Integration of Economical Optimization and Control for Intentionally Transient Process Operation

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Summary. This paper summarizes recent developments and applications of dynamic real-time optimization (D-RTO). A decomposition strategy is presented to separate economical and control objectives by formulating two subproblems in closed-loop. Two approaches (model-based and model-free at the implementation level) are developed to provide tight integration of economical optimization and control, and to handle uncertainty. Simulated industrial applications involving different dynamic operational scenarios demonstrate significant economical benefits.

1 Introduction

Increasing competition coupled with a highly dynamic economic environment in the process industry require a more agile plant operation in order to increase productivity under flexible operating conditions while decreasing the overall production cost [1]. The polymer industry is an illustrative example of this development. While on the one hand the product specifications for high-value products become tighter and tighter, on the other hand many of the specialty polymers are becoming commodities resulting in lower profit margins, thus requiring an efficient and cost-effective production [6]. Multi-product and multi-purpose plants have become common. Therefore, transient operational tasks involving sudden changes in production load, product grade (usually triggered by market conditions) are routinely performed. These scenarios demand integrated economical optimization of the overall plant operation.

Today's plant operation requires *real-time business decision making (RT-BDM)* tasks at different levels integrating planning, scheduling, optimization and control tasks. Figure 1 depicts a typical decision making and automation hierarchy. Due to a wide range of process dynamics, different time-scales are involved at each level such as fractions of seconds for base layer control, minutes for advanced control, hours for set-point/trajectory optimization, days for planning and scheduling, and months or even years for strategic corporate planning.

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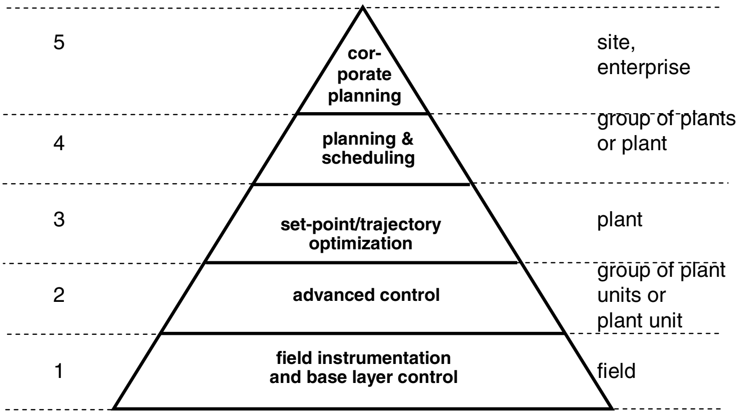


Fig. 1. Real-time business decision making and automation hierarchy

Accordingly, RT-BDM involves multiple decision making levels each with a different objective reflecting the natural time scales. Despite the decomposition in the implementation, there is a single overall objective for the complete structure, namely maximization of profitability and flexibility of plant operation.

In the last decades, technologies have been developed to solve operational problems at different levels of the automation hierarchy. However, most of them are segregated techniques, each one targeting a single problem independently and exclusively. For example, model predictive control technology using linear, nonlinear or empirical models [16, 17] is used to reject disturbances and to control the process at given target set-points (level 2 in Figure 1). The set-points are often the result of a *stationary real-time optimization* [15] using steady-state process models (level 3 in Figure 1). Alternatively, nonlinear model predictive control (NMPC) with an economical objective (referred to as *direct approach* in [9]; Figure 2) has more recently been suggested for transient processes [5] to solve the tasks on level 2 and 3 in Figure 1. On a moving horizon, NMPC repetitively solves a dynamic optimization problem with a combined economical and control objective. On a given time horizon $[t^j, t_f^j]$ with a sampling interval Δt, the corresponding dynamic optimization problem (denoted by the superscript j) reads as:

$$\min_{\boldsymbol{u}^j(t)} \Phi(\boldsymbol{x}(t_f)) \tag{P1}$$

$$\text{s.t.} \quad \dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{y}(t), \boldsymbol{u}^j(t), \hat{\boldsymbol{d}}^j(t)), \quad \boldsymbol{x}(t^j) = \hat{\boldsymbol{x}}^j, \tag{1}$$

$$\boldsymbol{0} \geq \boldsymbol{h}(\boldsymbol{x}(t), \boldsymbol{y}(t), \boldsymbol{u}^{\boldsymbol{j}}(t)), \quad t \in [t^j, t_f^j], \quad t_f^j := t_f^{j-1} + \Delta t, \tag{2}$$

$$\boldsymbol{0} \geq \boldsymbol{e}(\boldsymbol{x}(t_f^j)). \tag{3}$$

$\boldsymbol{x}(t) \in \mathbb{R}^{n_x}$ are the state variables with the initial conditions $\hat{\boldsymbol{x}}^j$; $\boldsymbol{y}(t) \in \mathbb{R}^{n_y}$ are the algebraic output variables. The dynamic process model (1) is formulated in $\boldsymbol{f}(\cdot)$. The time-dependent input variables $\boldsymbol{u}^j(t) \in \mathbb{R}^{n_u}$ and possibly the

