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Assessment of control techniques for the dynamic optimization of (semi-)batch reactors

Ergys Pahija^a

Flavio Manenti^{a,*}

Iqbal M. Mujtaba^b

^a Politecnico di Milano, Dipartimento di Chimica, Materiali e Ingegneria
Chimica “Giulio Natta”, Piazza Leonardo da Vinci 32, 20133 Milano, ITALY

^b School of Engineering Design & Technology, University of Bradford, West
Yorkshire BD7 1DP, UK

**Corresponding author:*

Phone: +39 02 2399 3273; Fax: +39 02 7063 8173; Email: flavio.manenti@polimi.it

Abstract

This work investigates how batch reactors can be optimized to increase the yield of a desired product coupling two appealing techniques for process control and optimization: the nonlinear model predictive control (NMPC) and the dynamic real-time optimization (D-RTO). The overall optimization problem is formulated and applied to calculate the optimal operating parameters of a selected case study and the numerical results are compared to the traditional control/optimization techniques. It has been demonstrated in our previous work (Pahija et al, Selecting the best control methodology to improve the efficiency of discontinuous reactors, *Computer Aided Chemical Engineering*, 32, 805-810, 2013) that the control strategy can significantly affect optimization results and that the appropriate selection of the control methodology is crucial to obtain the real operational optimum (with some percent of improved yield). In this context, coupling NMPC and D-RTO seems to be the ideal way to improve the process yield. The results presented in this work have been obtained by using gPROMS[®] and MS C++ with algorithms of BzzMath library.

Keywords

Dynamic optimization; batch reactors; control techniques; NMPC

1. Introduction

The growing competition and continuously more restricting regulations force improvement on chemical plants. Nowadays batch reactors play an important role in polymer, pharmaceutical productions, fine chemicals, and bioprocesses to quote a few. For instance, in the case of biofuels, discontinuous reactors are used for the deacidification of crude vegetable oils containing high amounts of free fatty acids (Boffito et al., 2013a, 2013b; Pirola et al., 2010). Improving models, simulation and optimization of batch processes is more problematic than continuous processes for the intrinsic dynamic nature of discontinuous operations and, hence, for the need of dynamic models that are usually hard to develop and evenly difficult to solve. In fact, many batch processes are based on heuristic optimization, exploiting the run-to-run method. Nevertheless, batch processes are extensively used in several fields such as the production of fine chemicals (Le Lann et al., 1999) or in the biomass pretreatment and conversion (Ranzi et al., 2013), where volumes are small and/or residence times are long. This is the reason for which great attention has been given to the modeling and optimization of batch processes in the last decades especially at the laboratory scale (Simon et al., 2007; Lima et al., 2009; Abel and Marquardt, 2003) leading to nonlinear models and, thus, to multi-dimensional constrained nonlinear programming problems. Nowadays, the computational effort and the numerical techniques allow solution of these problems easily by opening the possibility to implement novel coupled control/optimization methodologies (Buzzi and Manenti, 2010) that go beyond the traditional dynamic optimization based on conventional control loops; the coupling of NMPC and D-RTO is becoming feasible.

From this perspective, it is worth remarking that contrarily to the NMPC where manipulated variables are degrees of freedom of the optimization problems (Manenti, 2011) the dynamic optimization (D-RTO) has the setpoint trajectories as degrees of freedom. It implies that the control loops are open in the nonlinear model predictive control and the manipulated variables are the direct results of the (usually quadratic) optimization problems. On the other hand, the control loops are generally preserved (close) in dynamic optimization as they were originally conceived and they only receive new setpoints to be achieved for controlling and operating at best the discontinuous reactor (Bonvin, 1998). This work is focused on the implementation study of a coupled two-level dynamic optimization of batch reactors that benefit from the use of nonlinear model predictive control (NMPC) techniques. Actually, it has been demonstrated in our prior works (Pahija et al., 2013a, 2013b) that the final results of dynamic optimization significantly depend on the control technique **adapted** to manage the process and the NMPC is the ideal control technique to further improve the production yield. Literature batch systems (Zhang and Smith, 2004; Rohman et al., 2011) are adopted as validation case. The work is organized as follows: section 2) mathematical formulation of batch and semi-batch reactor models and optimization problems; section 3) optimization of the batch and semi-batch reactors (Rohman et al., 2011); section 4) assessment of different control techniques combined with dynamic optimization; and section 5) implementation of the combined NMPC and D-RTO technique.

2. General Mathematical Formulation

The optimization problem can be stated as follows:

- Given: the kinetic parameters for each reaction and the initial concentration of reactants.
- Determine: the optimal temperature profile for the batch reactors; the optimal temperature profile and the feed for the semi-batch reactor.
- Maximize: yield of the desired product.
- Subject to: reactant constraints and reactor model.

