Nonlinear model predictive control for batch processes using set-theory

Control predictivo basado en modelo para procesos por lotes utilizando teoría de conjuntos

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Abstract
The control problem of Batch Processes presents many challenges. In general, it must deal with the irreversible behaviour of state variables, limited corrective actions, and sensitivity regarding disturbances. In this paper, the Controllable Trajectory Set is applied to a Nonlinear Model Predictive Control to improve the control performance of Batch Processes. The main capability of the proposed controller is to operate over a safe trajectory and away from constraints by incorporating the Controllable Trajectory Set. When the optimization problem solution is feasible, it is possible to ensure the end batch point. Additionally, the Nonlinear Model Predictive Control uses Controllable Reference Trajectory as the desired trajectory to improve robustness. Controller characteristics are illustrated using a semibatch process under a disturbance scenario. The proposed scheme decreases the control indexes under the disturbance scenario, assuring the main control objectives.
Keywords: Reachable set; Controllable set; Controllable Reference Trajectory; Controllable Trajectory Set; Robustness; MPC.

Resumen
El problema de control de los procesos por lotes tiene varios desafíos. En general, es necesario lidiar con el comportamiento irreversible de las variables de estado, acciones correctivas limitadas y sensibilidad ante perturbaciones. En este artículo, el conjunto de trayectoria controlable se aplica a un control predictivo de modelo no lineal para mejorar el rendimiento del control de procesos por lotes. La principal capacidad del controlador propuesto es operar sobre una trayectoria segura y alejarse de las limitaciones mediante la incorporación del conjunto de trayectoria controlable. Cuando la solución del problema de optimización es factible, es posible asegurar el punto final del lote. Además, el control predictivo de modelo no lineal utiliza la trayectoria de referencia controlable como la trayectoria deseada para mejorar la robustez. Las características del controlador se ilustran mediante un proceso semi-lote en un escenario de perturbación. El esquema propuesto disminuye los índices de control bajo el escenario de perturbación, asegurando el alcance de los principales objetivos de control.
Palabras Clave: Conjunto alcanzable; Conjunto controlable; Trayectoria de Referencia Controlable; Conjunto de Trayectorias Controlables; Robustez; Control Predictivo.

1 INTRODUCTION

Batch Processes (BPs) have been widely used in the food, chemical, and pharmaceutical industries. In recent years, their use has increased due to their flexibility, i.e., their ability to handle different grades, types, and quantities of products with the same equipment. However, BPs control is still challenging because the control system must be designed over a time-dependent trajectory with irreversible states. A BP always has transitory dynamic and irreversible behaviour of at least one state [1]. These two specific characteristics are not frequently found in continuous processes, where the main problem is regulating variables around an equilibrium point. In BPs, the main control aim is to obtain a certain quantity and quality of product at the end of the batch, i.e., this is an endpoint problem [2].

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Regardless of the operation mode of the processes, batch or continuous, Model Predictive Control (MPC) stands as the most promising control technique. MPC is a family of techniques with a very high level of development. Much literature is devoted to theoretical results regarding MPC on continuous processes, such as feasibility and stability [3]–[9]. Unfortunately, although many emerging papers are concerned with this subject, theoretical results on BP control design are scarce.

The BPs control objective is to drive the process from an initial condition to a desired final state. An endpoint Nonlinear Model Predictive Control (NMPC) is the most suitable technique since it incorporates the final state of the systems in the cost function or constraints [10], [11]. However, NMPC applied to BPs usually is implemented through trajectory tracking, in which the controller has a desired trajectory [2], [12], [13]. Such a trajectory is computed offline following economic criteria. The technique is relatively easy to implement, but the obtained optimal often operates over the constraint with a low capability to react to disturbances, which may lead to an unfeasible control [12].

Up to now, there has yet to be an agreement about the best MPC technique for BPs. Each MPC technique offers a specific possibility that the other techniques cannot give [14]–[17]. The stability and controllability of many MPC proposals for BPs are often tested under simulation without theoretical developments due to the irreversible feature of the BPs [18]. BPs control is troublesome because it does not have a unique equilibrium point and is not controllable because it has irreversible states [19]. However, using the concept of local controllability along a trajectory proposed by [20] and applying other ideas from set-theoretic methods in control, a framework for BPs control analysis was proposed [12], [18], [19]. The central concept in that proposal is the Controllable Trajectory Set (CTS). This set is used as an index of the control capability of the BP operation. It can be interpreted as the feasibility of converging to a final desired state, maintaining it around a given trajectory. A similar concept is discussed in [21], addressing the stability issue in BP and its relation to reproducibility. Reproducibility is the issue of whether the trajectories at several BP runs will remain close during their time evolution when they have sufficiently close initial conditions and identical input profiles. In other words, stability in BPs can be related to the ability to reproduce the same or close trajectories despite the disturbance effect of the initial condition [21].

