lambda^t, \mathbf{u}_{PE}, k)$$

min $V_N^{EXC}(x, \lambda^t, \mathbf{u}_{PE}, k; \mathbf{u})$
 $x(0) = x,$
 $x(j + 1) = Ax(j) + Bu(j), \quad j \in \mathbb{I}_{0:N-1}$
 $x(j) \in \mathcal{X}, u(j) \in \mathcal{U}, \qquad j \in \mathbb{I}_{0:N-1}$
 $x(N) \in \lambda^{ter}$
(8)

Again, the control law, derived from the application of a receding horizon policy, is given by $\kappa_N(x, \lambda^t) = u^0(0; x)$, where $u^0(0; x)$ is the first element of the solution sequence $\mathbf{u}^{0}(x)$. The controller derived from this formulation ensures the convergence of the closed-loop system to the ISI set \mathcal{X}^{t} , and once the system is there, the persistent excitation of the system is performed. The following Theorem formalizes the properties of the proposed MPC controller:

Theorem 2. Consider that assumptions made in Section 2.1 hold, and consider an ISI set χ^t and a persistent excitation sequence \mathbf{u}_{PE} contained in the EIS set \mathcal{U}^t . Then, for any initial state $x \in \mathcal{X}^t$, the system controlled by the receding horizon MPC control law $\kappa_N(x, X^t)$, will be persistently excited inside χ^t . Furthermore, for any initial state $x \in$ $\mathcal{X}_N(\mathcal{X}^{ter}) \setminus \mathcal{X}^t, \mathcal{X}^t$ is locally attractive for the closed-loop system $x^+ =$ $Ax + B\kappa_N(x, \mathcal{X}^t)$

Proof. The proof can be found in [10]. \Box

What Theorem 2 states is similar to Theorem 1, but for the generalized equilibrium set (or invariant set) \mathcal{X}^{t} , which also includes the transient states trajectories of the system under input excitation.

Remark 1. The EIS and ISI sets, $\mathcal{U}^t \subset \mathcal{U}$ and $\mathcal{X}^t \subset \mathcal{X}$, are formally defined in [10]. The idea behind these definitions is that the ISI set is an Invariant set for any possible Persistent Excitation input signal, \mathbf{u}_{PF} , contained in the EIS set. These definitions capture the concept of persistent excitation conditions of the input sequence necessary to perform an identification [12,20], and propose an invariant set in this context.

Remark 2. One can define the Output Identification Set (OIS set) as $\mathcal{Y}^t = C\mathcal{X}^t \subset \mathcal{Y}$. This way, given that $\mathcal{X}^t \supset \mathcal{X}^t_{ss}$, it follows that $\mathcal{Y}^t \supset \mathcal{Y}^t_{ss} = C\mathcal{X}^t_{ss} = C(I_n - A)^{-1}B\mathcal{U}^t$. This implies that for any input sequence in \mathcal{U}^t , the state trajectory will be inside \mathcal{X}^t and the output sequence will be inside $\mathcal{Y}^t \subset \mathcal{Y}$, which is not true for the equilibrium output set \mathcal{Y}_{ss}^{t} .

Remark 3. In many cases, the excitation requirements for identification come from the output space, in such a way that some given output limit should not be violated during the excitation procedure. These limits define the (generally box-type) set \mathcal{Y} in the output space, and therefore, the set \mathcal{U}^t should be selected such that the set \mathcal{Y}^t is strictly inside \mathcal{Y} .

Fig. 1 shows a schematic plot of the sets \mathcal{U}^t , \mathcal{X}^t , \mathcal{X}^t_{ss} , \mathcal{Y}^t and \mathcal{Y}^t_{ss} , coming from a given 2-input, 2-output, 3-state system. Notice that for any input sequence inside \mathcal{U}^t , the state trajectory will be inside \mathcal{X}^t , and the output sequence will be inside \mathcal{Y}^t .

Fig. 1. Box-type set \mathcal{U}^t , and the corresponding sets \mathcal{X}^t , \mathcal{X}^t_{ss} , \mathcal{Y}^t and \mathcal{Y}^t_{ss} .

3. Target set X^t for model mismatch

The main parameter of the proposed MPC for re-identification is the ISI set \mathcal{X}^t . The invariant condition of this sets, as it is clear from its definition, depends on the EIS set, \mathcal{U}^t , and on the model. So, since the excitation scenario is precisely given when the current model is no longer valid, a certain robustness to model mismatch on the computation of \mathcal{X}^t is needed, in such a way that the computed set is not only invariant for the current model, but for a family of models around it. Consider a family of systems given by

$$x^+ = A(w)x + B(w)u, \qquad y = C(w)x, \qquad w \in \mathcal{W} \subseteq \mathbb{R},$$
(9)

where A(w), B(w) and C(w) are affine functions of w, i.e., A(w) = A + A(w) $\overline{A}w, B(w) = B + \overline{B}w, C(w) = C + \overline{C}w$, with w belonging to the set $W \subset$ \mathbb{R} . Assume that the Nominal model is given by $x^+ = A(w_N = 0)x + C(w_N = 0)x^+$ $B(w_N = 0)u = Ax + Bu$, $y = C(w_N = 0)x$, and the unknown Real model, is given by $x^+ = A(w_R)x + B(w_R)u$, $y = C(w_R)x$, for some $w_R \in \mathcal{W}$. In this model scenario, the following Theorem holds:

Theorem 3. Consider a X^t , that is not the minimal one, for $x^+ =$ $Ax + Bu, x \in \mathcal{X}, u \in \mathcal{U}$. Then, there exists a non-empty set $\mathcal{W} \subset \mathbb{R}$ for which the sets \mathcal{X}^t and $\mathcal{Y}^t = C \mathcal{X}^t$ are also an ISI and OIS sets for $x^+ =$ $A(w)x + B(w)u, y = C(w)x, x \in \mathcal{X}, u \in \mathcal{U}$, for all $w \in \mathcal{W}$.

Proof. The proof can be seen in [10]. \Box

What Theorem 3 shows is that the ISI set \mathcal{X}^t has an inherent robustness such that it is not only an ISI set for the model for which it was computed, but for a family of models in a non-null vicinity of this model. Theorem 3, however, shows only that such non-null vicinity exists (by continuity of the model family), but say nothing about how to measure this robustness and how to obtain a sufficiently large λ^t . Next, new results that extend the latter theorem are presented, which establish a form to evaluate the contractivity of an ISI set, and so, the robustness for a family of models.

Let us consider the identification map $\mathcal{R}(\cdot)$: $\mathcal{P}(\mathcal{X}) \rightarrow$ $\mathcal{P}(\mathcal{X}), \mathcal{R}(\cdot) \stackrel{\Delta}{=} A(\cdot) + B\mathcal{U}^t$, where $\mathcal{P}(\mathcal{X})$ is the set of all possible subsets in \mathcal{X} , i.e., the power set of \mathcal{X} . The contractivity of a set Ω under the map $\mathcal{R}(\Omega)$ is defined as the "minimal scaling" of the set, $\lambda \Omega$, such that it contains $\mathcal{R}(\Omega)$.⁴ Here, a modified contractivity (MC) of the set Ω under the *identification map* will be defined:

Definition 1. The modified identification contractivity (MC) of a set Ω , under the identification map $\mathcal{R}(\cdot)$, is defined as

$$\lambda \stackrel{\Delta}{=} \max\{\xi \ge 0 : A\Omega \oplus \mathcal{BU}^t \oplus \xi \mathcal{B} \subseteq \Omega\}.$$
(10)

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³ In [10], several alternatives for both, the generalized distance and the terminal cost function are given.

U ν \mathcal{U}^t v \mathcal{Y}_{*}^{t} х \mathcal{X}^t_{\circ}

⁴ Notice that if contractivity is defined as the "maximal scaling" of the map, $\lambda \mathcal{R}(\Omega)$, such that it is contained in Ω , the result is less conservative and different in general.

where \mathcal{B} is the unitary ball according to the 2-norm; $\mathcal{B} \stackrel{\Delta}{=} \{x \in \mathbb{R}^n : \|x\| \le 1\}$.

Given that \mathcal{B} is full dimensional in \mathbb{R}^n , if $\lambda > 0$, then the usual contractivity follows (with a possible different contractivity constant) from the modified one. Furthermore, given that \mathcal{B} is 0-symmetric, the fact $A\Omega \oplus \mathcal{BU}^{\ell} \oplus \lambda \mathcal{B} \subseteq \Omega$ is equivalent to $A\Omega \oplus \mathcal{BU}^{\ell} \subseteq \Omega \ominus \lambda \mathcal{B}$, since in this case, the Minkowsky addition and Pontryagin difference cancel each other. The benefit of the new definition is that $\lambda \mathcal{B}$ is a less conservative measure of the potentiality of the set Ω to be robustly invariant, than the one obtained with the contractivity constant of the usual definition. Next, this fact is clarified and used to characterizes the robustness of an ISI set.

Following a similar procedure to the one presented in Property 2, (4), in [10], let consider a set Ω which is contractive (now, according to the new definition) under the autonomous map $A(\cdot)$. This way, it follows that

$$A\Omega \oplus \delta \mathcal{B} \subseteq \Omega, \quad \delta > 0. \tag{11}$$

Such a set is easy to find given that *A* is assumed to be Schur. Now, the interesting point is that if the set Ω is scaled by a constant $\zeta > 1$ (i.e., enlarged), then the contractivity of the new set is enlarged. To see that, consider:

$$A\zeta\Omega \oplus \zeta\delta\mathcal{B} = \zeta[A\Omega \oplus \delta\mathcal{B}] \tag{12}$$

$$\subseteq \zeta \Omega,$$
 (13)

where the inclusion follows from (11). This means that the modified contractivity of $\zeta \Omega$ is given by $\lambda_1 \stackrel{\Delta}{=} \zeta \delta$, which is a greater constant than δ (since $\zeta > 1$). So, by means of a simply scaling, the contractivity constant of any contractive set can be indefinitely enlarged.