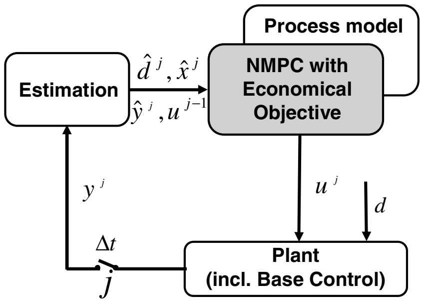


Fig. 2. NMPC with economical objective (or direct approach) using a process model

final time are the decision variables for optimization. Furthermore, equations (2) and (3) denote path constraints $\boldsymbol{h}(\cdot)$ on input and state variables, and end-point constraints $\boldsymbol{e}(\cdot)$ on state variables, respectively. Uncertainties of different time-scales $\boldsymbol{d}^j(t) \in \mathbb{R}^{n_d}$ (e.g. fast changing model parameters, disturbances, and relatively slow changing external market conditions) are also included in the formulation. In NMPC, measurements ($\boldsymbol{y}^j$) are used to estimate on-line the current states ($\hat{\boldsymbol{x}}^j$), outputs ($\hat{\boldsymbol{y}}^j$) and uncertainties ($\hat{\boldsymbol{d}}^j$). The inputs ($\hat{\boldsymbol{u}}$) are updated subsequently by an on-line solution of the dynamic optimization problem P1. For large-scale industrial applications, the NMPC problem is computationally expensive to solve though significant progress has been made in recent years (e.g. [2, 5, 18]). Due to the considerable computational requirements, larger sampling intervals (Δt) are required, which may not be acceptable due to uncertainty.

Functional integration can, alternatively, be achieved by a cascaded feedback structure maintaining the automation hierarchy that has been evolved in the process industry with the base layer control (level 1 in Figure 1) being the most inner and the corporate planning (level 5 in Figure 1) the most outer loop. The operational problem formulation (objective, constraints etc.) at each level should be *consistently* derived from its upper level. This is in contrast to the existing technologies used today in the automation hierarchy, where inconsistencies in objectives, constraints and process models exist at each of the different levels. Furthermore, uncertainties due to process disturbances, plant-model mismatch and changes in external market conditions need to be efficiently tackled. Though NMPC could be tailored to deal with the requirements, it is not a cascaded feedback control system which respects the established time-scale decomposition in the automation hierarchy. Furthermore, NMPC lacks functional transparency which complicates human interaction and engineering. Due to these concerns, the acceptance of such a monolith solution in industry is limited. Rather, a cascaded feedback optimizing control strategy is preferred, because it is less complex and computationally better tractable in real-time, but provides approximate control profiles of sufficient quality. In summary, *the overall problem of economical optimization and control of dynamic processes should be decomposed into consistent and simple subproblems, and subsequently re-integrated using* *efficient techniques to handle uncertainty.* This contribution reviews some of useful concepts to address the above mentioned requirements, and presents their application to simulated industrial case studies.

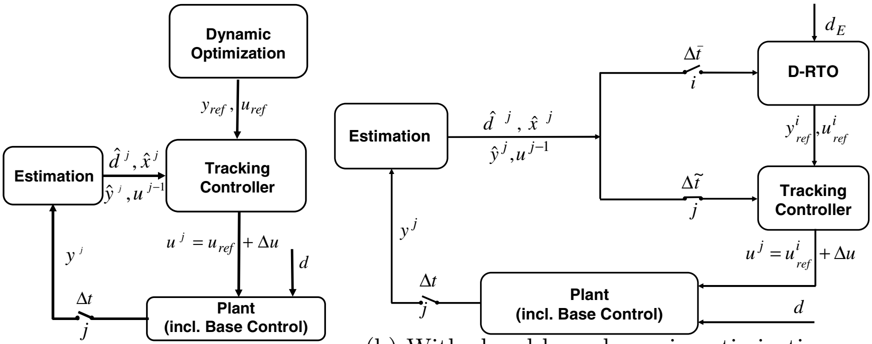
The paper is organized as follows: In Section 2, a two-level optimization and control strategy is presented. To handle uncertainty and tightly integrate the economical optimization and control levels, two strategies are presented in Section 3 and 4. In the first approach in Section 3, a strategy for a fast update of reference tracking trajectories with possible changes in the active constraints set (due to uncertainty) is presented. When the active constraint set is constant, an NCO tracking control approach (in Section 4) can be used, which does not require on-line solution of the dynamic optimization problem and uses only available measurements or estimates of the process variables. The two-level dynamic optimization and control strategy along with fast update and NCO tracking forms a cascaded optimizing control strategy that implements close-to-optimal plant operation. In each section, a simulated industrial application involving different types of transitions is presented.