This paper proposes an NMPC that combines endpoint control and trajectory tracking with CTS and Controllable Reference Trajectory (CRT) techniques. The proposed scheme obtains some robust characteristics, ensuring the achievement of the endpoint objective if the optimization problem reaches a feasible solution [4], [22], [23]. Section 2 describes the NMPC in BPs control problem to present our proposal. Section 3 presents the CTS and the CRT in terms of the Set theory framework. Then, Section 4 presents the proposed NMPC for BPs, and Section 5 shows some simulations, illustrating the benefits of the proposed strategy when controlling a BP. Finally, some conclusions are outlined.

2 NMPC IN BATCH PROCESS CONTROL

BPs dynamics are characterized by the existence of irreversible states which affect process controllability [1], [18]. Other works have highlighted the implications of such characteristics in the control system's performance [24]. Generally, BPs control is evaluated by its capacity to accomplish two kinds of objectives [25]:

- Trajectory tracking: The output variable must follow a particular set point trajectory during all the batch time.
- Endpoint shrinking: The output variable must shrink to a particular value at the end of the batch time.

However, in BPs control literature, control system performance is evaluated without disturbances because it dramatically impacts BPs dynamic and control system behavior. Only some authors apply disturbances to evaluate BPs control behavior [15], [24], [25]. The following section presents an application of NMPC in a BP control problem using a well-known semibatch model to illustrate NMPC behavior. First, we show the dynamic model and then the NMPC formulation with some simulations.

2.1 *Semibatch process dynamic simulation*

An isothermal semibatch stirred tank reactor dynamics is evaluated, where the elementary reaction ($A + B \rightarrow C$) takes place. The process considers that component A should be present in the reactor, while a continuous flow with B is added during the batch time to increase C productivity, which must reach 0.6 moles of C. The equations of this model, per [13], are:

$$\frac{dV}{dt} = q \tag{1}$$

$$\frac{dC_A}{dt} = -kC_AC_B - \frac{q}{V}C_A \tag{2}$$

$$\frac{dC_B}{dt} = -kC_AC_B + \frac{q}{V}(C_{Bin} - C_B) \tag{3}$$

where V is the volume, q is the inlet B component flow, C_{Bin} is the B component concentration in the feed flow, C_A and C_B are the respective A and B concentration, and k is a parameter related to the chemical reaction. This dynamic system has one input variable $(u = q)$ and three states,$[x_1, x_2, x_3]^T = [V, C_A, C_B]^T$. Product C is the output variable $(y = N_C)$ which is calculated using equation (4).

$$N_c = C_{A0}V_0 + C_{C0}V_0 - C_AV \tag{4}$$

where C_{A0} is the initial *A* concentration and C_{C0} is the initial *C* concentration, and V_0 is the initial volume. Simulation is performed during 22 hours of batch-time operation. This work focuses on control characteristics like the evaluation of trajectory tracking and endpoint shrinking [12], [18], [19]. Although the final condition can be obtained by finishing the process at the desired final C concentration, no matter the time used, we have set a finishing time to evaluate the control performance. As it is known, NMPC is suitable for accomplishing trajectory tracking and endpoint-shrinking objectives. The following section shows the NMPC general formulation and its application in this semibatch process control.

2.2 General NMPC formulation

The general NMPC formulation considers output variable error and the input and output as the minimum and maximum constraints. Moreover, we consider the minimum and maximum state constraints and dynamic models as equality constraints:

$$\min_{u} \sum_{i=1}^{N} \alpha_i \left(y_{k+i|k} - y_{ref}\right)^2 \tag{5}$$

Subject to:

$$u(t)_{max_{min}} \tag{6}$$

$$x(t)_{max_{min}} \tag{7}$$

$$y(t)_{max_{min}} \tag{8}$$

$$\dot{x}(t) = f(x(t), u(t)) \tag{9}$$

where *i=1,2…,* y_{ref} is the desired output reference, and *N* represents the discrete time steps until it reaches the final batch predictive horizon. The predictive horizon needs to be changed since BPs have a defined final time, and *N* will decrease until it reaches the final conditions. Equation 9 represents model dynamics, while equations 6, 7 and 8 represent input variables, state variables and output variables' maximum and minimum limits constraints, respectively. For instance, in the given semibatch process, the constraint for the volume variable $V \leq V_{max}$ is used. The NMPC was carefully tuned through simulation. In this process, α_i were set equal to 1000 for all i time steps, and the results should be the same for any value of α_i. However, providing the optimization methods with the major relevant position of numerical values produces better performance due to the sensibility function and the optimization method stop criteria. Furthermore, control performance could slightly change by selecting different α_i depending on the i time steps.

