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Defeating the Sustainability Challenge in Batch Processes through Low-Cost Utilities Usage Reduction

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A novel optimisation algorithm is proposed to simultaneously perform an online dynamic optimisation and control of batch processes while optimising the batch operation time as well. This new method is employed to reduce, in real-time, the environmental impact of discontinuous processes through a lower utility consumption, minimizing, at the same time, the consequences in terms of net income losses. Object-oriented programming and parallel computing are exploited to improve the algorithm efficiency. A simple but meaningful test case is used to prove the effectiveness of the proposed methodology.

1. Introduction

Discontinuous and multi-stage processes are often (and still) managed by means of traditional and heuristic recipes, conventional controls and/or manual operations. This is mainly due to their batch nature that requires frequent manual interventions, e.g., to switch from on (operating) to off conditions, to enable/disable cooling and heating operations or loading and unloading procedures. Moreover, the adopted control methodology is often only partially effective to handle the set-point changes dictated by the recipes of batch productions and the uncertainties typical of semi-batch operations. This common recipe-based management methodology, coupled with the conventional control schemes, also results in a significant utility consumption since all the process uncertainties are handled through an excessive usage of the utility fluxes (each uncertainty effect is typically balanced with the utility fluxes). For these reasons, many authors focused on batch processes to find efficient solutions to make them more automatic and better controlled but only with the principal aim of improving safety and reducing costs. A MPC algorithm for the optimal control of distillation columns, modelled through the wave theory, was developed in (Balasubramhanya and Doyle, 1997), a MPC procedure based on the differential flatness was studied in (Mahadevan et al., 2001), a scenario integrated MPC for batch reactors with the aim of avoiding the loss of control even in failure circumstances was addressed in (Abel and Marquardt, 2003) and, finally, a comparison between the efficiency of sequential and simultaneous methodologies for the dynamic optimisation of discontinuous processes was made in (Joly and Pinto, 2004). Several other authors, instead, have shown both the potential for applying the dynamic optimisation to batch systems, using either neural networks (Greaves et al., 2003) or standard simultaneous procedures (Zavala et al., 2005) or novel adaptive shooting techniques (Vite-Martínez et al., 2014), and the importance of selecting the most appropriate control methodology to be used (Pahija et al., 2013b). Much fewer works, instead, aim to develop optimisation and optimal control strategies based on both income and environmental impact, thus moving towards more sustainable discontinuous processes; developing one such strategy is the main goal of the current work. In supply chain management such a topic is now under development; indeed, a sustainable supply chain project for rubber seed oil is proposed in (Ng et al., 2012) and the study of an optimal supply chain management, which guarantees to minimize the transport environmental impact, is carried out in (Ng and Lam, 2013). In the batch systems field, instead, an offline optimal sustainable scheduling procedure has been investigated in (Yue and You, 2013) but no online studies have been

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found. The current work aims to propose a novel simultaneous real-time optimisation and control algorithm for discontinuous processes, which is able to overcome the drawbacks of the standard optimisation and control strategies, but, above all, to exploit this method in order to provide an on-line optimisation and control procedure whose goal is, in real-time, to both minimize the environmental impact of a batch process, through a utility usage reduction, and maximize the net income, taking also into account the effect of possible incoming perturbations. A test case, partially based on a literature well-known example, is exploited to prove the effectiveness of the proposed strategy.

2. Optimisation and control algorithm structure

The simultaneous model-based dynamic optimisation and control methodology (SMBO&C) proposed here derives from a coupling, a generalization and an extension of nonlinear model predictive control (NMPC) and dynamic real-time optimisation (DRTO) algorithms. The aim of SMBO&C is to provide, at the same time, an on-line optimisation and a process control for batch systems where the manipulated variable time-variant profiles and the batch operational time are simultaneously calculated by means of an optimisation procedure in which the objective function is partially assigned as an input data (most of the times the user defined objective function is an economic indicator for the process but in the following test case a miscellaneous economic-green objective function is employed). In order to introduce the formulation of SMBO&C algorithm, let $\mathbf{d}$, $\mathbf{m}$ and $\mathbf{w}$ be, respectively, the vectors of the perturbations, the manipulated variables and the dependent variables of a discontinuous process. Therefore the process model can be written as:

$$\begin{cases} \mathbf{I}_M \dfrac{d\mathbf{w}}{dt} = \mathbf{f}(\mathbf{w}(t), \mathbf{m}(t), \mathbf{d}(t)) \\ \mathbf{w}(\mathrm{t}_0) = \mathbf{w}^0 \end{cases} \tag{1}$$

where $\mathbf{I}_M$ is a diagonal matrix that can be either nonsingular, i.e. the process model is an ODE system, or singular, i.e. the process model is a DAE system. The proposed SMBO&C scheme is based on the steps indicated in Figure 1. First of all, an initial number of control intervals $\left(N_{CI}\right)$ and the standard length of each interval $\left(\Delta t_{CI}^0\right)$ are assigned as input data, then, starting from a general time instant $\left(t^*\right)$ where the process working point (i.e. $\mathbf{d}$, $\mathbf{m}$ and $\mathbf{w}$ values) is known, the optimal manipulated variable profiles $\left(\mathbf{m}_i^{opt}\right)$ and the optimal residual operational time $\left(\Delta t_{BC}^{opt}\right)$ are estimated through an optimisation procedure, described in Eq.(2) and analysed in detail later. To perform this optimisation the manipulated variable profiles are approximated via piecewise constant functions (Figure 1). The nearest computed optimal values of the manipulated variables $\left(\mathbf{m}_1^{opt}\right)$ are implemented to the controlled system for Δt_{CI} units of time and the response to the control actions measured; at the same time, the initial time value for the calculation of the next control move $\left(t_{new}^*\right)$ is evaluated and the number of control intervals is updated.
The evaluation/update logics of t_{new}^* and N_{CI} can be found in the block diagram in Figure 1: in detail, N_{CI} can only be reduced or kept constant in the proposed scheme. If the updated number of control intervals is zero, then the optimal operational time has been reached and the procedure of simultaneous control and optimisation is stopped, otherwise a new "iteration", which starts from the controlled system working point that relates to t_{new}^*, is executed. The overall algorithm is based on differential and differential-algebraic solvers and optimisers of BzzMath library (Buzzi-Ferraris and Manenti, 2012) to exploit object-oriented programming features and parallel computing.

After describing the SMBO&C algorithm structure in general, it is important to focus the attention on the optimisation sub-step; the objective function is constituted by two user-defined performance functions, i.e. f and g, an anti-ringing term - in the third line of Eq(2), and a third term - in the second line of Eq(2). This last term is quite important: its task is to avoid an excessive variation in the process variables due to a high sensitive response of the controlled system to the manipulated variables change, thus helping to achieve low-oscillating dependent variable profiles, as required in many applied circumstances.

The anti-ringing term is well-known in literature, thus it does not require any explanation.