2 A Two-Level Optimization and Control Strategy

2.1 Concept

For an integration of economical optimization and control, we consider the *two-level* strategy introduced in [9] and modified in [12]. Problem P1 is decomposed into an upper level economical dynamic optimization problem and a lower level tracking control problem, as shown in Figures 3(a) and 3(b). The dynamic optimization in the approach depicted in Figure 3(a) does not involve measurements feedback to update the model. Hence no re-optimization has to be performed on-line, but suboptimal behavior is unavoidable. Therefore, it is referred to as the two-level approach with open-loop dynamic optimization. In contrast, the approach shown in Figure 3(b) involves feedback and hence on-line re-optimization (D-RTO), but can cope with uncertainty. Consequently, it is referred to as the two-level approach with closed-loop dynamic optimization. Any controller, for example, a PID controller or a predictive controller using a linear, possibly time-variant, or even a nonlinear model-based controller may be used at the lower level to track the reference trajectories of the outputs $\boldsymbol{y}_{ref}$ and the controls $\boldsymbol{u}_{ref}$ which results from a solution of the D-RTO problem at the upper level. The concept of providing reference trajectories for tracking is similar to the calculation of constant targets of controls and outputs used in MPC [17]. Note that economical optimization is considered for the nominal model, at the D-RTO level in the simplest case only, while uncertainty is accounted for on the control level only. Hence, the process model used for the optimization has to have sufficient prediction quality and should cover a wide range of process dynamics. Therefore, a fundamental process model is a natural candidate.

This decomposition has two different time-scales, a slow time-scale denoted by $\bar{t}$ on the D-RTO level and a fast time-scale $\tilde{t}$ on the control level, with the corresponding sampling times $\Delta\bar{t}$ and $\Delta\tilde{t}$, respectively. As shown in Figure 3,



(a) With open-loop dynamic optimization (b) With closed-loop dynamic optimization

Fig. 3. Two-level dynamic optimization and control strategies

the solution of the upper level dynamic optimization problem determines optimal trajectories $\boldsymbol{u}_{ref}$, $\boldsymbol{y}_{ref}$ for all relevant process variables to minimize an economical objective function. The sampling time $\Delta\tilde{t}$ (the time interval between two successive re-optimizations performed in the approach in Figure 3(b)) has to be sufficiently large to capture the process dynamics, yet small enough to make flexible economic optimization possible. Depending on whether uncertainty affects the reference trajectories, the two-level approach can be implemented with open-loop (with $\Delta\bar{t} = \infty$) or closed-loop (with $\Delta\bar{t} = \Delta\bar{t}_0$) dynamic optimization depending on the requirements of the application at hand.

On the lower level, the control problem is solved in a delta mode to track the optimal reference trajectories (see Figure 3). The tracking controller calculates only updates $\Delta\boldsymbol{u}$ to $\boldsymbol{u}_{ref}$ (provided by the upper level as feed-forward part of the control) at every sampling time $\tilde{t}_j$ to minimize the deviation from $\boldsymbol{y}_{ref}$. Hence, the degree of optimality achieved by employing the two-level approach depends upon the reference trajectories provided by dynamic optimization at the upper level. The set of tracked variables in $\boldsymbol{y}_{ref}$ is selected from the important output variables available in the plant. The sampling interval $\Delta\tilde{t}$ has to be reasonably small to handle the fast, control relevant process dynamics. The values of the initial conditions $\hat{\boldsymbol{x}}^j$ and disturbances $\hat{\boldsymbol{d}}^j$ for the control problem are estimated from measurements by a suitable estimation procedure such as an extended Kalman filter or a moving horizon estimator.

2.2 Optimal Load Change of an Industrial Polymerization Process

An industrial polymerization process is considered. The problem has been introduced by Bayer AG as a test case during the research project INCOOP [11].

Process description: The flowsheet of this large-scale continuous polymerization process is shown in Figure 8. The exothermic polymerization involving multiple reactions takes place in a continuously stirred tank reactor (CSTR) equipped with an evaporative cooling system. The reactor is operated at an open-loop unstable operating point corresponding to a medium level of conversion. It is followed by a separation unit for separating the polymer from unreacted monomer and solvent. Unreacted monomer and solvent are recycled back to the reactor via a recycle tank, while the polymer melt is sent to downstream processing and blending units. For this process, the following measurements (or estimates) are considered to be available: Flowrates of recycle and fresh monomers, $F_{M,R}$ and $F_{M,in}$, flowrate of reactor outlet $F_{R,out}$, recycle tank holdup V_{RT}, reactor solvent concentration C_S, reactor conversion μ, polymer molecular weight M_W. The reactor holdup V_{RT} is maintained at a desired setpoint using a proportional control that manipulates the reactor outlet flowrate $F_{R,out}$. A rigorous dynamic process model consisting of about 2500 differential and algebraic equations is available from previous studies at Bayer AG [6].