General NMPC formulation is evaluated using a Minimum Time Reference Trajectory (MTRT) calculated by an optimization problem stated in [12]. In the reference, the authors look for the minimization of batch time for the described semibatch process. Under our considerations, the minimum batch time is 19.72 hours. The NMPC controller simulation is evaluated using the Integral Absolute Error (IAE) for tracking trajectory evaluation and the Final Absolute Error (FAE) for endpoint shrinking objective evaluation.

$$\mathrm{IAE} = \int_0^{t_f} |y(t) - y_{ref}|\, dt \tag{10}$$

$$\mathrm{FAE} = |y(t_f) - y_{ref}| \tag{11}$$

Low IAE represents good trajectory tracking, while low FAE represents suitable endpoint shrinking. Even though the performance is batch case dependent, our proposal aims to decrease both performance indexes, i.e., to improve trajectory tracking and endpoint shrinking approaches.

2.3 Batch processes with disturbance

The experiment is performed using a 20% disturbance change in the inlet flow at the 5th hour. The disturbance variable is C_{Bin}. NMPC can handle the volume constraint. However, trajectory tracking and shrinking endpoint have a negative impact.

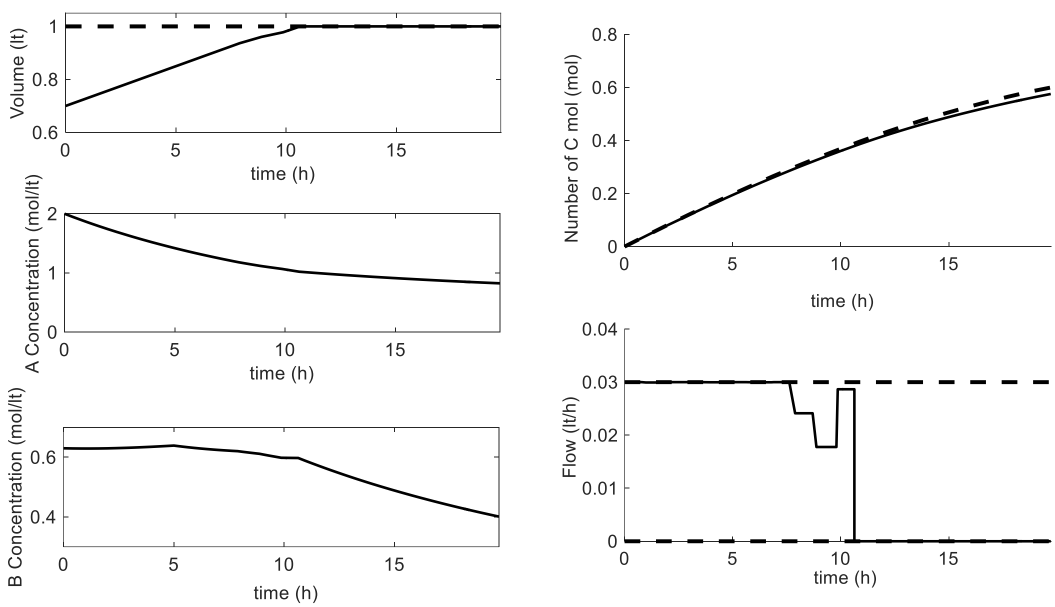

Figure 1. NMPC disturbance rejection

As a result, the values of error indexes were IAE=0.2007 and FAE=0.0244. Moreover, it is possible to see the input variable saturation, which is not desirable because there is no available input for control correction. Therefore, the NMPC alone cannot handle the problem in a disturbance scenario, as both IAE and FAE worsen. The NMPC with CTS presented in this work can decrease these indexes, simultaneously improving the trajectory tracking and the endpoint shrinking. Before presenting the CTS, the following section introduces some definitions of Set Theory. For further information, the reader may consider consulting the reference [22].

