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

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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. (2013). Selecting the best control methodology to improve the efficiency of discontinuous reactors. *Computer Aided Chemical Engineering, 32*, 805–810) 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.

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, Pirola, Galli, Di Michele, & Bianchi, 2013; Boffito, Crocella, et al., 2013; Pirola, Bianchi, Boffito, Carvoli, & Ragaini, 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, Cabassud, & Casamatta, 1999) or in the biomass pretreatment and conversion (Ranzi, Corbetta, Manenti, & Pierucci, 2014), 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 (Abel & Marquardt, 2003; Lima & Linan, 2009; Simon, Introvigne, Fischer, & Hungerbühler, 2008) 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-Ferraris & 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 receives 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

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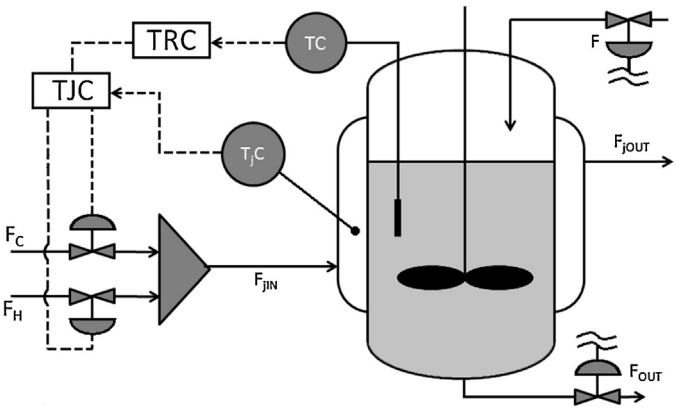

Fig. 1. Scheme of the batch reactor and the related control scheme.

of nonlinear model predictive control (NMPC) techniques. Actually, it has been demonstrated in our prior works (Pahija, Manenti, & Mujtaba, 2013a;Pahija, Manenti, & Mujtaba, 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 (Rohman, Sata, & Aziz, 2011; Zhang & Smith, 2004) are adopted as validation case. The work is organized as follows: Section 2 describes mathematical formulation of batch and semi-batch reactor models and optimization problems; Section 3 describes optimization of the batch and semi-batch reactors (Rohman et al., 2011); Section 4 describes assessment of different control techniques combined with dynamic optimization; and Section 5 describes 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 (Fig. 1) is described mathematically as:

Semi-batch reactor

$$\begin{aligned} &\text{OP} \quad \text{Yield} \\ &s.t. \quad \text{ODE(model equations)} \\ &\quad T_L \le T \le T_U; F_L \le F \le F_U \\ &\quad F_{\text{TOT}} \le F_{\text{LIMIT}} \end{aligned} \tag{1}$$

Batch reactor

$$\begin{aligned} &\text{OP} \quad \text{Yield} \\ &s.t \quad \text{ODE(model equations)} \\ &\quad T_L \le T \le T_U \end{aligned} \tag{2}$$

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:

$$\frac{dn_j}{dt} = F_j + V\sum_{i=1}^{Nr} \nu_{ij} r_i \tag{3}$$

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

$$r_i = k_i^0 \left(-\frac{E_i}{RT}\right) \prod_{j=1}^{Nc} C_j^{\nu_{ij}} \tag{4}$$

where $i = 1,\ldots,Nr$. 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:

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

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:

$$\frac{dT_j}{dt} = \frac{-Q_j}{V_j \rho_j Cp_j} + \frac{M_j \rho_j Cp_j (T_{jsp} - T_j)}{V_j \rho_j Cp_j} \tag{6}$$

where T_j, V_j are the temperature and the volume in the jacket respectively, while ρ_j, Cp_j are the density and specific heat of the fluid inside the jacket; M_j is the flow of water in the jacket. T_{jsp} 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:

$$\begin{cases} X_H + X_C = 1 \\ X_H T_H + X_C T_C = (X_H + X_C) T_j \end{cases} \tag{7}$$

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, Cabassud, Le Lann, Pibouleau, and Casamatta (1995). On the other hand, energy balances were suggested by Aziz, Hussain, and Mujtaba (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, Kittisupakorn, & Mujtaba, 2005) methodologies. Briefly, considering a process based on the following model equations:

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

$$y = h(x) \tag{9}$$

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