The Optimization Problem (OP) for the generic batch reactor (Figure 1) is described mathematically as:

	<u>Semi-Batch Reactor</u>		<u>Batch Reactor</u>	
OP	Max T, F Yield		OP Max T Yield	
s.t.	ODE (model equations) $T_L \leq T \leq T_U ; F_L \leq F \leq F_U$ $F_{TOT} \leq F_{LIMIT}$		s.t. ODE (model equations) $T_L \leq T \leq T_U$	[2]
	[1]			

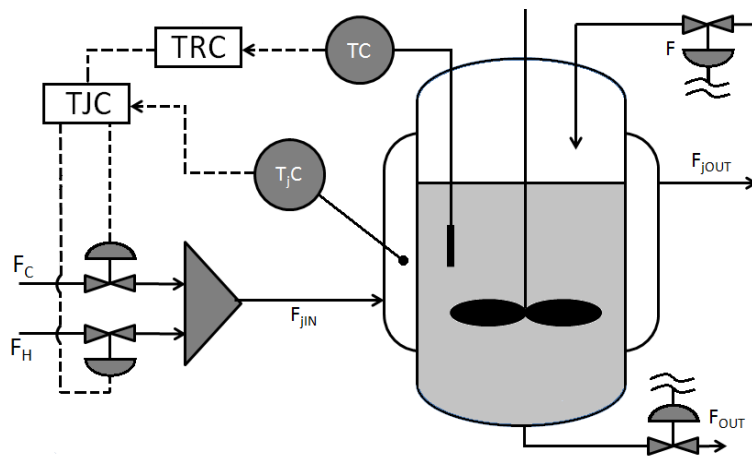


Fig. 1. Scheme of the batch reactor and the related control scheme.

Lower and upper bounds for the temperature, T_L and T_U , and inflow, F_L and F_U , are usually assigned. Specifically for the batch case the feed flow rate bounds are not necessary since the feed flow rate is null during the operations. The total amount of reactant B supplied to the reactor, indicated with F_{TOT} , must not exceed a specific threshold. Perfect mixing conditions are considered. Heat exchanges are neglected. Also the metal mass, which is often relevant in batch reactors with respect to the reactive volume, is neglected. The model equations (ODE system) are derived from the component continuity:

$$\frac{dn_j}{dt} = F_j + V \sum_{i=1}^{Nr} v_{ij} r_i \quad [3]$$

where $j = 1, \dots, Nc$; V is the volume of the reactor, F_j is the flow feed rate (null value for the batch case), v_{ij} is the stoichiometric coefficient of the compound j in the reaction i . Reaction rates r_i are calculated as follows:

$$r_i = k_i^0 \exp\left(-\frac{E_i}{RT}\right) \prod_{j=1}^{Nc} C_j^{v_{ij}} \quad [4]$$

where $i = 1, \dots, Nr$. T is the reactor temperature, E_i is the activation energy of the reaction i and C_j is the concentration of the compound j .

Other equations shall be written introducing the control system, such as the energy balances for the reactor and for the jacket.

Since the heat of reaction is negligible as well as the enthalpy related to the compound B fed to the reactor during the operations is rather small, the energy balance is reduced to:

$$\frac{dT}{dt} = \frac{Q_j}{(W_r * C_{pr})} \quad [5]$$

where Q_j is the heat exchanged with the jacket, W_r represents the total moles within the reactor, C_{pr} is the specific heat of the mixture inside the reactor. The energy balance for the jacket is:

$$\frac{dT_j}{dt} = \frac{-Q_j}{V_j \rho_j C_{p_j}} + \frac{M_j \rho_j C_{p_j} (T_{j_{sp}} - T_j)}{V_j \rho_j C_{p_j}} \quad [6]$$

where T_j , V_j are the temperature and the volume in the jacket respectively, while ρ_j , C_{p_j} are the density and specific heat of the fluid inside the jacket; M_j is the flow of water in the jacket. $T_{j_{sp}}$ is the setpoint temperature for the jacket. To manage the reactor temperature, hot and cold fluids entering the jacket can be opportunely mixed and a linear relationship can be used to model it:

$$\begin{cases} x_H + x_C = 1 \\ x_H T_H + x_C T_C = (x_H + x_C) T_j \end{cases} \quad [7]$$

where x_H and x_C are the fraction of hot and cold water respectively, used to obtain the desired temperature in the jacket. Specific heats are considered constant. The material balances were proposed and validated by Garcia et al. (1995). On the other hand, energy balances were suggested by Aziz et al. (2000).

3. Control Methodologies

Before presenting the analyzed case study, the control methodologies are illustrated below. The reactor temperature is controlled by means of Proportional (P), Proportional-Integral (PI), Proportional-Integral-Derivative (PID) (Stephanopoulos,1984) and Generic Model Control (GMC) (Arpornwichanop et al., 2005) methodologies. Briefly, considering a process based on the following model equations:

$$\frac{dx}{dt} = f(x, p, t) + g(x, t)u \quad [8]$$

$$y = h(x) \quad [9]$$

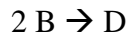
where x is a vector of state variables, y is a vector of output variables, u is a vector of input variables, p is a vector of process parameters and f , g and h are generally nonlinear function vectors (Arpornwichanop et al., 2005). As a general GMC controller the following algorithm is used:

$$\frac{dy}{dt} = K_1(y_{sp} - y) + K_2 \int_0^t (y_{sp} - y) dt \quad [10]$$

Where y is the controlled variable, y_{sp} is the set point of the controlled variable, K_1 and K_2 are tuning parameters and t is the cycle time.

4. Case Study

The case study analyzed is a parallel reaction scheme:



where C is the desired product to be maximized. The reaction conditions and kinetic parameters to perform the simulations are given in Table 1.

Table 1. Process conditions and kinetic parameters (Garcia et al., 1995).