3 SET THEORY AS A BP CONTROL FRAMEWORK

The absence of a steady state in a BP affects the theoretical analysis because controllability and stability are evaluated around the steady state. There are some proposals for controllability and stability analysis of BPs or systems without a steady state [19] [21] [26], but the problem still needs a complete solution. [20] proposed a definition of local controllability along a trajectory. In this case, it is possible to control "every initial state near the original initial state to every final state near the original final state and to be able to do so without deviating far from the original trajectory." By using Set Theory methods, a framework to formalize controllability has been developed [19]. Since it is impossible to evaluate the controllability in irreversible states, the set theory appears as a solution to evaluate the control capacity in this kind of dynamic systems. [19] proposed the evaluation of BPs control systems through the hypervolume of the CTS. Then, [12] proposed using the CTS to design the CRT as a trajectory for control purposes. This paper proposes to use both definitions in an NMPC formulation to improve the control performance.

3.1 Definitions of Basic Sets

Consider a nonlinear, continuous dynamic system, such as:

$$\dot{x}(t) = f\big(x(t), u(t)\big) \tag{12}$$

$u(t) \in \mathcal{U}$ is the control action vector; $\mathcal{U} \subset \mathbb{R}^m$ is a compact and simply connected set that represents the set of system admissible control actions; $x(t) \in \mathcal{X}$ is the state vector; $\mathcal{X} \subset \mathbb{R}^n$ is a closed and simply connected set of physical states that the system can take; and $f(\cdot,\cdot)$ is defined in the $\mathcal{X} \times \mathcal{U}$ space. For the dynamic system represented by equation (12), it is possible to evaluate the following sets [19],[22].

Definition: Reachable Set in i-steps. Given a set $\mathcal{P}$, the Reachable Set $\mathcal{R}^i(\mathcal{P})$ from $\mathcal{P}$ in i-steps is the state space subset, in which the system evolves from $\mathcal{P}$ in i sample times, (Δt), given the admissible control action sequence $[u_1, u_2, u_3, \dots, u_i]$ of size i.

$$\mathcal{R}^i(\mathcal{P}) = \{x(i \cdot \Delta t) \in \mathcal{X} \exists x(0) \in \mathcal{P} \wedge [u_1, u_2, u_3, \dots, u_i] \in \mathcal{U}: x(i \cdot \Delta t) = f(x(0), u_1, u_2, u_3, \dots, u_i)\} \tag{13}$$

Definition: Controllable Set in i-steps. Given a set $\mathcal{S}$, the Controllable Set $\mathcal{C}^i(\mathcal{S})$ towards$\mathcal{S}$ in i steps is the state space subset, in which the system evolves towards$\mathcal{S}$in i sample times, (Δt), given the admissible control action sequence$[u_1, u_2, u_3, \dots, u_i]$of size i.

$$\mathcal{C}^i(\mathcal{S}) = \{x(0) \in \mathcal{X} \exists x(i \cdot \Delta t) \in \mathcal{S} \wedge [u_1, u_2, u_3, \dots, u_i] \in \mathcal{U}: x(i \cdot \Delta t) = f(x(0), u_1, u_2, u_3, \dots, u_i)\} \tag{14}$$

3.2 Controllable Trajectory Set

The control analysis for BPs used here is mainly supported by the concept of CTS [19]. The CTS is the interception between the Reachable set from a given initial condition and the Controllable set to the final condition [12][19]. Each set in Figure 2 represents a CTS at a certain time step, where Q_0 represents a state-space set of initial conditions while Q_N represents a state-space set of final BP conditions. The CTS is like a tunnel where the states travel from an initial set to a final desired condition in a BP, given the admissible control action vector set. As a result, every state that belongs to the CTS can shrink to the final condition set considering its initial condition.

Using CTS in NMPC formulation would give extra information about the state of the BP to accomplish trajectory tracking and the best shrinking of the endpoints. Figure 2 shows a tunnel reconstruction through layers or views at different times of the intersection of controllable and reachable sets. Inside that tunnel, there are infinite CTSs. The calculation algorithm for CTSs is presented in [12].

Therefore, the ideal situation is that the designed control helps the states to remain inside the tunnel following one or more CTSs. Nowadays, there needs to be an analytical strategy to obtain the reachable and controllable sets for BP control analysis. Therefore, several numerical methods have been proposed. Unfortunately, the algorithms used to estimate the sets are affected by the curse of dimensionality [27]. This issue has impeded the application of Set Theory in Control Theory. However, randomized algorithms have been used to deal with high computational complexity [28], [29]. Current work uses a randomized algorithm method with the dynamic model of the process to obtain points in state space that belong to Reachable and Controllable sets [12]. Then, each set is characterized as a polytope using the convex hull method. The Reachable Set and Controllable Set were computed to obtain the CTSs as the intercept between those sets [12], [18], [19].