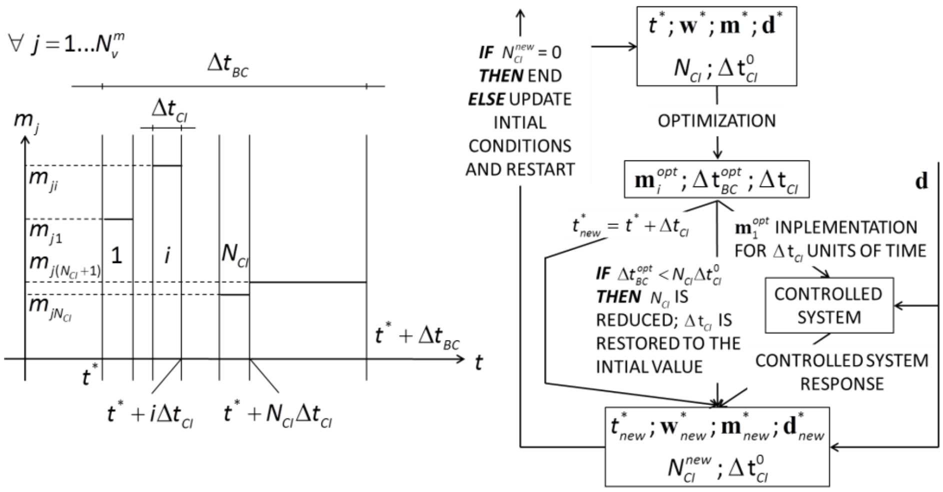

Figure 1: Manipulated variables discretization scheme and SMBO&C algorithm

The function g is the main objective function and its purpose is to constitute a quantitative indicator of the controlled batch process degree of performance, most of the times in a single cycle; the lower the value of g is, the higher the system optimality degree must be. The complementary function f, instead, is used for scheduling purposes and it often represents the number of batch cycles that can be carried out inside a certain campaign time. It is clear that, through a proper definition of f and g, it is possible to model each existing single-cycle or scheduling-based optimisation and control problem, thus the structure described in Eq(2) allows SMBO&C algorithm to be very flexible.

$$
\begin{cases}
\underset{m_{ji};\Delta t_{BC};\mathbf{w}}{Min}\left[\begin{array}{l}
f\left(\Delta t_{BC}, t^*, \mathbf{w}\left(t^* + \Delta t_{BC}\right)\right) g\left(\Delta t_{BC}, t^*, \mathbf{w}\left(t^* + \Delta t_{BC}\right)\right) + \\
+ f\left(\Delta t_{BC}, t^*, \mathbf{w}\left(t^* + \Delta t_{BC}\right)\right) \sum_{k=1}^{N_v^w} Dc_k \left(\dfrac{w_k\left(t^* + \Delta t_{CI}\right) - w_k(t^*)}{\Delta t_{CI}}\right)^2 + \\
+ f\left(\Delta t_{BC}, t^*, \mathbf{w}\left(t^* + \Delta t_{BC}\right)\right) \sum_{j=1}^{N_v^m} ARc_j \sum_{i=1}^{N_{CI}+1} \left(m_{ji} - m_{j(i-1)}\right)^2
\end{array}\right] \\
s.t. \\
\begin{cases}
\mathbf{I}_M \dfrac{d\mathbf{w}}{dt} = \mathbf{f}(\mathbf{w}(t), m_{ji}, \mathbf{d}^*) \\
\mathbf{w}(t^*) = \mathbf{w}^*
\end{cases} \\
m_{ji} \in \left[m_{ji}^{MIN}; m_{ji}^{MAX}\right]; \Delta t_{BC} \in \left[\Delta t_{BC}^{MIN}; \Delta t_{BC}^{MAX}\right]; w_k \in \left[w_k^{MIN}; w_k^{MAX}\right]
\end{cases}
\tag{2}
$$

In conclusion, the SMBO&C algorithm is an optimisation tool, which is able to drive a discontinuous process to profitable operating conditions (not only in terms of income), and, at the same time, a control tool, which can handle random perturbations entering into the controlled system, providing just-in-time optimal corrections; at last, it continuously re-optimise the optimal batch operation time according to the variations of trajectories, together with manipulated variables and process uncertainties. Therefore, this method is able to simultaneously handle, in real-time, both the manipulated variables level and the batch cycle duration level as no other existing algorithm is able to do.

3. A sustainable choice for f and g

Each discontinuous process exploits in general external utilities, such as cooling and heating fluids, that are fundamental for the operations which the process itself is made of. A way to improve a batch process sustainability is to decrease its environmental impact, through a utility consumption reduction, by keeping almost the same economic profitability level. This aim can be realized thanks to the usage of SMBO&C

algorithm where the objective function g is formulated as the sum of both a process income term and a utilities global usage term; this second member groups all the penalty terms related to each utility consumption, each of which conveniently scaled with a penalty coefficient to avoid an excessive negative effect on the process income. The objective function f, instead, must not be modified by a utilities global usage penalty term inclusion. If N_U is the number of different required utilities, $F_{U,\mathrm{q}}$ is the flow of the q-th utility entering into the batch controlled system, λ_q is the penalty coefficient relating to $F_{U,\mathrm{q}}$ and NI^P is the net income of the controlled process, the sustainable formulation of g is the one described in Eq(3).