Results: The following scenario is a typical example for an intentionally dynamic mode of operation. Due to changed demand from the downstream processing unit, the polymer load needs to be instantaneously changed from 50% load to 100% load and back to 50% load after a given time interval. It is desired, if possible at all, to produce on-spec polymer during the transition and thereafter. Otherwise, the total amount of off-spec polymer produced during the transition should be minimized. At the end of the transition and thereafter, the process is required to be at the given steady-state operating point. The polymer quality variables, reactor conversion and polymer molecular weight, are allowed to vary in a band of ±2% around their specifications. Three input variables $\boldsymbol{u}$ are available: Flowrate of fresh monomer $F_{M,in}$, catalyst feed stream $F_{C,in}$ and flowrate of recycled monomer $F_{M,R}$. Path and end-point constraints on five process variables need to be respected during the load change operation. Various uncertainties and disturbances in the form of unknown solvent concentration and initial conditions, measurement errors need to be considered during the transition.

The two-level strategy with open-loop dynamic optimization and control ($\Delta\bar{t} = \infty$; cf. Figure 3(a)) has been implemented in a software environment and applied to the simulated polymerization process for the load change scenario. For this transitional scenario, off-line optimization studies have shown that the prevalent uncertainties and disturbances have an insignificant effect on the optimal reference trajectories. Only representative results from the closed-loop control simulation are reported in Figure 4 (see [6] for further details). The solid lines in the plots show the optimal reference trajectories which are calculated by solving a dynamic optimization problem that employs the nominal process model. The lower level of the two-level strategy involving estimation and control was run in a closed-loop simulation in order to verify its capabilities to follow the reference trajectories in the presence of the various process disturbances. A linear time-variant model derived repetitively on-line along the reference trajectories is employed in the tracking controller. The optimization of the load transitions led to significantly improved operation of the plant, when compared to the conventional strategies used by the operators. The transition time is drastically reduced, and the production of off-spec material can be completely avoided, which also could not be ensured in conventional operation.

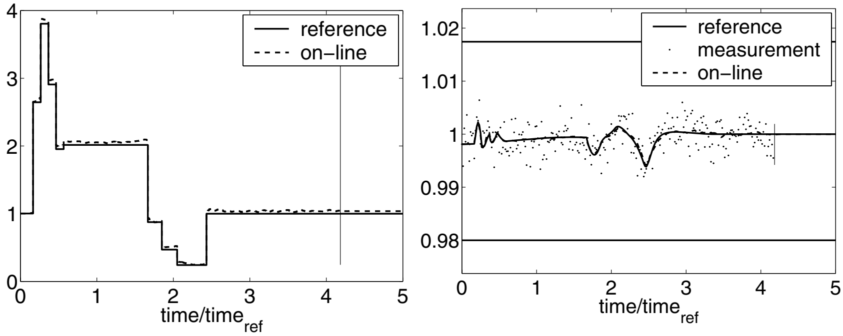


Fig. 4. Results using the two-level strategy with open-loop dynamic optimization: Fresh monomer flowrate $F_{M,in}$ (left) and polymer molecular weight M_W (right)

2.3 Tight Integration and Uncertainty Handling

The two-level strategy is essentially a *cascaded optimizing feedback control system* which generalizes steady-state RTO and advanced predictive control of intentionally dynamic processes. In this approach, the overall problem is *decomposed* into two sub-problems (with *consistent* objectives) that need to be subsequently *re-integrated* in closed-loop. Furthermore, to consider effects of uncertainty, the tracking reference trajectories can be updated by repetitive re-optimization using the feedback (state and eventually model update) provided at a constant time interval $\Delta\bar{t}$. However, a repetitive re-optimization is not always necessary. Rather, it can be systematically triggered by analyzing the optimal reference trajectories based on the disturbance dynamics and its predicted effect on the optimality of P1 if needed. Two strategies are proposed for uncertainty handling and tighter integration of the two-levels of dynamic optimization and control subsequently. In the first approach introduced in Section 3, a neighboring extremal control approach is used for linear updates of the reference trajectories even in case of active inequality constraints. In the second approach presented in Section 4, a solution model is derived from a nominal optimal solution of the dynamic optimization problem. The resulting solution model is used to implement a decentralized supervisory control system to implement a controller with close-to-optimal performance even in case of uncertainty.

3 Sensitivity-Based Update of Reference Trajectories

3.1 Concept

Due to uncertainty, the reference trajectories of the inputs and outputs need to be updated. So far, the update is done via repetitive re-optimization, which can be computationally expensive. Furthermore this may not be necessary as the updated solution and the predicted benefits (objective function) may not be significantly different from the reference solution. Parametric sensitivity analysis