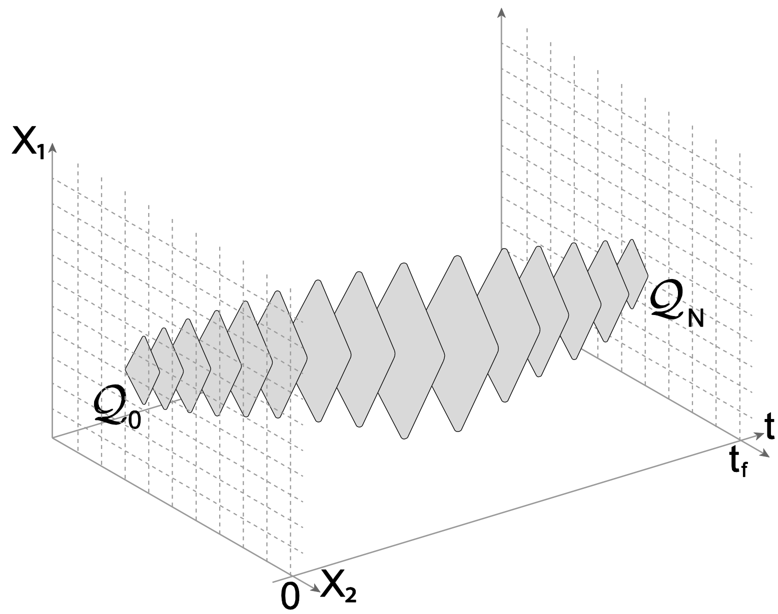

Figure 2. Controllable Trajectory Set

3.3 Controllable Reference Trajectory

Another critical issue concerning the NMPC proposal is the application of a Controllable Reference Trajectory (CRT), which was proposed in [12] and applied in [24]. The existence of the CTS produces two kinds of control actions, one driving the states outside the CTS and the other maintaining the states inside the CTS. When the state is inside the CTS, it has an available control action [12]. This kind of control action produces the Available Control Action Set (ACAS) defined in [12]. ACAS hypervolume depends on the trajectory [12]. Hence, we can search for the BP dynamics trajectory that can maximize the ACAS hypervolume, as shown in [12]. This optimal trajectory is the CRT ensuring the maximum ACAS series in the BP. CRT application allows the control system to improve trajectory tracking and endpoint shrinking, as it is shown in [24]. This trajectory is possible by the set theory analysis of BP dynamics.

Using the CRT in the NMPC proposal, it is possible to provide some robustness characteristics to the control system because it has all the BP control possibilities to face a disturbance [24]. However, it is essential to say that such a reference trajectory cannot assure maximum benefits (maximum productivity or minimum batch time) [12]. As a result, a CRT always works in a suboptimal condition for benefits but maintains the process stability.

4 NMPC PROPOSAL FOR BPS

The proposed NMPC includes two new features in its formulation, the CTSs, and a CRT. It is important to remember that CTSs and CRT are obtained offline. We used the same NMPC formulation shown in Section 2.2 in equations 5-9, including a new constraint for the states (equation 12). The prediction horizon needs to be changed since BPs have a defined final time, and N will decrease until it reaches the final conditions. y_{ref} is parameterized by the CRT definition. α_i are tunable coefficients which are used to give weight to a specific i-step error. The α_i value was selected as 1000 for all the sample times, to compare with classic NMPC.

$$x(t_i) \in \mathcal{Q}_i \tag{15}$$

The main idea is that the controller must maintain the process states inside the CTS tunnel to obtain the final desired conditions. The use of equation 15 as a constraint permits the controller to follow the reference trajectory, helping the irreversible state to approach the desired final state safely. Note that any kind of MPC formulation is prone to be used. Moreover, equation 15 is easier to evaluate if the CTS is a convex set. Therefore, this proposal does not add computational complexity to the NMPC.

As was previously said, the proposed NMPC includes two new features in its formulation to provide robustness and feasibility when applied to BP control. These characteristics are obtained by including the CTSs and a CRT, as explained below.

4.1 Robustness

Considering that the CRT is inherently robust, the typical disturbances and uncertainties of the BP model are covered by using it in NMPC. Generally, reference trajectory design in BPs assumes no disturbances during the batch time, so it is designed to operate under a favorable scenario. The mentioned CRT considers disturbance events taking place during the running of the BP. As a result, using the CRT in NMPC formulation gives robustness to NMPC.