Now, consider the minimal ISI set, \underline{X}^t for system $x^+ = Ax + Bu$, which means that $\mathcal{R}(\underline{X}^t) \subseteq \underline{X}^t$ minimally, i.e., the modified contractivity of \underline{X}^t is null. Then, the ISI set $\underline{X}^t \oplus \zeta \Omega$, where Ω is the set defined before, has the modified contractivity $\lambda_1 = \zeta \delta$ under the map \mathcal{R} . That is,

$$\mathcal{R}(\underline{\lambda}^{t} \oplus \zeta \Omega) \oplus \lambda_{1} \mathcal{B} = A[\underline{\lambda}^{t} \oplus \zeta \Omega] \oplus B \mathcal{U}^{t} \oplus \lambda_{1} \mathcal{B}$$
(14)

$$= \overbrace{A\underline{\lambda}^{t} \oplus B\underline{\lambda}^{t}}^{\subseteq \underline{\lambda}^{t}} \oplus \overbrace{A\zeta\Omega \oplus \lambda_{1}B}^{\subseteq \zeta\Omega}$$
(15)

$$\subseteq \lambda^t \oplus \zeta \Omega, \tag{16}$$

where it should be noticed that contractivity λ_1 can be enlarged by the arbitrary parameter $\zeta > 1$.

With this results, it will be provided next a new form to compute a robust ISI set for the system family (9).

Theorem 4. Consider an ISI set given by $\chi^t \triangleq \underline{\chi}^t \oplus \zeta \Omega$ which, as before, is a modified contractive set under the nominal identification map $\mathcal{R}_{nom}(\cdot) \triangleq A(\cdot) \oplus \mathcal{BU}^t$. Consider also the constant λ_2 given by $\lambda_2 \triangleq \min\{\xi \ge 0 : \xi B \supseteq \overline{\mathcal{R}}(\chi^t)\}$, where $\overline{\mathcal{R}}(\cdot) \triangleq \overline{A}(\cdot) \oplus \overline{\mathcal{BU}}^t$ is the identification map corresponding to the uncertain term of model family (9). Then, χ^t and $\chi^t = C\chi^t$ are ISI and OIS sets, respectively, of $x^+ = A(w)x + B(w)u$, for all $w \in \mathcal{W} \triangleq \{w \in \mathbb{R} : w \le \frac{\lambda_1}{\lambda_2}\}$, where λ_1 can be arbitrary selected.

Proof. Let define the complete map according to the model family $x^+ = A(w)x + B(w)u$ as $\mathcal{R}(\cdot) \stackrel{\Delta}{=} A(w)(\cdot) \oplus B(w)\mathcal{U}^t$. Then:

$$\mathcal{R}(\mathcal{X}^{t}) = A(w)\mathcal{X}^{t} \oplus B(w)\mathcal{U}^{t}$$

$$= A\mathcal{X}^{t} \oplus B\mathcal{U}^{t} \oplus w(\overline{A}\mathcal{X}^{t} \oplus \overline{B}\mathcal{U}^{t})$$
(17)
(17)
(17)
(17)
(17)

$$\subseteq \mathcal{X}^{t} \ominus \lambda_{1} \mathcal{B} \oplus w \lambda_{2} \mathcal{B}$$
⁽¹⁹⁾

$$\subseteq \lambda^t$$
, (20)

where the last inclusion follows from the fact that $w \le \lambda_1/\lambda_2$. Then, since $\mathcal{R}(\mathcal{X}^t) \subseteq \mathcal{X}^t$, \mathcal{X}^t is an ISI set of $x^+ = A(w)x + B(w)u$, for all $w \in \mathcal{W}$. The OIS condition of $\mathcal{Y}^t = C\mathcal{X}^t$ follows directly. \Box

Remark 4. This last result means that, given a model family (i.e., a model family of the form (9), for a given set W) no matter how small the nominal target set \underline{A}^t is, it can be enlarged by a simple scaling, in such a way that the so obtained enlarged target set is not only invariant for the nominal system, but for the entire model family. More precisely, the enlarged target robust ISI set can be computed as $\lambda^t = \underline{A}^t \oplus \zeta \Omega$, where Ω is an arbitrary contractive set and ζ is an appropriated constant.

