2017 21st International Conference on Process Control (PC)
June 6–9, 2017, Štrbské Pleso, Slovakia

Closed-loop dynamic optimization of a polymer grafting batch reactor

R. Bousbia-Salah, F. Lesage, M.A. Latifi
Laboratoire Réactions et Génie des Procédés,
CNRS – ENSIC, Université de Lorraine
Nancy, France
abderrazak.latifi@univ-lorraine.fr

M. Fikar
Faculty of Chemical and Food Technology
Slovak University of Technology
Bratislava, Slovakia
miroslav.fikar@stuba.sk

***Abstract*— A dynamic real-time optimization (D-RTO) methodology has been developed and applied to a batch reactor where polymer grafting reactions take place. The objective is to determine the on-line reactor temperature profile that minimizes the batch time while meeting terminal constraints on the overall conversion rate and grafting efficiency. The methodology combines a constrained dynamic optimization method and a moving horizon state estimator within a closed-loop control. The results show very good performances in terms of state estimation, constraints fulfillment and computation load.**

Keywords— Dynamic real-time optimization, Moving horizon state estimator, Polymer grafting batch reactor

I. INTRODUCTION

Real-time optimization (RTO) has emerged as an essential technology for optimal process operation in the chemical industry. It is a closed-loop optimizer based on a steady-state model. The most common RTO method used in industrial applications is the two-step approach. It consists of solving two optimization problems: the first one is a parameter estimation to update the model, and the second one is the resolution of an optimization problem to minimize the cost function, using the updated model to find new improved operating points [1]. Thus, as the number of iterations increases, the model becomes more accurate. Another interesting RTO method is the modifier adaptation approach that modifies, at each iteration, the optimization problem in order to match the real-plant to the Karush−Kuhn−Tucker (KKT) point, upon convergence. It is noteworthy that RTO has demonstrated its performance in many industrial applications, but has also shown its limitations for processes with frequent transitions and long transient dynamics. Recent advances have transformed the steady-state RTO to dynamic real-time optimization (D-RTO) based on a dynamic process model, hence allowing the performance indices evaluation with higher frequency [2]. Furthermore, D-RTO makes use of the online available measurements to maximize a process performance index while meeting environmental and operating constraints. On the other hand one of the most interesting features of D-RTO is the use of a more general cost function that represents the process economics rather than the tracking error [3]. This is referred to as economic model predictive control (eMPC) [4-6]. In the present paper, a D-RTO methodology has been developed and applied to a grafting polymerization batch reactor. The objective is to minimize the batch period subjected to some terminal industrial specifications (i.e. conversion rate and grafting efficiency) with the reactor temperature and batch period as decision variables.

II. DYNAMIC REAL-TIME OPTIMIZATION APPROACH

The D-RTO approach consists in coupling an on-line dynamic optimization method with a moving horizon estimator (MHE) in a closed loop control as presented in Figure 1.

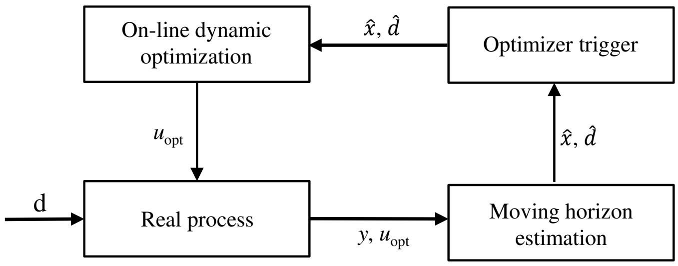

Fig. 1. Block-diagram of the D-RTO approach

A. *On-line dynamic optimization*

The on-line dynamic optimization block consists of an optimization problem where the objective function is optimized (maximized or minimized) under different constraints. The problem is solved using the control vector parametrization (CVP) method [7] which is based on the approximation of decision variables by means of piece-wise constant functions over the optimization horizon. The resulting approximated optimization problem is a nonlinear programming problem (NLP) which is solved using a gradient-based optimization method (e.g. SQP). The gradients of the objective function and constraints with respect to the decision variables are computed by means of the method of sensitivities.

B. *Real Process*

The process is a batch reactor where polymer grafting reactions take place. The objective is to value the used ground tire rubber (GTR) [8]. The latter results from grounding of the rubber part of used tires which retain excellent elasticity. The idea is to take advantage of its elasticity to toughen brittle polymers such as polystyrene upon incorporating GTR into them. The kinetic scheme and reaction rates as well as reactor design equations are detailed in [8].