$$g = -NI^P + \sum_{q=1}^{N_U} \lambda_q \int_{t^*}^{t^*+\Delta t_{BC}} F_{U,q}(t)dt \tag{3}$$

It is relevant to highlight that the utilities global usage penalty term must be added to the process net income, thus possible utility costs must be also considered in the computation of NI^P.

4. Test case

A jacket-cooled batch reactor with a two exothermic reactions kinetic scheme in series is considered as a test case for the proposed methodology. Most of the system data, summarized in Table 1, and the reactor configuration itself are taken from a well-known literature case (Pahija et al., 2013a); please refer to that paper also for a graphical insight of the reacting system. The reactor model, instead, developed assuming perfect mixing both in the reacting mixture and in the cooling jacket and temperature-independent thermodynamic properties, is reported in Eq(4).

Table 1: Process and structural data, components economic value and coolant usage penalty coefficient

Kinetic scheme and parameters	Thermodynamic properties	Structural parameters, reacting volume and molar masses	Initial and boundary conditions plus variable bounds	Economic values and coolant penalty coefficient
$A+B \xrightarrow{R_1} C$	$\Delta H_{R,1} = -1.835E+5$	$D_R = 0.75$	$C_a^0 = 1$	$EV_a = 0.15$
$C \xrightarrow{R_2} D$	$\Delta H_{R,2} = -2.25E+5$	$H_R = 3$	$C_b^0 = 1$	$EV_b = 0.25$
		$V_j = 0.08$	$C_c^0 = 0$	$EV_c = 1$
$R_1 = k_1 C_a C_b$	$Cp_a = 75.31$	$U = 9.842$	$C_d^0 = 0$	$EV_d = 0.05$
$R_2 = k_2 C_c$	$Cp_b = 167.36$		$T_R^0 = 340$	$EV_{coolant} = 0$
$k_1 = k_1^0 \exp\left(-\frac{E_1}{RT}\right)$	$Cp_c = 217.57$	$V_R = 1$	$T_j^{OUT,0} = 340$	$\lambda_{coolant} = 0 \to 0.1$
	$Cp_d = 334.73$		$T_j^{IN} = 340$	
$k_2 = k_2^0 \exp\left(-\frac{E_2}{RT}\right)$		$PM_a = 30$		
	$Cp_j = 4.186$	$PM_b = 100$		$\left.\begin{matrix} EV_a, EV_b \\ EV_c, EV_d \end{matrix}\right\} \to [-]$
	$\rho_j = 1E+3$	$PM_c = 130$	$T_R^{MIN/MAX} = 330/378$	
$E_1 = 7.9E+4$		$PM_d = 130$	$T_j^{OUT,MIN/MAX} = 315/378$	$EV_{coolant} \to \frac{kg}{m^3}$
$E_2 = 1.1E+5$			$F_j^{MIN/MAX} = 1E-5/0.2$	
$k_1^0 = 5.55E+8$	$\Delta H_{R,1}, \Delta H_{R,2} \to \frac{kJ}{kmol}$	$D_R, H_R \to m$		$\lambda_{coolant} \to \frac{kg}{m^3}$
$k_2^0 = 1.35E+12$	$\left.\begin{matrix} Cp_a, Cp_b \\ Cp_c, Cp_d \end{matrix}\right\} \to \frac{kJ}{kmol*K}$	$V_j, V_R \to m^3$	$\left.\begin{matrix} C_a^0, C_b^0 \\ C_c^0, C_d^0 \end{matrix}\right\} \to \frac{kmol}{m^3}$	
		$U \to \frac{kW}{m^2*K}$		
$E_1, E_2 \to \frac{kJ}{kmol}$	$Cp_j \to \frac{kJ}{kg*K}$	$\left.\begin{matrix} PM_a, \mathrm{PM}_b \\ PM_c, \mathrm{PM}_d \end{matrix}\right\} \to \frac{kg}{kmol}$	$\left.\begin{matrix} T_R^0, T_j^{OUT,0} \\ T_j^{IN}, T_R^{MIN/MAX} \\ T_j^{OUT,MIN/MAX} \end{matrix}\right\} \to K$	
$k_1^0 \to \frac{m^3}{kmol*s}$	$\rho_j \to \frac{kg}{m^3}$			
$k_2^0 \to s^{-1}$			$F_j^{MIN/MAX} \to \frac{m^3}{s}$	