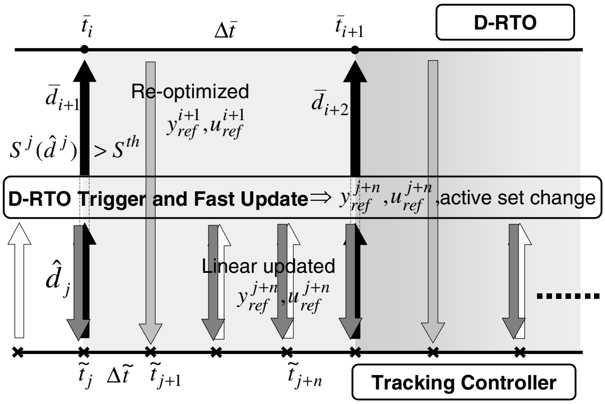


Fig. 5. Schematic of D-RTO trigger and fast update strategy

[7] is a strong tool to analyze an optimal solution for perturbations of parameter values. Consequently, this analysis has been extensively used in steady-state and dynamic optimization for calculating updates due to parametric perturbations or parametric uncertainty (cf. [4]) because it demands only negligible computational time. The applicability of parametric sensitivity techniques, also referred to as *neighboring extremal control*, depends upon the strong assumption that the active constraint set does not change with perturbations, which is often quite restrictive. The assumption is only valid for sufficiently small perturbations entering the optimization problem.

A trigger strategy is suggested in the two-level strategy in Figure 3(b) to initiate a solution of the D-RTO problem only if necessary, otherwise it provides linear updates to $\boldsymbol{u}_{ref}, \boldsymbol{y}_{ref}$ based on the neighboring extremal control with the handling of possible changes in the active constraints set. A schematic of the D-RTO trigger and fast update strategy is given in Figure 5. The reader is referred to [10] for algorithmic details. An optimal solution is available at the nominal values of uncertainty parameters from the previous optimization at time $\bar{t}_i$ and updates at time $\tilde{t}_j$. At each sampling time $\tilde{t}_j$, reference trajectories of the controls are updated as u_{ref}^{j+1}, and the changed active constraint set is calculated using the neighboring extremal control strategy with inequality constraints [10]. Simultaneously, sensitivities S^j of the Lagrange L^j of P1 are evaluated as $S^j = \frac{\partial L^j(u_{ref}^{j+1}, \hat{d}^j)}{\partial u}$, where L^j is calculated for the updated controls u_{ref}^{j+1} and the uncertainty estimate $\hat{d}^j$. A D-RTO trigger criteria ($S^j > S^{th}$ with S^{th} as threshold value) is defined to analyze the updated control for optimality of P1. If the criteria is met, a linear update is not sufficient and a re-optimization is performed to calculate new reference trajectories $\boldsymbol{u}_{ref}^{i+1}, \boldsymbol{y}_{ref}^{i+1}$.

3.2 Productivity Maximization of a Semi-batch Reactor

Problem description: A semi-batch reactor is considered here, which is derived from the continuous Williams-Otto benchmark reactor [8]. The following reactions are taking place in the reactor: $A{+}B \xrightarrow{k_1} C,\ C{+}B \xrightarrow{k_2} P{+}E,\ P{+}C \xrightarrow{k_3} G$. The reactor is fed initially with a fixed amount of reactant A; reactant B is fed continuously. The first-order reactions produce the desired products P and E. Product G is a waste. As the heat generated by the exothermic reactions is removed through the cooling jacket by manipulating the cooling water temperature. During reactor operation, path constraints on the feed rate of reactant B ($F_{B_{in}}$), reactor temperature (T_r), hold-up (V) and cooling water temperature (T_w) have to be respected. $F_{B_{in}}$ and T_w are the manipulated variables. The operational objective is to maximize the yield of the main products at the end of batch. A measurable disturbance ΔT_{in} affects the feed temperature at $t =$ 250 sec during batch operation. Furthermore, the parameter b_1 in the reaction kinetic equation $k_1{=}a_1 \exp(\frac{b_1}{T_r+273.15})$ is assumed to vary about $\pm 25\%$ from its nominal value $b_1 = 6666.7$ sec^{-1}.

Results: The economical optimization problem is solved using DyOS [19] to obtain the optimal solution for nominal values of the uncertain parameters. The nominal optimal control and constraint profiles are depicted in Figure 6 by solid lines. These profiles have different arcs corresponding to active and inactive parts of the path constraints, which are characterized as follows: $F_{B_{in}}$ is initially kept at its *upper bound* and then switched to its *lower bound* when the *reactor volume* (V) reaches its *upper bound*. The second control variable T_w is manipulated to move the *reactor temperature* (T_r) to its lower bound at t=140 sec and keep it there. At the switching time t=360 sec, T_r is moved away from its lower bound by *manipulating* T_w in a bang-bang profile with the switching times computed implicitly by optimization. Note that T_w is at its lower bound at t=0 sec and quickly switched to its upper bound.

The profiles shown by a solid line with dots in Figure 6 depict the response of the neighboring extremal control update and D-RTO trigger strategy in the presence of uncertainty and disturbances. Only once a re-optimization was triggered in this episode. It can be observed in the figures that the closed-loop linearly updated solution is almost identical to the synchronously re-optimized solution (depicted by dashed lines). Note that the structure of the true optimal solution under uncertainty and disturbances is drastically different from that of the nominal solution. Most interestingly, $F_{B_{in}}$ is stopped at t=282 sec, and again switched back to its upper bound at t=656 sec until the reactor hold-up reaches its upper bound. Furthermore, the reactor temperature is never at either of its bounds, while T_w is at its lower bound throughout the operation. These changed active sets are correctly and timely detected by the sensitivity based-update strategy, and the batch operation is optimized in real-time. It is shown that by using the D-RTO trigger and the linear fast update in two-level integrated dynamic optimization economical and control, large uncertainty and disturbances can be effectively handled.