Remark 5. This last results allow us, under some mild conditions, to find robust ISI sets under other kind of uncertainty, as the parametric uncertainty given by: $x^+ = Ax + Bu$, where $A = \sum_{i=1}^{r} \epsilon_i A_1$, $B = \sum_{i=1}^{r} \epsilon_i B_1$, with $\epsilon_i \ge 0$ and $\sum_{i=1}^{r} \epsilon_i = 1$. This alternative, however, will not be analyzed in this work.

Remark 6. Another question that remains open at this stage, and needs to be studied in future works, is the effect of a state observer in the whole aforementioned analysis.

This flexibility in computing the robust ISI sets involved in the proposed MPC formulation is one of the key points of the easy applicability of the controller. The Simulation section presented next will show how to use these results in computing appropriated robust ISI sets for a (nonlinear) polymerization reactor.

4. The styrene polymerization reactor

The polymerization reactor is usually the heart of the polymer production process and its operation may be difficult as it involves exothermic reactions, unknown reaction kinetics and high viscosity [1]. Most styrene polymers are produced through batch or continuous polymerization processes. The present work considers the free-radical bulk and solution styrene polymerization in a jacketed CSTR. As shown in Fig. 2, the CSTR has three feed streams: the pure styrene monomer, the 2,2'-azoisobutyronitrile (AIBN) initiator dissolved in benzene, and the pure benzene solvent. The exit stream contains polymer, un-reacted monomer, initiator, and solvent. The kinetic mechanism used for this homopolymerization



Fig. 2. Process diagram for the styrene polymerization reactor.

Table 1

Process parameters for the polymerization reactor.

Variable	Symbol	Value	Units
Frequency factor for initiator decomposition	Ad	2.142×10^{17}	h^{-1}
Activation energy for initiator decomposition	E_d	14,897	К
Frequency factor for propagation reaction	A_p	3.816×10^{10}	$L mol^{-1} h^{-1}$
Activation energy for propagation reaction	E_p	3557	К
Frequency factor for termination reaction	A _t	$4.50 imes 10^{12}$	$L mol^{-1} h^{-1}$
Activation energy for termination reaction	E_t	843	К
Initiator efficiency	f_i	0, 6	
Heat of polymerization	$-\Delta H_r$	$6.99 imes 10^4$	J mol ⁻¹
Overall heat transfer coefficient	hA	$1.05 imes 10^6$	$J K^{-1} h^{-1}$
Mean heat capacity of reactor fluid	ρC_p	1506	$J K^{-1} L^{-1}$
Heat capacity of cooling jacket fluid	$\rho_c C_{pc}$	4043	$J K^{-1} L^{-1}$
Molecular weight of the monomer	M_m	104.14	g mol ⁻¹

process is very general and can be described by the following steps [17]:

 $I_{i}^{f_{i},k_{d}} 2R \text{ (initiator decomposition)}$ $M + R \xrightarrow{k_{i}} P_{i} \text{ (chain initiation)}$ $P_{n} + M \xrightarrow{k_{p}} P_{n+1} \text{ (propagation)}$ $P_{n} + P_{m} \xrightarrow{k_{td}} T_{n} + T_{m} \text{ (termination by disproportionation)}$ $P_{n} + P_{m} \xrightarrow{k_{tc}} T_{n+m} \text{ (termination by combination)}$

The two initiation reactions involve the decomposition of initiator I to produce radicals R, which react with the monomer molecules M to initiate new live (radical) polymer chains P_n , $n \ge 1$. During the propagation step, monomer molecules M are added, one at a time, to the live-polymer chains $Pn(n \ge 1)$. The growth of the chains terminates when the propagating radicals lose their activity through any termination reaction, resulting in dead-polymer chains, $T_n(n \ge 1)$. The nonlinear model that represent the dynamic of the reactor is defined by the following equations [21]:

$$\frac{d[I]}{dt} = \frac{(Q_i[I_f] - Q_t[I])}{V} - k_d[I]$$
(21)

$$\frac{d[M]}{dt} = \frac{(Q_m[M_f] - Q_t[M])}{V} - k_P[M][P]$$
(22)

$$\frac{dT}{dt} = \frac{Q_t(T_f - T)}{V} + \frac{(-\Delta H_r)}{\rho C_P} k_p[M][P]$$
(23)

$$-\frac{hA}{\rho C_P V}(T-T_c) \tag{24}$$

$$\frac{dT_c}{dt} = \frac{Q_c(T_{cf} - T_c)}{V_c} + \frac{hA}{\rho_c C_{pc} V_c} (T - T_c)$$
(25)

Table 2

Steady-state operational condition for the polymerization reactor.

where

$$[P] = \left[\frac{2f_i k_d[I]}{k_t}\right]^{0.5}$$
(26)

$$k_j = A_j \exp\left(\frac{-E_j}{T}\right), \quad j = d, p, t$$
 (27)

$$Q_t = Q_i + Q_s + Q_m \tag{28}$$

The definition of the parameters and variables involved in the equations above can be found in Tables 1 and 2, respectively. The moment equations for the dead polymer are written as follows:

$$\frac{dD_0}{dt} = 0.5k_t[P]^2 - \frac{Q_t D_0}{V}$$
(29)

$$\frac{dD_1}{dt} = M_m k_p[M][P] - \frac{Q_t D_1}{V}$$
(30)

$$\frac{dD_2}{dt} = 5M_M K_p[M][P] + 3M_M \frac{{K_p}^2}{k_t} [M]^2 - \frac{Q}{V} D_2$$
(31)

 D_0 , D_1 and D_2 represent the zero, the first and the second order moment of the dead polymer, respectively.