$$\begin{cases} \dfrac{dC_i}{dt} = \sum_{j=1}^{N_R} \nu_{ij} R_j \\ \dfrac{dT_R}{dt} = \dfrac{4U}{D_R \sum_{i=1}^{N_C} C_i Cp_i}\left(T_j^{OUT} - T_R\right) - \dfrac{\sum_{j=1}^{N_R} \Delta H_{R,j} R_j}{\sum_{i=1}^{N_C} C_i Cp_i} \\ \dfrac{dT_j^{OUT}}{dt} = \dfrac{F_j}{V_j}\left(T_j^{IN} - T_j^{OUT}\right) + \dfrac{4UV_R}{D_R V_j \rho_j Cp_j}\left(T_R - T_j^{OUT}\right) \\ j = 1,2;\; i = a,b,c,d \end{cases} \tag{4}$$

Finally the user-defined performance functions of the SMBO&C algorithm, formulated as described in section [3] and employed for the current test, are summarized in Eq(5). The secondary performance indicator is set to 1, so a single-cycle optimisation and control problem is dealt with.

$$\begin{cases} f = 1 \\ g = \mathrm{V}_R \left(\begin{array}{l} \mathrm{C}_a^0 \mathrm{PM}_a \mathrm{EV}_a + \mathrm{C}_b^0 \mathrm{PM}_b \mathrm{EV}_b - \mathrm{C}_c\left(t^* + \Delta t_{BC}\right)\mathrm{PM}_c \mathrm{EV}_c + \\ -\mathrm{C}_d\left(t^* + \Delta t_{BC}\right)\mathrm{PM}_d \mathrm{EV}_d + \dfrac{\mathrm{EV}_{coolant} + \lambda_{coolant}}{\mathrm{V}_R} \displaystyle\int_{t^*}^{t^*+\Delta t_{BC}} F_j\, dt \end{array} \right) \end{cases} \tag{5}$$

The performed test case is divided into two different sub-cases: in the first sub-case (solid lines) the only perturbation affecting the controlled system, i.e. the jacket coolant inlet temperature $\left(T_j^{\mathrm{IN}}\right)$, is kept constant to its nominal value (see Table 1) while in the second sub-case (dashed lines) the perturbation is given a piece-wise constant profile; each of the two sub-cases is also carried out for three different values of $\lambda_{coolant}$, i.e. 0 (I), 0.01 (II) and 0.1 (III); therefore, a group of six different optimisation and control simulations is executed through the SMBO&C method application. All the achieved trends and the computed numerical results are reported, respectively, in Figure 2 and in Table 2.