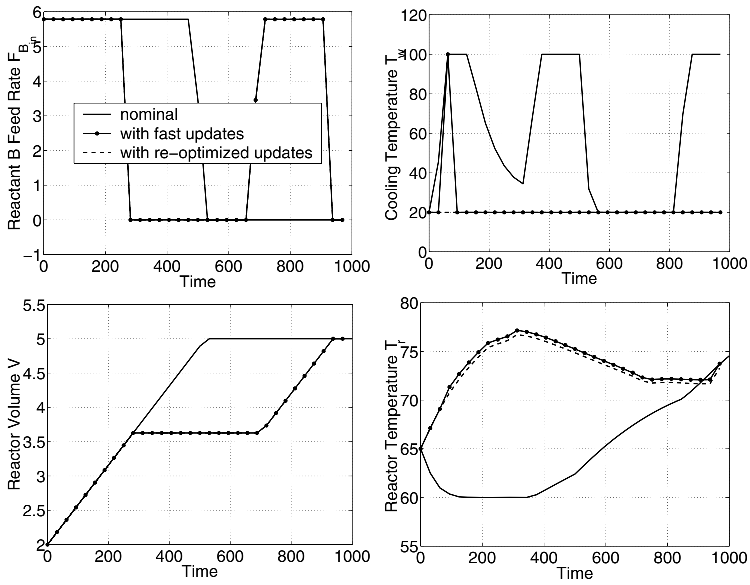


Fig. 6. Nominal and closed-loop optimization profiles of controls and constraints

4 Solution Model-Based NCO Tracking

4.1 Concept

Instead of using *uncertainty-variant* tracking reference trajectories as presented in Sections 2 and 3, a *combination of uncertainty-variant and uncertainty-invariant* arcs of the optimal solution is deduced for the tracking control problem. The approach is termed *NCO tracking* [20] as it adjusts the inputs by means of a decentralized control scheme in order to track the necessary conditions of optimality (NCO) of problem (P1) (cf. Table 1 [3]) in the presence of uncertainty. As shown in Figure 7, measurements ($\boldsymbol{y}$) are employed to directly update the inputs ($\boldsymbol{u}$) using a parameterized solution model obtained from off-line numerical solution of problem (P1) [21]. This way, nearly optimal operation is implemented via feedback control without the need for solving a dynamic optimization problem in real-time. The real challenge lies in the fact that four different objectives (Table 1) are involved in achieving optimality. These path and terminal objectives are linked to active constraints (row 1 of Table 1) and sensitivities (row 2 of Table 1). Hence, it becomes important to appropriately parameterize the inputs using time functions and scalars, and assign them to the different objectives. There results a solution model, i.e. a decentralized self-optimizing control scheme, that relates the available decision variables (seen as inputs) to the NCO (seen as measured or estimated outputs).

Table 1. Separation of the NCO into four distinct parts

	Path objectives	Terminal objectives
Constraints	$\boldsymbol{\mu}^T \boldsymbol{h} = 0$	$\boldsymbol{\nu}^T \boldsymbol{e} = 0$
Sensitivities	$\frac{\partial H}{\partial \boldsymbol{u}} = \boldsymbol{0}$	$H(t_f) + \frac{\partial \Phi}{\partial t}\Big\vert_{t_f} = 0$

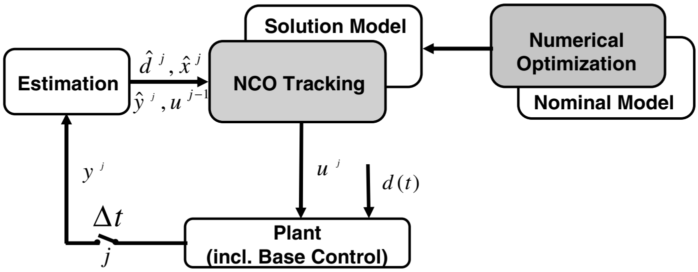


Fig. 7. D-RTO via numerical optimization of a nominal model and NCO tracking

The generation of a solution model includes two main steps:

- *Input dissection:* Using the structure of the optimal solution provided by off-line numerical optimization, this step determines the so-called fixed (uncertainty-invariant) and free (uncertainty-variant) arcs of the inputs. In some of the arcs, the inputs are independent of the prevailing uncertainty, e.g. in arcs where the inputs are at their bounds, and thus can be applied in an open-loop fashion. Hence, the corresponding input elements can be considered as fixed in the solution model. In other arcs, the inputs are affected by uncertainty and need to be adjusted for optimality based on measurements. All the input elements affected by uncertainty constitute the *decision variables* of the optimization problem.