The weight-average molecular weight is obtained as:

$$\overline{M}_W = M_m \frac{D_2}{D_1} \tag{32}$$

For on-line control, it is more common to measure the viscosity as a substitute for the average molecular weights [1]. In this work, it is assumed that an online viscosimeter provides reliable measurements of the intrinsic viscosity η . The following correlation is used to simulate the measurement of the viscosity [8]:

$$\eta = 0.0012 M_w^{0.71} \tag{33}$$

Variable	Symbol	Value	Units
Flow rate of initiator	Qi	108	$L h^{-1}$
Flow rate of solvent	Q_s	459	$L h^{-1}$
Flow rate of monomer	Q_m	378	$L h^{-1}$
Flow rate of cooling jacket fluid	Q_c	471.6	$L h^{-1}$
Reactor volume	V	3000	L
Volume of cooling jacket fluid	Vc	3312.4	L
Concentration of initiator in feed	$[I_f]$	0.5888	$mol L^{-1}$
Concentration of monomer in feed	$[M_f]$	8.6981	$mol L^{-1}$
Temperature of reactor feed	T_f	330	К
Inlet temperature of cooling jacket fluid	T_{cf}	295	K
Concentration of initiator in the reactor	[1]	$6.6832 imes 10^{-2}$	$mol L^{-1}$
Concentration of monomer in the reactor	[<i>M</i>]	3.3245	mol L ⁻¹
Temperature of the reactor	Т	323.56	К
Temperature of cooling jacket fluid	T _c	305.17	К
Molar concentration of dead polymer chains	D_0	$2.7547 imes 10^{-4}$	$mol L^{-1}$
Mass concentration of dead polymer chains	D_1	16.110	$g L^{-1}$

5. Linear model for predictions

Here, the polymer intrinsic viscosity η and the reactor temperature T are defined as the controlled outputs. For controlling $y_1 = \eta$ and $y_2 = T$, the controller manipulates the initiator flow-rate $(u_1 = Q_i)$ and the liquid flow rate of the cooling jacket $(u_2 = Q_c)$. The remaining inlet flow-rates Q_s and Q_m are related to Q_i by ratio control. So as to improve the performance of the controller, the ratio between the initiator flow rate Q_i and monomer flow rate Q_m is maintained fixed, then:

$$Q_m = \frac{Q_m}{\overline{Q_i}} Q_i \tag{34}$$

where \overline{Q}_m and \overline{Q}_i are the nominal values of Q_m and Q_i , respectively. On the other hand, the solvent volume fraction should be maintained at 0.6 to avoid the gel effect [14], then a control law for the solvent flow rate is implemented as:

$$Q_s = 1.5Q_m - Q_i \tag{35}$$

To evaluate the proposed controller a linear model of the styrene reactor is required. This model was obtained by subspace identification techniques. The nominal point where the identification was performed is given by: $u_{ss}^1 = \begin{bmatrix} 0.030 & 0.131 \end{bmatrix}$ and $y_{ss}^1 = \begin{bmatrix} 3.8968 & 323.56 \end{bmatrix}$. The nominal model, denoted as M_1 , was obtained by means of the N4SID identification procedure [24], in open-loop, and it is as follows:

$$A_{1} = \begin{bmatrix} 0.95804 & 0.055977 & 0.0019812 \\ -0.001159 & 0.87878 & 0.002076 \\ 0.023994 & -0.061489 & 0.91569 \end{bmatrix},$$
 (36)

$$B_{1} = \begin{bmatrix} 20.024 & -2.4812 \\ -12.813 & -2.7082 \\ -13.692 & 0.51582 \end{bmatrix},$$
(37)
$$C_{1} = \begin{bmatrix} -0.075737 & 0.044659 & -0.1073 \\ 0.60234 & -0.27493 & -0.025648 \end{bmatrix},$$
(38)

5.1. Constraints and system sets

The state and input constraints, and the output zones are given by $\mathcal{X} = \begin{bmatrix} -20 & -20 & -20 \end{bmatrix}^T \le x \le \begin{bmatrix} 20 & 20 & 20 \end{bmatrix}^T$, $\mathcal{U} = \begin{bmatrix} -0.016 & -0.080 \end{bmatrix}^T \le u \le \begin{bmatrix} 0.016 & 0.080 \end{bmatrix}^T$ and $\mathcal{Y} = \begin{bmatrix} -3 & -0.35 \end{bmatrix}^T \le y \le \begin{bmatrix} 3 & 0.35 \end{bmatrix}^T$, respectively.