Kinetic parameters	$k_1^0 = 7.55 \times 10^8 \text{ m}^3 \text{ kmol}^{-1} \text{ s}^{-1}$ $k_2^0 = 5.75 \times 10^{11} \text{ m}^3 \text{ kmol}^{-1} \text{ s}^{-1}$ $E_1 = 7.90 \times 10^4 \text{ kJ kmol}^{-1}$ $E_2 = 9.80 \times 10^4 \text{ kJ kmol}^{-1}$
Initial concentrations	$C_A^0 = 1.0 \text{ kmol m}^{-3}$ $C_B^0 = 1.0 \text{ kmol m}^{-3}$
Reaction volume	$V = 1.0 \text{ m}^3$
Reaction temperature bounds	$313.15 \text{ K} \leq T \leq 393.15 \text{ K}$
Batch cycle time	$t_s = 3600 \text{ s}$
Global exchange coefficient [kJ/(s m ² °C)]	$U = 40.842$
Specific heats [kJ/(kmol °C)]	$C_{pA} = 75.31$ $C_{pB} = 167.36$ $C_{pC} = 217.57$ $C_{pD} = 334.73$
Densities [kg/m ³]	$\rho = 1000$ $\rho_f = 1000$
Volume [m ³]	$V = 1$
Molar weight [kg/kmol]	$MW_A = 30$ $MW_B = 100$ $MW_C = 130$ $MW_D = 160$
Temperatures [K]	$T_H = 400.15$ $T_C = 313.15$
Initial temperatures (reactor - jacket) [K]	$T_0 = 350.15$ $T_{j0} = 340$

Performing the D-RTO, the initial control tuning parameters are $kc = 5$, $\tau_I = 30$ [s⁻¹], $\tau_D = 20$ [s], according to the conventional methodology P, PI and PID, respectively; tuning parameters for the GMC are $K_1 = 5$ [s⁻¹] and $K_2 = 1.0e-5$ [s⁻²]. The batch cycle time of 3600 s is discretized into 5 intervals of 720 s each. The SRQPD optimizer implemented in gPROMS and the BzzRobustMinimization optimizer implemented in BzzMath library are jointly used to handle the numerical problems. The initial reactor temperature is $T = 350.15$ K and the initial jacket temperature is $T_j = 340$ K. T_j is obtained mixing hot water ($T_H = 400.15$ K) and cold water ($T_C = 313.15$ K). Runs 1 to 4 (simulation and optimization) are performed on both batch and semi-batch reactors, Run 5 (D-RTO) simulates only the batch reactor, while the last run that couples the NMPC and the D-RTO is applied to the semi-batch reactor only highlighting the effectiveness of the proposed approach.

4.1. RUN 1: Process Simulation

Fig. 2 shows the numerical results assuming constant temperature $T = 350.15$ K for 5400 s (batch time), as proposed in the works of Garcia et al. (1994) and Zhang and Smith (2004). In the semi-batch case, the temperature is 393.15 K while the initial concentration of B is null and the compound is gradually fed during the operations for 3600 s, using a constant flow rate ($F_B = 2.778e-4$ kmol/s). Fig. 3 shows the numerical results for the semi-batch case. Comparative results for the two configurations are given in Table 2 (RUN 1). The numerical results are also compared to the results previously obtained by Garcia et al. (1994) and Zhang-Smith (2004). It is worth noting that Jackson et al. (1971) have observed that for reaction schemes with two parallel reactions (considering the first reaction having activation energy E_1 and the second

reaction having activation energy E_2), with reactant order m for the side-reaction and yield maximization as target, two cases are possible:

- $E_2/E_1 < m$, the reactant must be added gradually during the reaction, maintaining the temperature at its upper bound;
- $E_2/E_1 > m$, the reactant must be added at the beginning of the batch, optimizing the temperature.

For this particular reaction (RUN 1), $m = 2$, $E_2/E_1 = 1.24$. A comparison between the batch reactor (5400 s) and semi-batch-reactor (3600 s) shows that the semi-batch reactor works for 1800 s less than the batch reactor and the numerical results of RUN 1 reported in Table 2 highlight it as the best choice in this case, in good agreement with Jackson's directives.

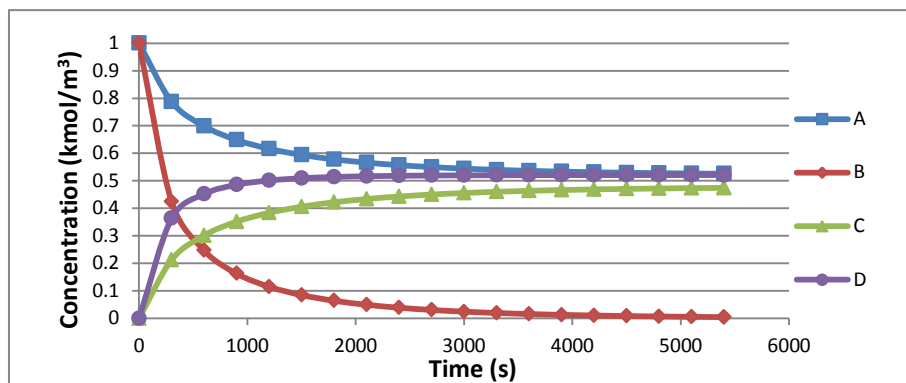


Fig. 2 Batch (5400 s) concentrations.