4.2 Feasibility

The CTSs are used in the controller structure to guarantee feasibility in the optimization problem. The feasibility of NMPC with CTS formulation requires that, given any feasible initial state, its terminal region will be an invariant set. Like the MPC feasibility formulation based on Set Theory for continuous processes [4], [23], the aim of using the CTSs is to force the variables to remain in a secure zone. In a continuous process, the secure zone is an invariant set. However, note that due to inherently irreversible state variables of BP, the proposed NMPC approach cannot assure stability as defined in traditional MPC stable formulation [20]. However, if the process state variables remain inside the CTSs, the optimization problem solution is feasible. This feasibility was demonstrated by [11], as reproduced in the following theorem. This remark implies stable operation conditions (reproducibility) under robust NMPC-BP operation.

> **Theorem** [11]. Consider a dynamical system that represents a batch process under the NMPC law of Equations 5-9 and 15. If and only if $x(0) \in \mathcal{Q}_0$, the optimization problem defining the NMPC law in Equations 5-9 and 15 remains feasible for all $i = 1,2,3...,N$ steps and $x(N) \in \mathcal{Q}_N$.
>
> *Remark.* Other authors named the Controllable Set the *Reverse Time Reachability Region* [11]. This set contains all the states that can reach a given objective set $\mathcal{S}$ within a defined time and with the given admissible control set. [11] used this definition in their RNMPC formulation to handle the shrinking of the endpoint.

This theorem formalizes that when states belong to the CTS regions, it is a necessary and sufficient condition to guarantee the desired endpoint. Hence, if any state is driven outside the CTS region, the desired endpoint is not reached in the time batch. The convergence and stability of the method cannot be assured. However, since every CTS is a subset of a controllable set, it is possible to say that every CTS is a pseudo-invariant controllable set in N steps [18]. As a result, if there is a feasible solution, the closed-loop solution will maintain the states in the CTSs toward the final desired state.

5 NMPC PROPOSAL SIMULATION RESULTS

The following simulations seek to evaluate the two features of the proposed NMPC. The semibatch process control scenario shown in Section 2 is used. NMPC formulation with CTSs and CRT is tested using a disturbance rejection scenario to evaluate the advantages of the new NMPC proposal. The NMPC was tuned through simulation seeking good performance at the trajectory tracking control objective despite disturbances. The performance of the NMPC to trajectory tracking control is presented in Figure 3. This simulation does not experience any disturbance during the process.

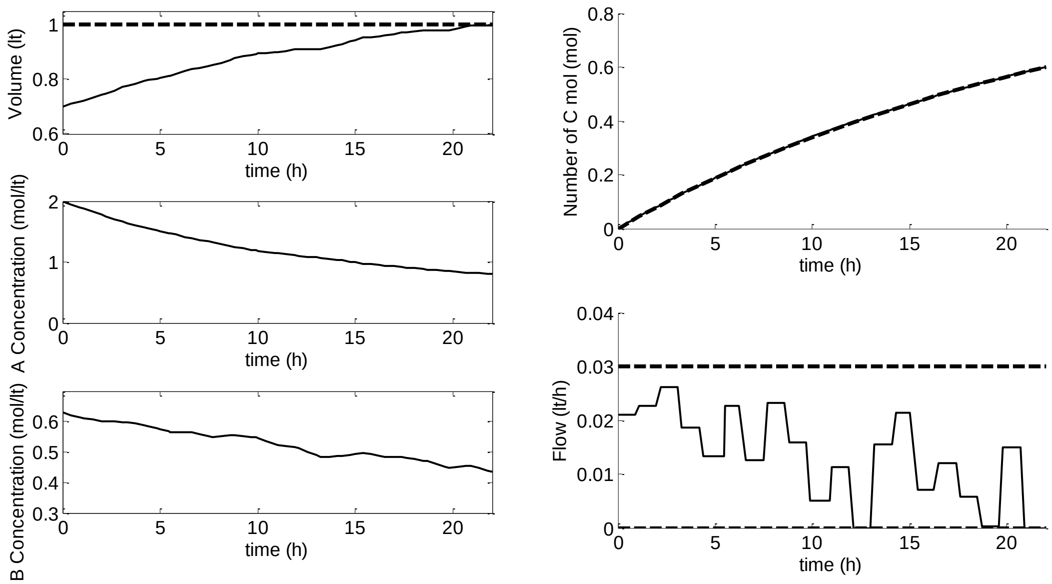

Figure 3. NMPC with CTS and CRT trajectory tracking.