The persistent excitation set (EIS), \mathcal{U}^t , was computed according to the knowledge of the usual operation of the process, and it is given by $\mathcal{U}^t = \begin{bmatrix} -0.0060 & -0.0197 \end{bmatrix}^T \le u \le \begin{bmatrix} 0.0060 & 0.0197 \end{bmatrix}^T$, while the persistent excitation signal used for future excitations is given by a pseudo-random binary signal (PRBS signal).

The ISI set \mathcal{X}^t is computed according to \mathcal{U}^t , and by means of the procedure described in 3, it was extended to achieve a satisfactory degree of robustness. Here it is important to remark that given a model family of the form (9) – that can be estimated from practical tests – and given that the state constraint set \mathcal{X} is large enough, it is always possible to find an appropriated robust ISI set. This is what Theorem 4 shows. Then, it is not necessary to compute the set \mathcal{W} into which the uncertain parameter w should be contained. If one knows approximately the state space region that the system move to under usual operating point changes (which is an estimate of the model family for a certain \mathcal{W}), then it is not difficult, for instance, to enlarge a given ISI set, \mathcal{X}^t (not necessarily the minimal one), by adding a set as the one defined in Theorem 4, in such a way that the enlarged ISI set covers (approximately, or even, conservatively) the entire regions. This was the procedure adopted in the simulations



presented in the next section, in such a way that the ISI set is not only an ISI for model M_1 , but also for other models corresponding to different operating points. This procedure was selected to explicitly show that the use of invariant sets is not a main issue to apply the proposed strategy.

Fig. 3 shows the state constraint set, \mathcal{X} , the ISI set, \mathcal{X}^t and the CES set \mathcal{X}_{ss}^t . Fig. 4, on the other hand, shows the output constraint set \mathcal{Y} , the output target set $\mathcal{Y}^t = C\mathcal{X}^t$ and the Output Equilibrium set $\mathcal{X}_{ss}^t = C\mathcal{X}_{ss}^t$.

6. Simulation results

6.1. Nominal operating point operation

In this section some results are presented to evaluate the proposed control structure applied to the polymerization reactor. The different operating points are assumed to be known – these points come from a real time optimization (RTO) problem, solved in an upper control levels – and the simulations start at the nominal operating point $u_{ss}^1 = \begin{bmatrix} 0.030 & 0.131 \end{bmatrix}$ and $y_{ss}^1 = \begin{bmatrix} 3.8968 & 323.56 \end{bmatrix}$. Under this operating condition, model M_1 , given by (36)–(38), is used as the nominal prediction model of the MPC. All along the simulation, output white noise – with zero mean and standard deviation of 0.001 for y_1 and 0.01 for y_2 – will be considered.

Simulations were designed to show the MPC controller working in the *Re-identification Operation Mode* in both cases, when the system is outside and inside the ISI set. As it can be seen in Fig. 5, different feasible states in $\mathcal{X} \setminus \mathcal{X}^t$ are steered into the objective ISI set \mathcal{X}^t , and once they are inside this set, the excitation procedure (autonomously) starts.



Fig. 4. Output sets $\mathcal{Y}, \mathcal{Y}^t$ and \mathcal{Y}^t_{ss} .



Fig. 5. State trajectory outside X^t .



Fig. 6. State trajectory around χ_{ss}^{t} , inside χ^{t} .

Fig. 6 shows the ISI set X^t and the equilibrium set X_{ss}^t , together with the parametric state evolution. Notice that the state trajectories move around X_{ss}^t while the system is excited, which means that the system cannot be driven entirely inside the control equilibrium set (CES); i.e., the system cannot be driven from one equilibrium point to another (transient regime) without leaving the equilibrium set. This shows that it is not possible to use X_{ss}^t as an objective set

for an MPC suitable for re-identification and justifies the inclusion of invariant sets in the formulation.

Furthermore, notice that once the state trajectory enters \mathcal{X}^{t} , it cannot leave the set, due to the *robust invariance condition* under the excitation input. Without the invariant property, a switching scenario may appear: once the state enters \mathcal{X}^{t} the excitation procedure starts, and the same excitation may steer the state outside \mathcal{X}^{t} , where the excitation is aborted. Then, the controller would drive the state back into \mathcal{X}^{t} , and the cycle would be repeated again and again, producing an undesirable closed-loop behavior.

Notice also that the invariant set \mathcal{X}^t , which was computed based on a linear model, ensures invariance also for the entire family of models that describe the nonlinear system, given that it was computed to be robust.