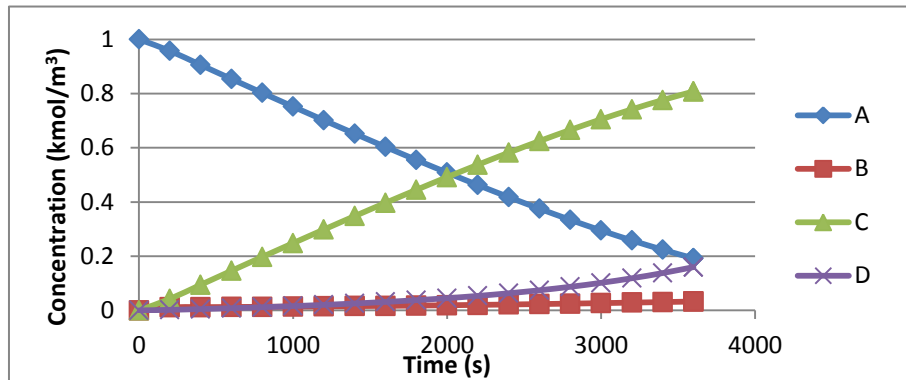


Fig. 3 Semi-batch (3600 s) concentrations.

4.2. RUN 2: Optimization

The batch reactor (batch cycle time 5400 s) and the semi-batch reactor (operation time 3600 s) studied in the Run 1 are optimized in this section. As optimization strategy, the reactor temperature profile is selected as degree of freedom for the batch case, whereas the temperature and the feed flow rate are selected as degrees of freedom for the semi-batch case. The systems are subject to the temperature bounds reported in Table 1. In addition, the semi-batch system is subject to the constraint of 1 kmol of B. The total batch cycle time is split into 10 intervals. Garcia et al. (1995) and Zhang and Smith (2004) have implemented a Generalized Reduced Gradient (GRG) method. In this paper, we adapted the SRQPD implemented in the gPROMS optimization tool improved by means of the very robust optimizers included in the BzzMath library (Buzzi-Ferraris and Manenti, 2010, 2012; Manenti, 2011). The optimal profiles of the reactor temperatures are reported in Fig. 4; the optimal feed flow rate is shown in Fig. 5 for the semi-batch reactor. The optimization results are showed in Table 2. It is worth saying that selecting only 2 discretization intervals for the optimization rather than the 10 intervals

selected here, the yield is still higher than 0.51. The yield in C is shown in Table 2 (RUN 2).

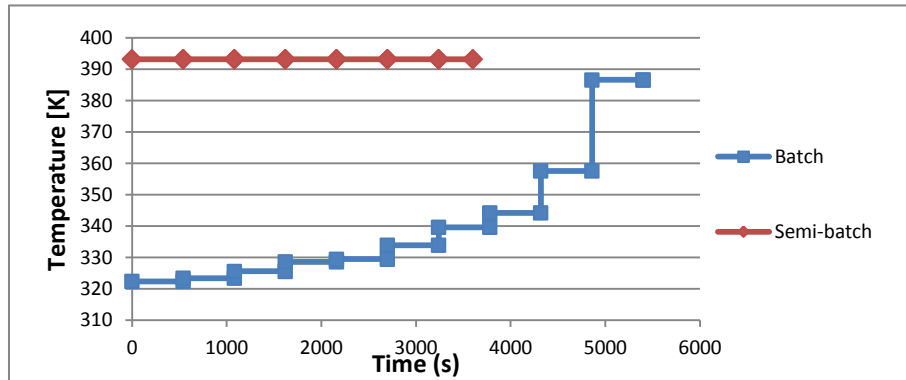


Fig. 4 Optimal temperature profiles.

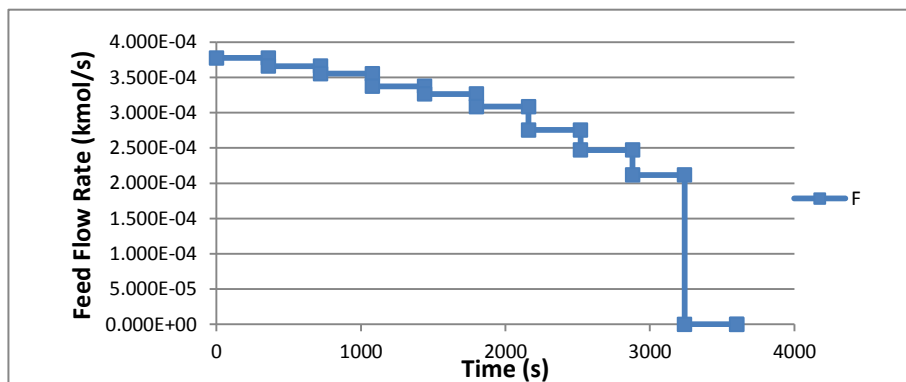


Fig. 5 Optimal feed rate.

4.3. RUN 3 : Simulation and Optimisation

This section is an extension of RUN 1 and RUN 2. Differently from the previews runs, where the batch cycle time was 5400 s while the semi-batch cycle time was 3600 s, in this run the cycle time for the batch reactor is 3600 s, while the cycle time for the semi-batch reactor is 5400 s. These runs were considered also by Garcia et al. and Zhang-Smith. The reaction and the parameters are the same used for RUN 1 and RUN 2. Looking at the results in Table 2 (RUN 3), increasing the operating time

leads to higher values of yield as expected. For this run, the component B is still a constrained value.