The resulting process model may be written in the following general form of nonlinear ordinary differential equations (ODEs):

$$\dot{x} = f(x,u) \quad \text{with} \quad x(0) = x_0 \quad \text{and} \quad y = h(x) \qquad (1)$$

where x, u and y are the vectors of states, decision variables, and process outputs, respectively. The model consists of 20 ODEs involving 24 unknown parameters which are previously estimated from experimental measurements [8].

The real process is represented by the set of nonlinear dynamic equations (1).

C. Estimation block

The estimation block is a moving horizon estimator (MHE) necessary to compute an estimate $\hat{x}$ of the current state x that cannot be measured directly on the process [9, 10] and possibly an estimate $\hat{d}$ of the disturbances [11]. It is then used for our model-based optimizer implemented within the D-RTO loop. The estimation can be done using the input and measurement variables u and y respectively.

The MHE provides an estimation of the states and unknown parameters (if any) of the nonlinear process model by minimizing a cost function over the receding horizon of fixed length H_e. The cost function used is a measure of the distance between the output from the real process and the output of the model over some time horizon preceding the time instant at which the state estimates and unknown parameters are required. The results of the observer are then sent to the dynamic optimizer to re-evaluate the input optimal profiles.

D. Trigger block

The trigger block acts like a switch in order to run the optimization when requested. The switching process can be based on a time criterion (predefined switching frequency) or on the disturbance dynamics.

III. FORMULATION OF THE OPTIMIZATION PROBLEM

The dynamic optimization problem of the polymerization reactor considered here may be formulated as

$$\min_{\theta, t_f} J = t_f \qquad (2)$$

Subject to

$$\dot{x} = f(x,\theta) \qquad (3)$$

$$x(t_k) = \hat{x}_k \qquad (4)$$

$$GE(t_f) \geq 0.75 \qquad (5)$$

$$X(t_f) \geq 0.95 \qquad (6)$$

$$\theta \leq \theta_{max} \qquad (7)$$

where $\theta = (T_1, T_2, \dots, T_{n_\theta})^T$ is the vector of time-independent parameters used to approximate the reactor temperature by means of piece-wise constant functions and x the vector of state variables. GE and X are the measured process outputs and are the polymer grafting efficiency and the monomer conversion rate respectively. $(\theta_{max})_i = T_{max}$ is the temperature upper bound.

The gradients of the objective function and constraints with respect to piece-wise constant functions are computed through the integration of sensitivities at each iteration of the optimizer. The sensitivities are defined as

$$s(t) = \frac{\partial x(t)}{\partial \theta} \qquad (8)$$

$$\dot{s} = \frac{\partial f}{\partial x} s + \frac{\partial f}{\partial \theta} \qquad (9)$$

$$s(t_k) = 0 \qquad (10)$$

Note that they are integrated from t_k to t_f at each iteration.

A. D-RTO implementation

The D-RTO loop proceeds as follows. Starting from the real process to which the optimal decision variables are applied at a sampling time t_k, the outputs as well as inputs are used to estimate, over an estimation horizon H_e, the state vector $\hat{x}_k$ that will be used as the initial condition for the next optimization at the sampling time t_{k+1}. The corresponding initial condition for the sensitivities is always taken equal to zero.

The prediction horizon H_p starts at the trigger time and ends always at t_f. The control horizon H_c specifies the number of piece-wise constant functions of the decision variable to be computed in order to minimize the performance index. Once the optimal decision variables are computed, only the first piece-wise constant value is applied to the process. When the optimization process is not triggered, the last values of the decision variables are applied to the process.

It is noteworthy that the state estimation does not need to be known at every sampling time, it may be carried out periodically with a predefined frequency E_p depending on the disturbance dynamics.

IV. RESULTS AND DISCUSSION

The details of the process model equations as well as the values of the parameters θ are given in [8]. The on-line optimization parameters are summarized in Table 1.

Figures 2-4 present some of D-RTO results obtained.

TABLE I. ON-LINE OPTIMIZATION PARAMETERS

Parameter	***Value***
Control horizon H_c	3
Trigger frequency	100 min
Estimation frequency E_p	3 min
T_{max}	150°C
Initial value of t_f	9 hours
Initial value of T	100°C
Sampling period Δt	3 min
Estimation horizon H_e	3