  Input dissection is based on off-line numerical optimization using a nominal process model. The resulting optimal solution consists of various arcs or intervals [3]. The information on the type of arcs can be deduced from the numerical solution of (P1). Schlegel and Marquardt [18] have proposed a method that automatically detects the control switching structure even for large-scale problems with multiple manipulated variables as well as path and endpoint constraints. The structure detection algorithm also provides the dissected optimal input profiles that are re-parameterized with a small number of parameters: $\boldsymbol{u}(t) = \mathcal{U}(\boldsymbol{\eta}(t), \boldsymbol{\mathcal{A}}, \boldsymbol{\tau})$, where $\boldsymbol{\eta}(t) \in \mathbb{R}^L$ are the time-variant arcs, $\boldsymbol{\tau} \in \mathbb{R}^L$ the switching times, and L the total number of arcs. The set of decision variables is comprised of $\boldsymbol{\eta}(t)$ and $\boldsymbol{\tau}$. The boolean set $\boldsymbol{\mathcal{A}}$ of length L describes the type of each particular arc, which can be of the type $\{u_{min}, u_{max}, u_{state}, u_{sens}\}$ depending on whether the corresponding input u_i

is at its lower or upper bound, determined by a state constraint or such that it is adjusted to minimize the objective function.

- *Linking the decision variables to the NCO:* The next step is to provide a link between every decision variable and each element of the NCO as given in Table 1. The active path and terminal constraints fix some of the time functions $\boldsymbol{\eta}(t)$ and scalar parameters $\boldsymbol{\tau}$, respectively. The remaining degrees of freedom are used to meet the path and terminal sensitivities. Note that the pairing is not unique. An important assumption here is that the set of active constraints is correctly determined and does not vary with uncertainty. Fortunately, this restrictive assumption can be relaxed by considering a *superstructure of the solution model* and process insight, which takes into account foreseen changes in the nominally active constraints set.

A designed solution model in the form of input-output pairing provides the basis for adapting the decision variables by employing appropriate controllers and measurements or estimates of its related NCO element as feedback. On-line implementation requires reliable on-line measurements of the corresponding NCO parts. In most applications, measurements of the constrained variables are available on-line. When on-line measurements of certain NCO parts are not available (e.g. sensitivities and terminal constraints), a model can be used to predict them. Otherwise, a run-to-run implementation that uses measurements at the end of the run becomes necessary.

4.2 Optimal Grade Transition of an Industrial Polymerization Process

The same polymerization process presented in Section 2.2 is used to produce different grades of polymer. Therefore, grade changes are routinely performed in this process. The optimization of grade transition is considered in this study. The task is to perform a change from polymer grade A of molecular weight $\bar{M}_{W,A} = 0.727 \pm 0.014$ to grade B of molecular weight $\bar{M}_{W,B} = 1.027 \pm 0.027$ in minimum time. During the transition, operational constraints are enforced on the state and input variables. Additionally, there are endpoint constraints on the reactor conversion μ and the polymer molecular weight $M_{W,B}$ that are more strict than those enforced on these quantities during the transition. For a detailed discussion on this case study and the complete set of results, the reader is referred to [13].

The optimal grade change problem is solved numerically using the dynamic optimizer DyOS [18]. To find an accurate optimal solution with an identifiable control structure, a wavelet-based adaptive refinement method combined with an automatic control structure detection algorithm [18, 19] is applied. The nominal optimal solution and its automatically detected structure are characterized, and a solution model linking inputs to parts of the NCO is derived. As certain nominally inactive path constraints can become active in the presence of model and process uncertainties, a superstructure solution model (to consider *foreseen* changes in nominally active constraints set) is developed. The input-output links

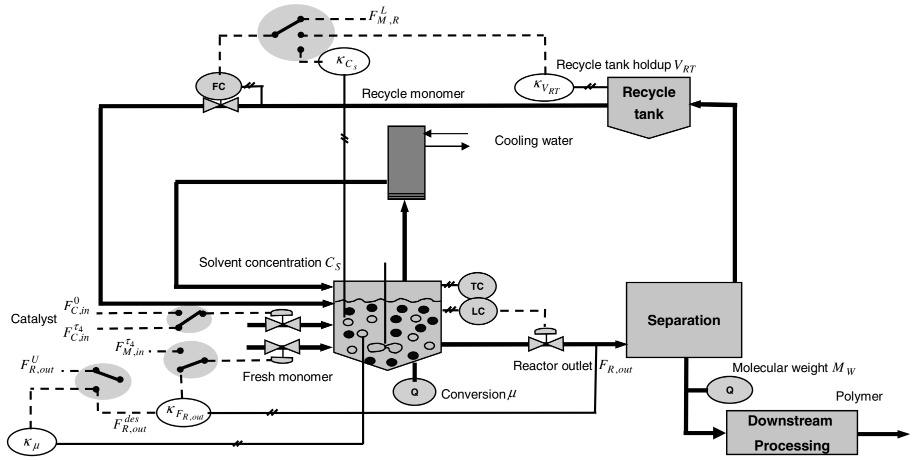


Fig. 8. Process schematic with the NCO tracking controllers and triggers

in the solution model are implemented using the controllers $\mathcal{K}$ as depicted in Figure 8. In this study, PI-type controllers are used employing the nominal input profiles as feedforward terms. Advanced controllers could also be used for improved tracking performance (cf. Section 2.2 and [6]). In the designed control superstructure, depending upon the state of the process, one controller *overrides* the other. In the classic process control terminology, this type of control structure is referred to as *overriding* or *signal-select* controller [14]. Reliable on-line measurements or estimates of the constrained variables are necessary for implementing the NCO tracking strategy using the superstructure solution model.