Table 2. Yield of C (desired product) from B. (* Run 1, ** Run 2, *** Run 3)

		Yields by Simulation			Yields by Optimization		
CASE	Time (s)	Garcia et al.	Zhang - Smith	This work	Garcia et al.	Zhang - Smith	This work
Batch	5400	0.4764*	0.491*	0.4744*	-	-	0.5361**
Semi-batch	3600	0.8109*	0.804*	0.8078*	0.8306**	0.822**	0.8293**
Batch	3600	0.4602***	0.473***	0.4637***	-	-	0.5197***
Semi-batch	5400	0.8414***	0.835***	0.8383***	0.8612***	0.853***	0.8617***

4.4. RUN 4 : Optimisation (improvement of RUN 2)

The optimization of the semi-batch reactor in RUN 2 is constrained by 1 kmol of B. Solving the semi-batch cases without constraints, it is possible to improve considerably the yield. For the 3600 s (semi-batch) case and 5400 s (batch), optimizing temperature for both cases and feed rate without constraints, the yields obtained respectively are 0.9716 and 0.9967. In the former case the total amount of B supplied is 1.77 kmol, whereas it is 2.33 kmol for the latter case. The unreacted A is reduced with respect to the constrained cases. For instance, using a cycle time of 3600 s with constraint, the residual of A is 0.171 kmol; on the other hand, the unconstrained case leads to residual A equal to 0.029 kmol. The dimensions of the reactor increase so that it can accommodate a higher amount of B. The effective dimensions of the reactor will depend on the densities of the species inside it.

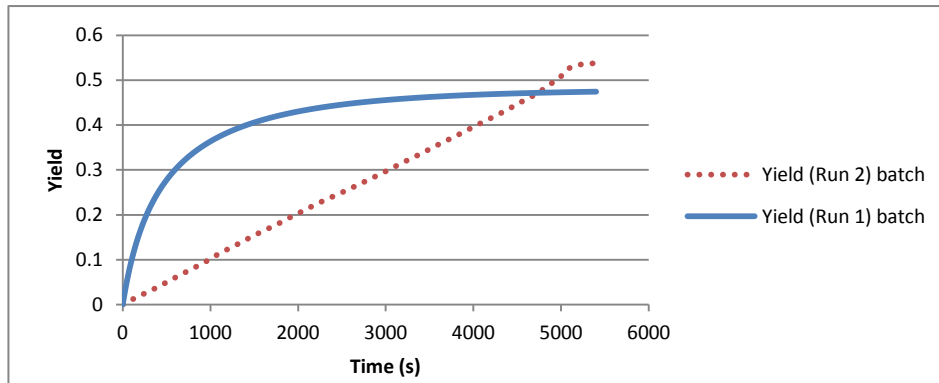


Fig. 6 Yields - batch case (5400s) Run 1 - Run 2.

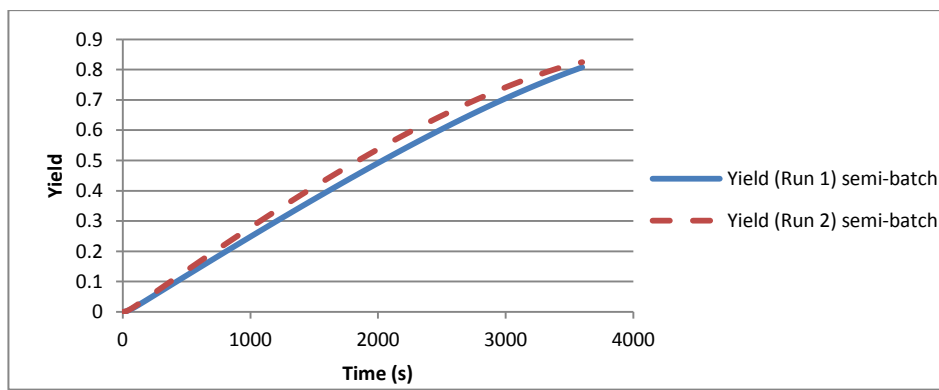


Fig. 7 Yield - semi-batch case (3600s) Run 1 - Run 2.

Fig. 6 shows the difference between the variation of the yield (of the desired product from C) maintaining the constant value of temperature inside the reactor (that is a given parameter equal to 350.15 K) (Run 1) and optimizing it through a piecewise constant optimization criterion (Run 2). Note that the yield of the optimized reactor is almost everywhere lower than the yield obtained by the regular simulation. It means that the optimal temperature profile obtained through the optimization will change if we change the total batch time; for instance, it is unsuitable to maintain the same trend of temperature otherwise the system will not achieve any yield improvement. Conversely, Fig. 7 shows the yield for the semi-batch case; the optimal yield (Run 2) is significantly higher than the yield obtained using a constant temperature

(Run 1) and a constant feed rate (that are given parameters equal to 393.15 K and 2.778e-4 kmol/s).

4.5. RUN 5 : D-RTO Control

As already introduced, this run is applied only to the batch reactor (3600 s) to make easier the discussion and highlight the benefits. Figs. 8 to 13 shows the process dynamics of the batch reactor obtained applying the D-RTO based on the aforementioned control methodologies. Specifically, the fractions of hot and cold water (manipulated variables) are reported in Fig. 8. The fraction of cold water decreases to let the reactor temperature progressively achieving higher values, as imposed by the dynamic optimizer that defines the reactor temperature optimal profile. Fig. 9 to 13 report the responses of the system to perform the servomechanism problems imposed by the dynamic optimizer. It is important to say that the trends are rather close to each other since the tuning parameters are optimized for each single control methodology. Nevertheless, responses are different according to the control methodology. It unavoidably means that the optimization is performed accounting for the controller feedback and the results is not purely economic, as it happens in the real-time optimization, but it is spoiled by control actions. It is surprising that the P controller, which has certain well-known relevant lacks with respect to the other methodologies (i.e. the offset), has superior performances when it is coupled with a dynamic optimizer. Actually, the use of P control coordinated by a dynamic optimizer leads to the highest yield of C (51.38%) with respect to the performance of the GMC (51.36%), PID (51.30%) and PI (51.27%). To better understand this fact, Fig. 13 show this difference comparing the optimal setpoints according to the control methodology. The setpoints obtained with the dynamic optimizer (D-

RTO) using the P controls are far from the other ones especially in the first and the last periods.