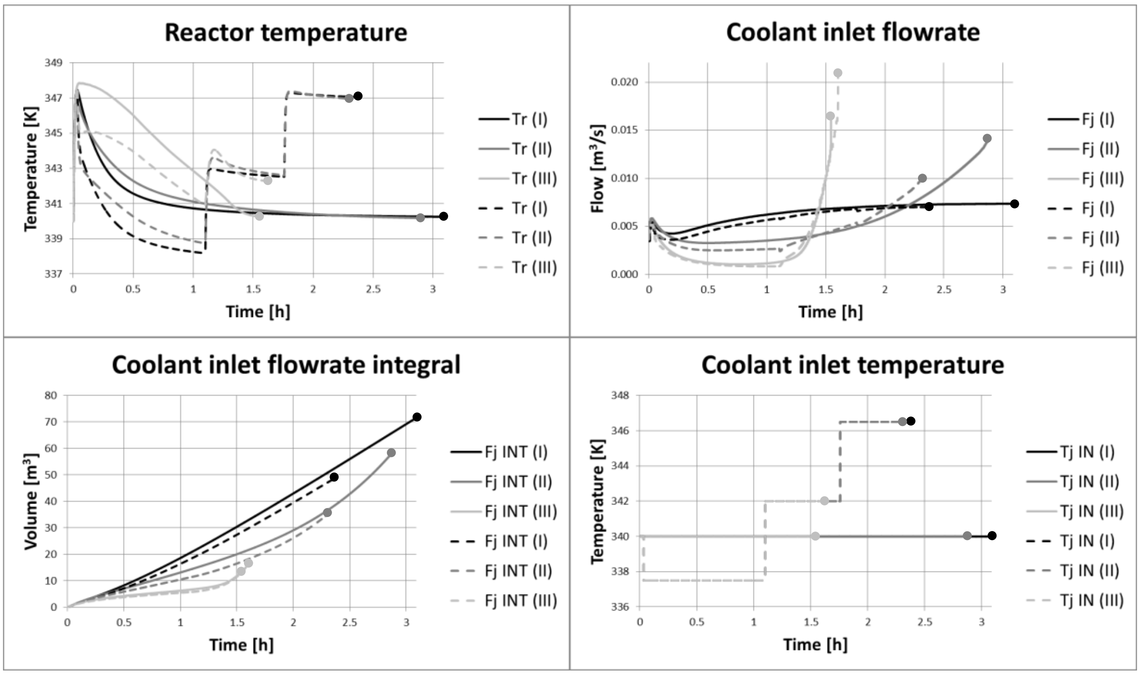

Figure 2: Test case trends summary

Table 2: Test case numerical results

-	$\chi_{a/b}$ [−]	η_c [−]	η_d [−]	NI^P [kg]	F_j^{INT} [m^3]	$\frac{NI^P - NI^P_{MAX}}{NI^P_{MAX}}$ [%]	$\frac{F_j^{INT} - F_j^{INT,MAX}}{F_j^{INT,MAX}}$ [%]
Sub-case 1, I	0.831	0.707	0.124	63.24	71.56	0	0
Sub-case 1, II	0.824	0.706	0.117	63.11	58.01	-0.211	-18.93
Sub-case 1, III	0.763	0.683	0.080	59.82	13.72	-5.412	-80.83
Sub-case 2, I	0.813	0.696	0.118	61.71	48.73	0	0
Sub-case 2, II	0.811	0.696	0.115	61.69	34.89	-0.037	-28.40
Sub-case 2, III	0.755	0.681	0.073	59.57	16.50	-3.472	-66.13

As clearly suggested by Figure 2 and Table 2, as $\lambda_{coolant}$ increases both F_j^{INT} and NI^P decrease, along with the optimal batch cycle duration, but with different slopes: the coolant flow integral is much faster reducing than the net income. Indeed, for a 0.01 value of $\lambda_{coolant}$ the batch cycle results almost as economically profitable as if no utility consumption control mechanism is enabled but, at the same time, much more sustainable because the coolant usage is reduced by about 20 %. The presence of coolant inlet temperature changes appears not to be very relevant on the above-mentioned trends thanks to the SMBO&C algorithm ability of handling the perturbations and developing proper adjustments in real-time. Finally, the proposed sustainable optimisation and control methodology seems to be effective and flexible.

5. Conclusions

An on-line all-in-one optimisation and control method for batch systems, which handles both the manipulated variables and the batch duration levels and appears to drive to sustainable process management rules, has been developed and tested on a batch reactor. The achieved results prove that the proposed methodology is effective and flexible (about 20 % utility consumption reductions with almost constant net income) and suggest that a sustainable batch process management is essentially feasible.

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