Figs. 7 and 8 show the time evolution of the input and output, respectively. In these figures two different sub-modes can be clearly seen: first, from time step k = 0 to k = 6, the system is steered to the ISI set (with a decreasing cost) and then, from time k = 6 on, the system is persistently excited (with a null cost function). This last period corresponds to the injection of a previously defined PRBS signal, \mathbf{u}_{PE} , to the system. Notice that the inputs are close to their limits at the beginning, since the controller tries to do its best to drive the system to the objective ISI set. Then, after time step k = 6, the inputs remain inside the EIS set \mathcal{U}^t – which is plotted in dotted lines in Fig. 7. Fig. 9 shows the first 20 time step evolution of cost.

The selected PRBS signal is of a relatively slow frequency. This implies that the state trajectory under this excitation is relatively close to stationary behavior, and so, it covers almost entirely the so called minimal invariant set of the system. Otherwise, the state evolution will be even smaller than the one shown in Fig. 6. The robustness condition of the invariant set, however, makes that the minimal invariant set is only a (conservative) small subset of χ^{ℓ} .

Finally, it should be noticed that it is easy to show that the input and output signal during the excitation procedure are uncorrelated, which allows one to implement any known identification method. In the next subsection the subspace identification method will be implemented with the input–output collected data.

6.2. Changing the operating point

In this section, a change of operating point is simulated, to evaluate the controller in a sever model-mismatch scenario. Given



Fig. 7. Input time evolution. From time step k = 10 on, input data set.



Fig. 8. Output time evolution. From time step k = 10 on, output data set.



Fig. 9. Cost time evolution: first 20 samples, when only control actions are implemented.

the system nonlinearity, the new operating point, which is given by $u_{ss}^2 = \begin{bmatrix} 0.0330 & 0.1245 \end{bmatrix}$ and $y_{ss}^2 = \begin{bmatrix} 3.7621 & 324.66 \end{bmatrix}$, places the system in a region where the original model cannot make accurate predictions. As usual in process operation, operating point changes are frequent, and so, the need for a model update (a reidentification) becomes apparent.

The constraint sets and the excitation set EIS will remain unmodified in this simulation. The state, input and output trajectories, going from the nominal to the new operating point, can be seen in Figs. 10–12, respectively. The system is steered by the MPC in the *Control Operation Mode*, which is the mode of the controller when no re-identifications are needed. Figs. 10 and 11 show that



Fig. 10. Input time evolution corresponding to the change of the operating point (from time step k = 100 to k = 200) and the new re-identification input data set (from time step k = 200 to k = 500).



Fig. 11. Output time evolution corresponding to the change of the operating point (from time step *k* = 100 to *k* = 200) and the new re-identification input data set (from time step *k* = 200 to *k* = 500).

at time step k = 100 the system starts to be driven from the nominal operating point, $[u_{SS}^1 y_{SS}^1]$, to the new point, $[u_{SS}^2 y_{SS}^2]$. This transient period is relatively short, so in approximately 50 time steps the new point is reached. Then, at time step k = 200 the controller is switched to the *Re-identification Operation Mode* (*Problem* $P_N^{EXC}(x, X^t, \mathbf{u}_{PE}, k)$), where the excitation procedure starts. In fact, as it was described, two conditions are needed for the excitation to start: the controller must be in the *Re-identification Operation Mode* and the state must be in χ^t . Otherwise, if the controller is switched to *Re-identification Operation Mode* when the state is outside χ^t , then the controller steers first the state to it, and then starts the excitation. This excitation permits, as explained, generating uncorrelated input–output data to obtain a new process model for the controller.

At this point it is important to remark that, given the robustness of the controller design, the new state trajectory (corresponding to the persistent excitation procedure) is completely inside the (robust) ISI set χ^t . This is so because this last set is not the minimal invariant set for identification (ISI set) associated to model M_1 , but a robust invariant set obtained by the addition of other invariant set. Given that the excitation input signal is a PRBS signal of relative low frequency in comparison with the system response, the state trajectories cover almost entirely the minimal invariant sets of each models, including regions close to the boundaries (i.e., the minimal ISI set for model M_1 , \underline{X}_1^t , being model M_1 an approximation of the nonlinear model at point x_{ss}^1 , and the minimal ISI set for model M_2 , \underline{X}_2^t , being model M_2 an approximation of the nonlinear model at point x_{ss}^2 , which was not identified yet). This way, the minimal invariant sets of each model are polytopes that tightly envelope the state trajectories shown in Fig. 13. Notice that although the minimal invariant sets for each model are quite different (black and white trajectories), the ISI set is only one for every model, and it is no necessary to re-adapt it.

6.3. Disturbance rejection under the identification procedure

Next, the controller performance will be evaluated in a disturbance scenario, given by a disturbance entering the system during the re-identification procedure. It is given by a state change that pushes the state outside the ISI set, \mathcal{X}^t . The state trajectory for this case is shown in Fig. 14. There, it can be seen that the controller – always in the *Re-identification Operation Mode* – aborts the excitation procedure to exclusively control the system back to the ISI set \mathcal{X}^t . It takes to the MPC controller about 10 time steps to reach the ISI set again. Once the system is inside the set, the MPC controller resumes the persistent excitation of the system by means of the



Fig. 12. State trajectory corresponding to the change of the operating point, from x_{ss}^1 to x_{ss}^2 .