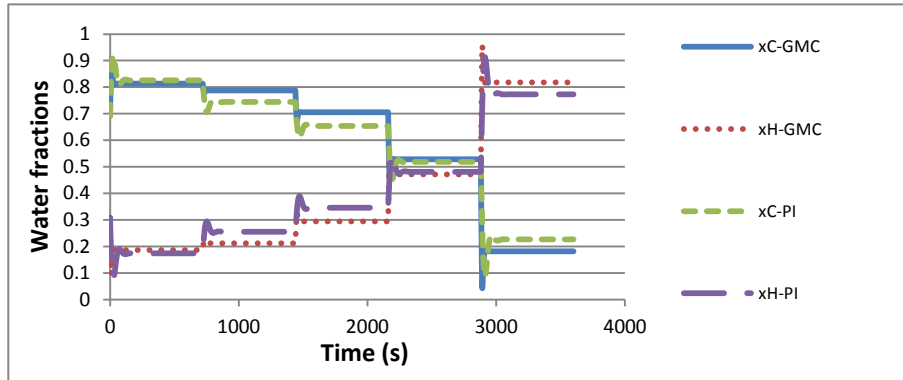


Fig. 8 Fractions of hot and cold water (xH , xC) with GMC and PI controls.

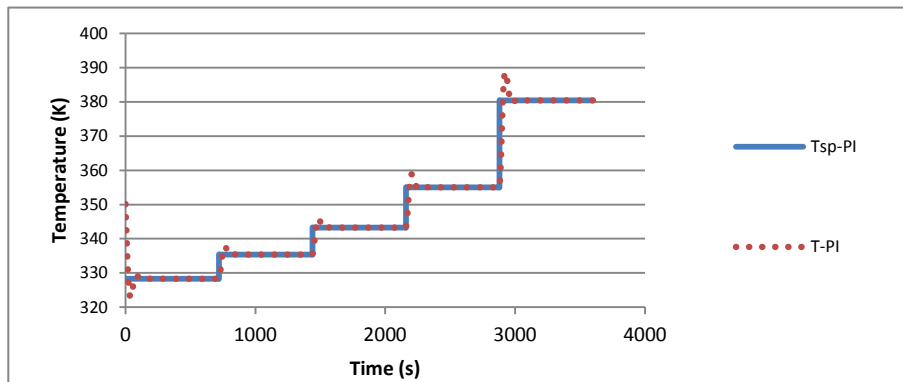


Fig. 9 Temperature setpoint ($Tsp-PI$) and reactor temperature ($T-PI$) with PI control.

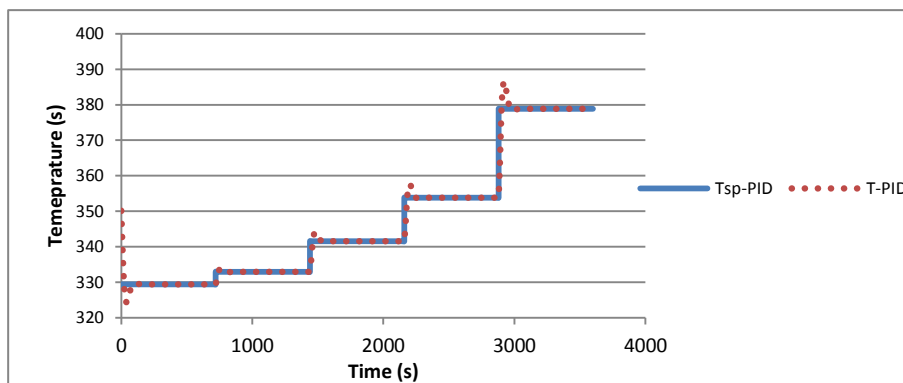


Fig. 10 Temperature setpoint ($Tsp-PID$) and reactor temperature ($T-PID$) with PID control.

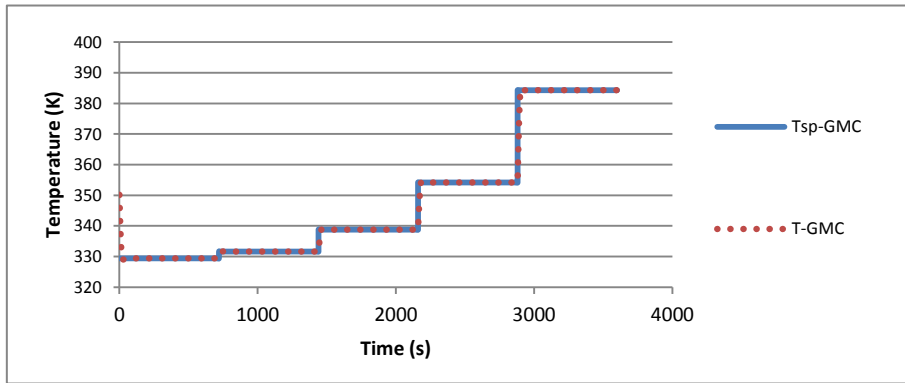


Fig. 11 Temperature setpoint (T_{sp-GMC}) and reactor temperature ($T-GMC$) with GMC control.