The calculated values of performance indexes were 0.0208 for IAE and 8.57×10-6 for FAE. The proposed NMPC with CTS and CRT generates movements of manipulated variables far from the maximum limit avoiding the limited-corrective action problem. The inlet concentration of B (C_{Bin}) is treated as a disturbance for the semibatch system, to test controller robustness. Two events are simulated at ten hours of batch operation, changing C_{Bin} from a nominal value to a value 10% below and above its nominal value (Figures 4 and 5). It is noticeable that, besides some points, the input variable does not reach its saturated value, indicating that we still have some control maneuverability. The same is true when initial conditions are changed. Moreover, we have included a scenario where initial conditions are changed (Figure 6). Control behavior accomplishes that the volume is less than 1 L and the final output condition reaches the desired 0.6 mol of C value.

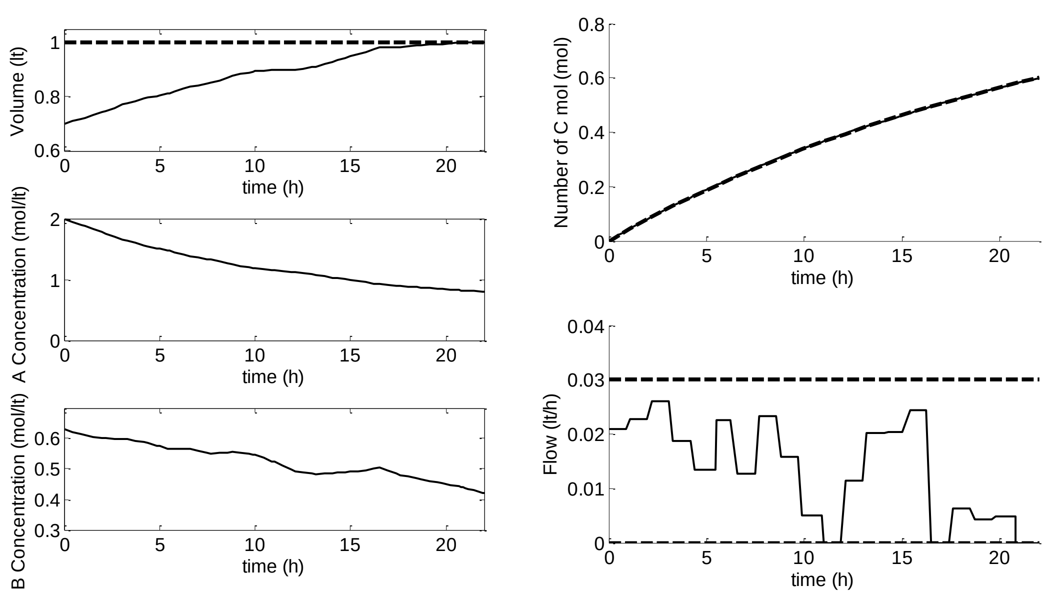

Figure 4. NMPC proposal with disturbance rejection: 10% below C_{Bin} nominal value.