Fig. 13. State trajectories around x_{ss}^1 (white signal) and x_{ss}^2 (black signal) corresponding to Model M_1 , and the new model, respectively.



Fig. 14. State trajectory corresponding to the Re-identification Operation Mode when a disturbance enters the system.

PRBS input signal. The so-obtained data, in cases where a disturbance pushes the system outside the ISI set \mathcal{X}^t , should be collected in such a way that data corresponding to no-excitation periods are discarded. Figs. 15 and 16 show the input and cost time evolution, respectively.

The new model is obtained in the same way as the nominal model, by exciting the system around the new operating point with a (uncorrelated) PRBS signal, and using the subspace identification method known as N4SID [24]. The PRBS signal is designed according to the largest settling time of the input–output system relations. This way, the gain estimation made in the experiment is prioritized, which is of crucial importance in most model-based dynamical and economic optimization. This kind of signal not only provides a persistent excitation of the system, but also permits to preserve the validity of the linear approximation of process: given that the input signal switches from one value to another (i.e., it is a binary signal) and covers an appropriate range, the linear approximation around a given operating point is accurate, which means that approximately constant estimation of the gains are obtained (Fig. 17).

The reason why uncorrelated signals are used is that most industrial identification practices continue to rely on uncorrelated input test signals, even though some benefits of the use of higher correlated signals are now known [4], mainly to 'generate more excitation to be applied in the weak gain direction of the process'. In fact, to design this latter kind of signals, it is necessary to know *a priori* the system gain, in order to estimate the weak directions, which increases the complexity of the method.

Although the system could be considered in closed loop, while the states are inside x^t there is no feedback that correlates with



Fig. 15. Input evolution corresponding to the Re-identification Operation Mode when a disturbance enters the system. The shadowed period corresponds to the period where the state is outside λ^{t} , and the input should not be considered as input data set.



Fig. 16. Cost evolution corresponding to the Re-identification Operation Mode when a disturbance enters the system. The shadowed period corresponds to the period where the state is outside λ^{t} .









Fig. 19. Step response of the old model M_1 (blue) and the re-identified model M_2 (red). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the inputs, and so, the subspace identification method will give an unbiased model. The first 800 input–output samples of the excitation procedure are used for the excitation procedure itself, while the last 400 are used for validation proposes. The new 3rd-order identified model, M_2 , is given by:

$$A_2 = \begin{bmatrix} 0.8841 & 0.1096 & 0.02627 \\ 0.0121 & 0.682 & -0.09175 \\ 0.177 & 0.2813 & -0.06919 \end{bmatrix},$$
(39)

$$B_2 = \begin{vmatrix} 43.18 & -8.723 \\ -27.06 & -5.337 \\ -26.27 & 19.12 \end{vmatrix},$$
(40)

$$C_2 = \begin{bmatrix} -0.07372 & 0.03907 & -0.06153\\ 0.6035 & -0.2271 & -0.06025 \end{bmatrix},$$
(41)

A cross-validation method was applied to the new and old model. This procedure is considered to be the best in order to validate models and the only one that can find actual general application [20]. Fig. 18 shows the comparison between the validation of the old (M_1) with the new (M_2) model, taking into account the new set of data. As it can be seen, the FIT coefficient for model M_2 is 86% (mean for the two outputs), while the FIT for M_1 is 41%. This fact clearly shows the necessity of a new identification each time the operating point changes.

Fig. 19 shows the step response of model M_1 (blue) and model M_2 (red).

7. Conclusions

In this work, new theoretical results related to robustness of Model Predictive Controller suitable for closed-loop re-identification were presented. Furthermore, the proposed MPC was applied to a nonlinear polymerization reactor simulator, in order to study the controller performance under different identification scenarios.

The apparent conflict between exciting and controlling a system is avoided by means of the use of a robust invariant set as a MPC target set – instead of using target equilibrium points that do not correspond to an excitation scenario. Closed-loop feasibility and attractivity of the target set is guaranteed when the system is outside the set. Furthermore, the identification procedure can be made in open-loop fashion when the system is inside the target set, given that no control actions correlate the system inputs and outputs in this region.

Although a comparison with other MPC's for re-identification is not valid – since none of them account for stability properties, and furthermore, the excited input–output data are correlated by the feedback – the simulation results show that the controller can be easily applied to the nonlinear simulated system, producing as expected, uncorrelated input–output data sets, even when the system operating point changes significantly.

Future works include the study of an adaptive scheme to improve the accuracy of the model by a recursive identification procedure.

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