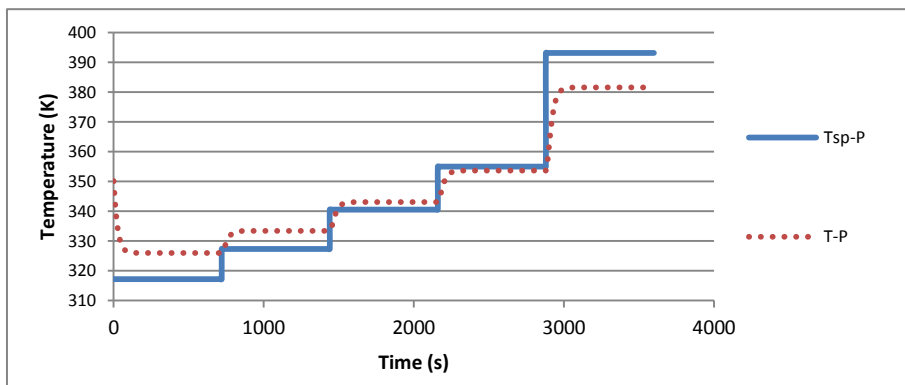


Fig. 12 Temperature setpoint (T_{sp-P}) and reactor temperature ($T-P$) with P control.

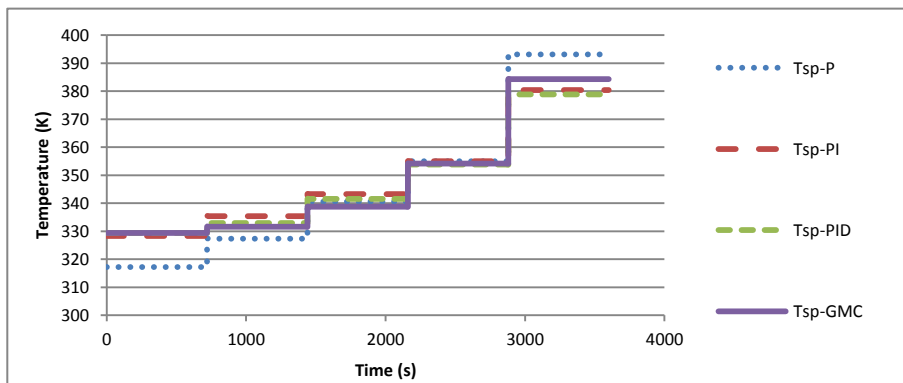


Fig. 13 Temperature setpoints for P, PI, PID and GMC controllers.

This is due to the offset of the P controls. Nevertheless, whenever the P controller is coupled with an optimizer such as in the dynamic optimization, the offset is directly handled and compensated by the same optimizer, which calculates a setpoint trajectory intentionally spoiled by the offset of the P controller, therefore zeroing the gap with respect to the other control methodologies. By doing so, certain good properties of P controls are fully exploited. The theory is easily confirmed by introducing the tuning parameters of the PID control, opportunely bounded, as additional degrees of freedom of the aforementioned optimal problem. Integral and derivative times of PI and PID controls tend to their upper and lower bounds respectively and, hence, the PID control tends to the P control. The optimal tuning parameters obtained are [kc=2.73 (P)], [kc=9.61, $\tau_I=53.77 \text{ s}^{-1}$ (PI)], [kc=19.93, $\tau_I=27.14 \text{ s}^{-1}$, $\tau_D=7.97 \text{ s}$ (PID)], [$k_1=3.99 \text{ s}^{-1}$, $k_2=2.82\text{E-}5 \text{ s}^{-2}$ (GMC)].

4.6. RUN 6 : NMPC and D-RTO

This run assesses the coupling of the NMPC with the D-RTO (Fig. 14). The semi-batch reactor is selected in this case (RUN 5, 3600 s). The setpoint profiles of the feed flowrate and the reactor temperature are obtained from the previous D-RTO. The optimization problem is formulated merging the economic target of D-RTO and the quadratic target of NMPC:

$$\max_{x_{set}} C_{yield}$$

$$\begin{aligned}
s. t. \quad & \min_{\bar{u}(k) \dots \bar{u}(k+h_c-1)} \left\{ \sum_{j=k+1}^{k+h_p} \omega_j (\bar{x}_j - x_j^{set})^2 + \sum_{l=k}^{k+h_p-1} \omega_{1,l} (\bar{u}_l - u_l^{tar})^2 \right. \\
& \left. + \sum_{l=k}^{k+h_p-1} \omega_{2,l} (\bar{u}_l - u_l^{(i-1)})^2 \right\} \\
s.t \quad & \begin{cases} x_j^{min} \leq \bar{x}_j \leq x_j^{max} \\ u_l^{min} \leq \bar{u}_l \leq u_l^{max} \\ \Delta u_l^{(i),min} \leq \Delta \bar{u}_l^{(i)} = \bar{u}_l^{(i)} - \bar{u}_l^{(i-1)} \leq \Delta u_l^{max} \\ \text{Model} \end{cases}
\end{aligned} \tag{11}$$

where *set* is the setpoint; u_l is the manipulated variable; $\bar{x}_j - x_j^{set}$ is the deviation between the control variable and its setpoint; $\bar{u}_l - u_l^{tar}$ is the deviation between the manipulated variable and its steady-state target; $\bar{u}_l - u_l^{(i-1)}$ is the incremental variation between i th and $(i-1)$ th time intervals of the l th manipulated variable; and ω are the weighting factors. Several simulations have been performed; the one reported in Fig. 15 has been obtained with a discretization horizon (integration step) equal to 36 s, the control horizon equal to 180 s and the prediction horizon equal to 800 s. **Control and prediction horizon are selected in accordance with heuristic methods reported in the literature (Manenti, 2011).** As the batch time is smaller than the control and prediction horizons, they are progressively reduced up to the end of simulation. This coupled approach results in a more effective batch production; actually, the production yield is 0.813, which is larger than the yield of 0.806 obtained in the best previous case (proportional control combined with D-RTO – **Run 5**).