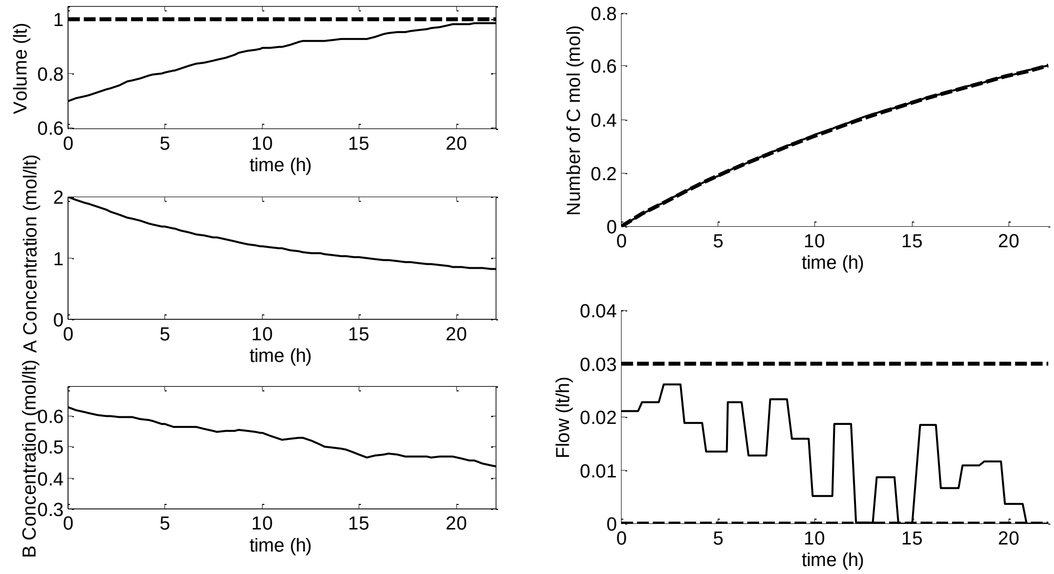

Figure 5. NMPC proposal with disturbance rejection: 10% above C_{Bin} nominal value.

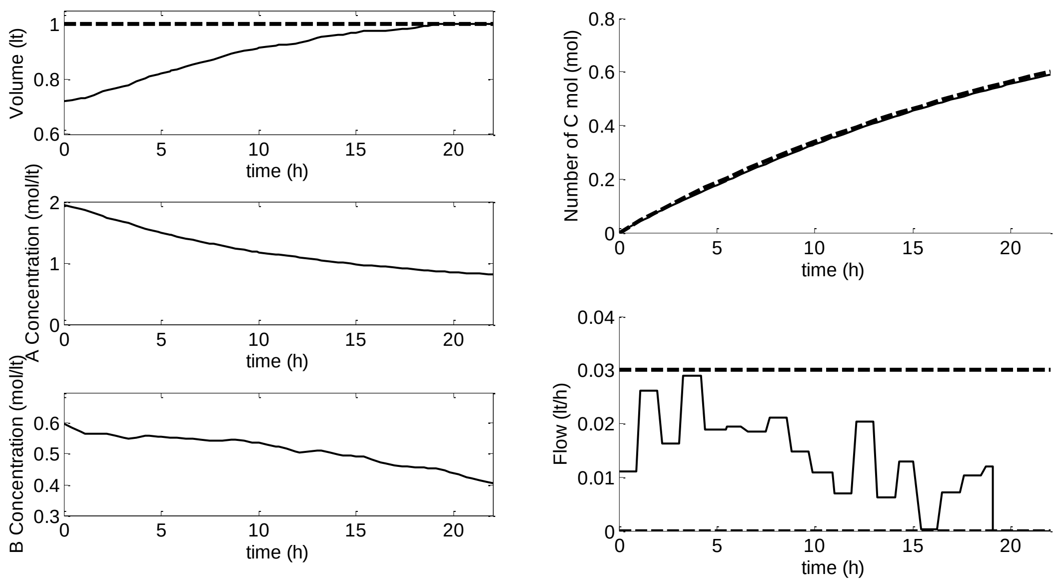

Figure 6. NMPC proposal with disturbance rejection: change in initial conditions.

Table 1 compares the performance of the general NMPC controller against the NMPC with CTS and CRT formulation throughout different disturbance scenarios. The performance index is less in the NMPC with CTS and CRT. The error indices are small for both controllers, showing that the general NMPC is suitable for BP control. Nevertheless, the proposed NMPC proposal improves the performance and can be a suitable solution for BPs with control problems. By enhancing the trajectory tracking and endpoint shrinking control problem, we can also improve the BPs reproducibility.

Tabla 1
NMPC Performance index comparison under different events

Controller	10% below CBin nominal value		10% above CBin nominal value		Changed initial conditions		Without disturbance	
NMPC	IAE	0.0661	IAE	0.0513	IAE	0.2206	IAE	0.0628
	FAE	0.0054	FAE	0.0025	FAE	0.0205	FAE	0.0044
NMPC with CTS and CRT	IAE	0.0203	IAE	0.0275	IAE	0.1848	IAE	0.0208
	FAE	0.0013	FAE	6.2x10-4	FAE	0.0116	FAE	8.57×10-6

6 CONCLUSIONS

A NMPC with CTS and CRT for BPs control was proposed and tested regarding disturbance rejection. It includes two new features in its formulation: the CTSs, and the CRT used to ensure controller feasibility and robustness, respectively. The NMPC improvement is focused on the limited corrective action challenge in BP control. Through the application of the CTSs and the CRT, the proposed NMPC can manage the irreversibility characteristic of every BP. The proposed NMPC uses the CTS to ensure the control feasibility, i.e., if the NMPC with CTS optimization solution is feasible, the endpoint condition will be assured. As a result, NMPC with CTS and CRT control has some robustness and reproducibility characteristics.

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