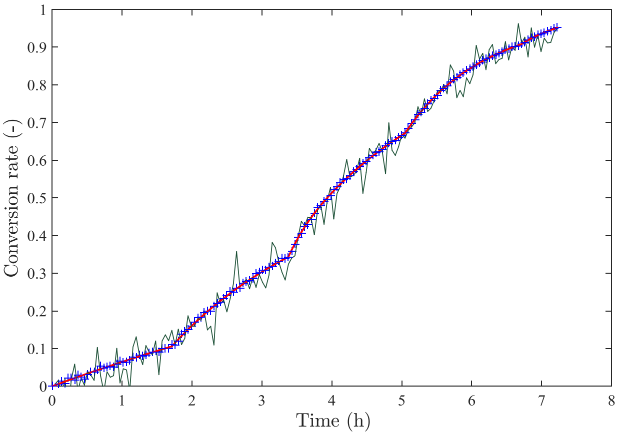

Fig. 2. Time-varying profile of overall conversion rate

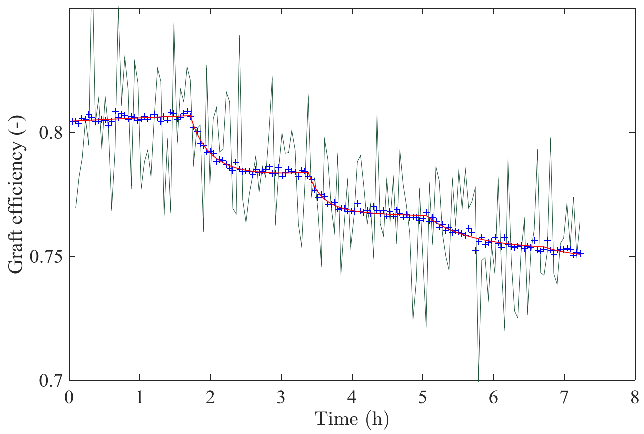

Fig. 3. Time-varying profile of grafting efficiency

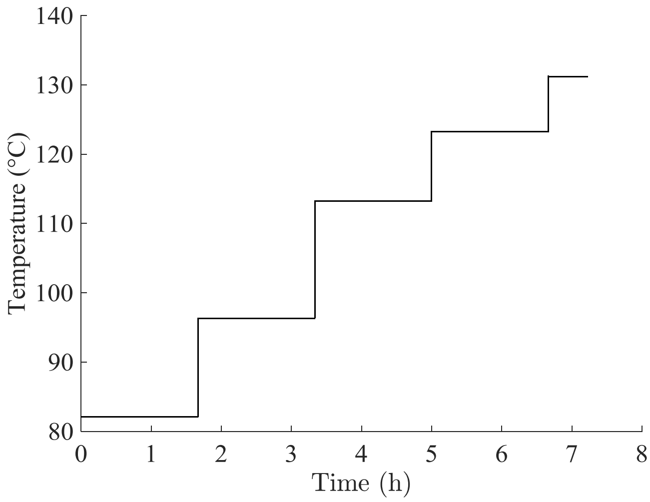

Fig. 4. Optimal profile of reactor temperature

Figures 2 and 3 show the time-varying process outputs, i.e. conversion rate and grafting efficiency respectively, with three different profiles. The "true" profile (in red) is given by integration of the process model equations (1), the estimated profile (in blue) and the "measured" profile (in green). The "measured" profiles are obtained by adding 5% noise to the "true" ones. The resulting optimal-time profile of the decision variable, i.e. temperature, is presented in Figure 4. The computed optimal value of the performance index, i.e. batch period t_f, is equal to 7.2 hours and is substantially reduced compared to its initial value, i.e. 9 hours.

By analyzing the results, it can be seen that the terminal inequality constraints on both process outputs are satisfied. On the other hand, the small difference between the "true" and "estimated" values shows that the estimator achieves very good performances.

The temperature profile exhibits a regular increase in order to fulfill the required monomer conversion rate and grafting efficiency. This shape of optimal temperature is meaningful since at constant temperature, the conversion rate increases with time whereas the grafting efficiency decreases. Therefore the temperature should increase in order to achieve the desired conversion rate but not too much in order to guarantee the specified terminal value of grafting efficiency.

V. Conclusion

A dynamic real-time optimization approach was developed for optimal control of a batch polymerization reactor where a grafting reaction takes place. It consists of a combination of a constrained shrinking horizon dynamic optimization method and a moving horizon state estimator within a closed-loop control. The process model used was previously developed, identified and validated with experimental measurements. The results show very good performances in terms of state estimation, constraints fulfillment and computation load. The stability of the computed optimal decision variables is not an issue since the process studied is of the batch type and the shrinking optimization horizon covers the whole operational time. However the likely process disturbance should be accounted for in the control loop prior to any experimental implementation which will be the next step of the work.

Acknowledgment

The authors gratefully acknowledge the contribution of the PHC STEFANIK joint project 2015/2017 (Campus France N° 35817XD and Slovak Research and Development Agency under the bilateral project SK-FR-2015-0001 and project APVV 15-0007).

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