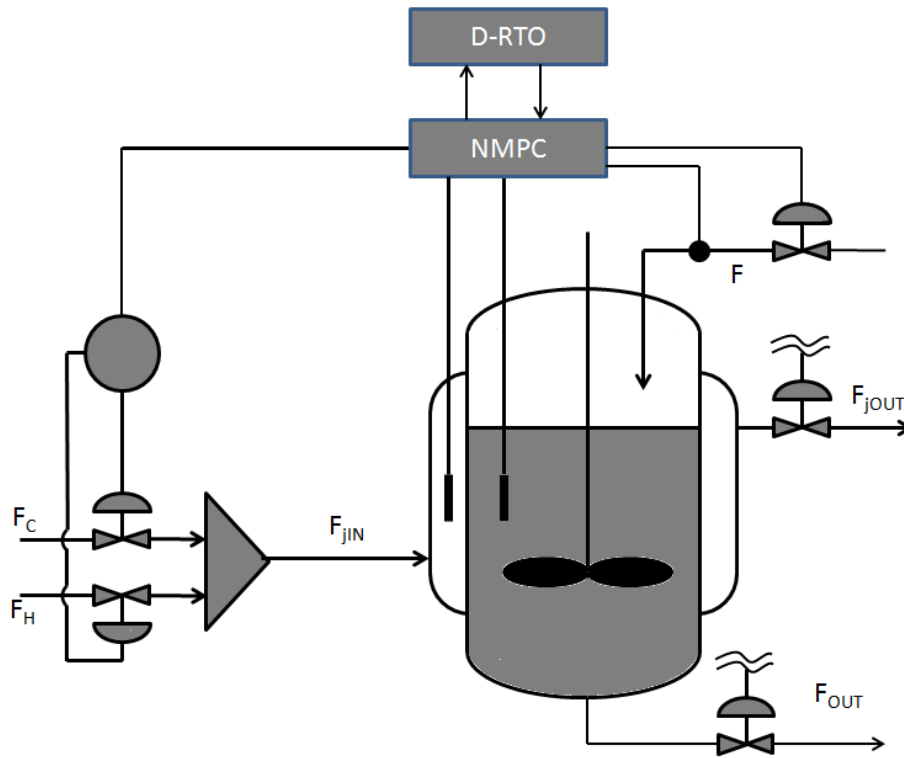


Fig. 14 Scheme of the Semi-Batch reactor and the related coupled optimization strategy (NMPC+D-RTO).

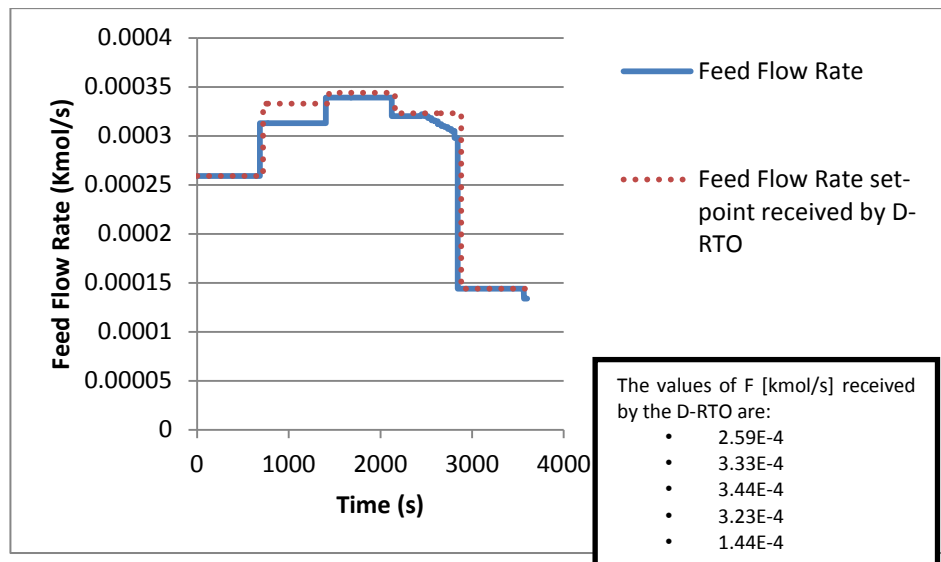


Fig. 15 The NMPC maintain the optimal trajectory received by the D-RTO.

5. Conclusions

Although the optimal conditions and setpoint trajectories to operate batch reactors are defined by means of dynamic optimization, they could be further improved by selecting the most appealing control technique. It was already demonstrated in our prior work (Pahija et al., 2013b) that the operations of batch systems can be improved simply considering the tuning parameters as degrees of freedom of the dynamic optimization problem. This paper has extended this concept by assessing different control techniques combined with dynamic optimization, showing that the proportional control is the most appealing one among the conventional control techniques and that its well-known offset issues are absorbed by the dynamic optimizer, making it very effective. At last, the preliminary results of coupling the dynamic optimization and nonlinear model predictive control for batch reactors have shown further potential.

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