A considerable amount of uncertainty due to different than nominal initial conditions and reactor solvent concentration is present in practice. The proposed NCO tracking superstructure for optimal grade transition is tested for its performance in the presence of uncertainty using the simulated plant model. The PI controllers are tuned for the nominal case. The simulated NCO tracking profiles of fresh monomer flowrate $F_{M,in}$ and polymer molecular weight M_W are depicted by dash-dotted lines in Figure 9. The transition time t_f for the uncertainty case is considerably larger than that for the nominal case, which is calculated on-line in simulation by using the solution model. The performance of the NCO tracking solution is compared to a robust solution and optimization with known uncertainty in Table 2. The robust solution (column 2 of Table 2) represents a single strategy computed off-line which is feasible for both the nominal and perturbed cases. Such an approach is often used in industrial practice to avoid real-time optimization. The NCO tracking approach (column 3 of Table 2) is computed using the decentralized control structure presented in Figure 9. Finally, the numerical optimal solution (column 4 of Table 2) corresponds to the best possible solution that can be computed using full knowledge of the uncertainty. Table 2 shows that the robust solution is rather poor. In

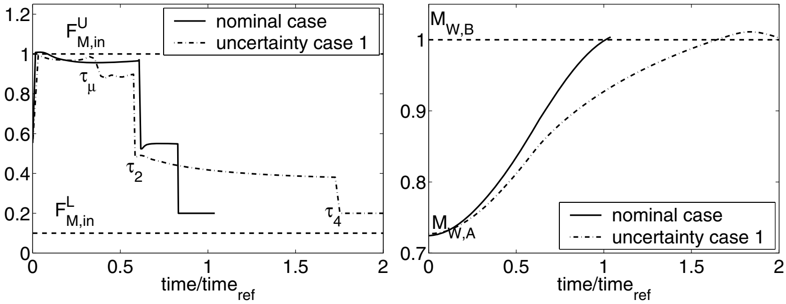


Fig. 9. NCO tracking solution profiles for nominal and uncertainty case 1: Fresh monomer flowrate $F_{M,in}$ (left) and polymer molecular weight M_W (right)

Table 2. Transition times using different optimization strategies; two distinct case of uncertainty are considered, each with different initial conditions corresponding to different solvent concentrations

Case	Robust solution (uncertainty known)	NCO tracking (uncertainty unknown)	Num. optimization (uncertainty known)
nominal	≥ 5	1.008	1.0
uncertainty 1	≥ 5	2.03	1.81
uncertainty 2	≥ 5	0.938	0.915

contrast, NCO tracking comes very close to the best possible solution, without knowledge of the uncertainty but at the expense of on-line measurements and (possibly) state estimations.

The results have demonstrated that a simple decentralized control strategy using a solution model and measurements can implement a complex grade transition. It must be re-emphasized that the generation of the solution model as well as its superstructure requires the optimal solution for the nominal case and process insights that help to simplify it. However, the economic benefits in terms of transition time reduction, and thus the amount of off-spec material, is quite significant compared to the conventional approach practiced in the plant. For limited grade transitions, nominal optimal solutions can be calculated off-line and implemented on-line using NCO tracking controllers. However, reliable on-line measurements or model-based estimates of certain variables are required. Furthermore, the solution model has to be tested and validated for different realization of uncertainty as an online re-optimization is not considered.

5 Conclusions

In this contribution, it is emphasized that the scope of NMPC needs to be broadened from its classic roles of set-point tracking and disturbance rejection. In the context of real-time business decision making (RT-BDM) implemented in the automation hierarchy, a cascaded optimizing feedback control strategy is necessary for economical and agile plant operation. A two-level decomposition strategy of dynamic optimization and control of transient processes is suggested. The overall objectives of profitability and flexibility with respect to scheduled or un-scheduled transitions are maintained consistently at two optimization and control levels. For tighter integration and effective uncertainty handling, two approaches based 1) on neighboring extremal control with inequality constraints and 2) on decentralized control for tracking the necessary conditions of optimality of the economical optimization problem are used. The simulated industrial applications for different transitions have shown significant economical benefits. The case studies show the potential of the suggested approaches. Obviously, there are many opportunities for the further development of an integrated dynamic optimization and control system implemented in multiple levels that consistently solves simple level-specific problems as part of the automation hierarchy.

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