SENSITIVITY-BASED SOLUTION UPDATES IN CLOSED-LOOP DYNAMIC OPTIMIZATION

Jitendra V. Kadam* **and Wolfgang Marquardt** *,[1]

* *Lehrstuhl für Prozesstechnik, RWTH Aachen University*
Turmstr. 46, D-52064 Aachen, Germany
{kadam,marquardt}@lpt.rwth-aachen.de

Abstract: The challenge for real-time optimization-based control systems is to efficiently handle uncertainty. A novel approach for closed-loop optimization is presented that systematically combines a fast update strategy with rigorous optimization when necessary. A parametric sensitivity-based technique is used to calculate optimal first-order updates to a nominal reference solution. The technique does not assume that the active constraint set remains the same after changes in uncertain parameters. In closed-loop, the approach is very effective to handle uncertainty while requiring only a minimum number of full real-time optimizations reducing the on-line computational expense. The approach is illustrated by simulations of closed-loop real-time optimizations of a semi-batch reactor described by a model with different kinds and ranges of parametric uncertainty. It is observed that the closed-loop updated solution is almost identical to the true optimal solution corresponding to uncertainty.

Keywords: dynamic real-time optimization, input adaptation, parametric sensitivity analysis, uncertainty, unknown active set

1. INTRODUCTION

Increasing competition requires a more agile chemical plant operation in order to increase productivity under flexible operating conditions while decreasing the overall production cost (Backx *et al.*, 1998). This demands an integration of economic optimization and control. However, existing applications use either stationary real-time optimization or off-line dynamic optimization together with linear model-based control. These techniques are limited with respect to the achievable flexibility and economic performance, especially when considering intentionally dynamic processes such as continuous processes during transitions or batch processes. Off-line dynamic optimization and trajectory tracking is not fully satisfactory for on-line application in the plant due to model uncertainty, process disturbances and changes in the external market conditions (e.g. future product demand). A basic schematic of dynamic real-time optimization (D-RTO) is shown in Figure 1 (left); its structure is identical to nonlinear model predictive control (NMPC) with output feedback. It is referred to as *single level D-RTO*. Controls are determined at the j^{th} sampling time t_j by solving a dynamic optimization problem that minimizes an economical objective using a nonlinear process model on the prediction horizon $[t_j, t_{f_j}]$. The prediction horizon can be fixed (for continuous processes) or shrinking (for optimal transitions with fixed final time, e.g. batch operations). Estimates of the current process states ($\hat{x}^j$) and disturbance predictions ($\hat{d}^j(t)$) are provided by the solution

[1] Corresponding author. Tel: +49-241-8096712

of an estimation problem e.g. by means of an extended Kalman filter. Only the control (u) residing on the first sampling interval $[t_j, t_j+\Delta\tilde{t}]$ is implemented in the plant. The problem is thus repetitively solved to use the feedback through measurements. For large-scale industrial applications, the D-RTO problem is computationally expensive to solve even if the solution on a previous horizon is used to initialize the algorithm on the current horizon (Binder *et al.*, 2002). Due to the large computational requirements larger sampling intervals are demanded which may not be acceptable due to uncertainty. On the other hand, the current solution may not significantly differ from the previous one. Due to the complexity of D-RTO its acceptance in industry is limited. Hence, an integrated economic optimization and control strategy is required, which is less complex and hence computationally tractable in real-time, and which provides approximate control profiles of sufficient quality. We consider the *two-level D-RTO* strategy (Kadam *et al.*, 2002) shown in Figure 1 (right) to address these requirements. A

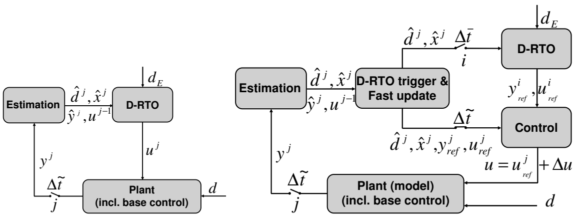

Fig. 1. Single level and two-level D-RTO

simple controller such as a PID controller or a predictive controller using a linear, possibly time-variant, model is used at the lower level to track the reference trajectories of the outputs y_{ref} and the controls u_{ref} provided by D-RTO at the upper level. To reject uncertainty, the reference solution is updated by a *fast update* technique at every sampling time t_j with the corresponding sample interval $\Delta\tilde{t}$. A so-called *D-RTO trigger* analyzes the updates in real-time for optimality and validity. When an estimate of an uncertain parameter differs from its nominal value, a re-optimization, denoted by the counter i, is triggered at non-equidistant sampling intervals $\Delta\bar{t} \geq \Delta\tilde{t}$ if the optimality criteria is not met. Moreover, the closed-loop strategy trades systematically off optimal solution accuracy for computational efficiency.

Parametric sensitivity analysis (Fiacco, 1983) is a strong tool to analyze an optimal solution for perturbations at a set of parameter values. Consequently, this analysis has been extensively used in steady-state and dynamic optimization for calculating updates due to parametric perturbations (cf. Büskens and Maurer (2002)) because it demands only negligible computational time. Diehl *et al.* (2002) use such an approach to provide updates as part of an NMPC algorithm tailored to large–scale nonlinear processes. 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. In this paper we focus on a *sensitivity-based fast solution update* in case of a *changing set of active constraints* in combination with a *D-RTO trigger to initiate rigorous re-optimization.* The paper is organized as follows: Section 2 presents a D-RTO problem formulation and discusses its numerical solution. The sensitivity analysis is given in Section 3. It is followed by the presentation of an algorithm integrating the techniques into the two-level approach. An illustrative example of dynamic real-time optimization of a semi-batch reactor is presented in Section 5.

2. PROBLEM FORMULATION AND SOLUTION

The main objectives of a D-RTO are minimization of operating cost and flexible and feasible operation in the presence of uncertainties. At t_j, the closed-loop single-level or two-level D-RTO problem with a fixed final time t_f, denoted by the counter j and i respectively, reads as

$$\min_{u(t)} \Phi(x(t), u(t), \hat{d}^j(t)) \qquad \text{(P)}$$

$$\text{s.t. } \bar{f}(\dot{x}(t), x(t), y(t), u(t), \hat{d}^j(t)) = 0;\; x(t_j) = \hat{x}^j,$$
$$\bar{g}(y(t), u(t), \hat{d}^j(t)) \geq 0;\; t \in [t_j, t_{f_j}].$$

For simplicity of notation, the superscript j of all the quantities in the this problem formulation is omitted. In closed-loop, the problem is solved repetitively at every t_j after a set of measurements (as feedback after the implementation of the control $u(t_{j-1})$) and a subsequent estimation of the initial state $\hat{x}^j$ and uncertainty $\hat{d}^j(t)$ are available. Due to the fixed final time considered here, at $t_{j+1}{=}t_j{+}\Delta\tilde{t}$, the previous time horizon $[t_j, t_{f_j}]$ is reduced by one sample interval $\Delta\tilde{t}$, i.e. $t_{f_{j+1}}{=}t_{f_j}$. In this formulation, Φ is a scalar *economic objective function* to be minimized over the time horizon $[t_j, t_{f_j}]$. $x(t) \in \mathbb{R}^{n_x}$ denote the system states with consistent initial conditions $\hat{x}^j$ at time t_j; and $y(t) \in \mathbb{R}^{n_y}$ are the algebraic variables. While, $u(t) \in \mathbb{R}^{n_u}$ denote the control variables. $\bar{f}(\cdot) : \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_d} \to \mathbb{R}^{n_x+n_y}$ contains a differential-algebraic (DAE) process model. Any operational (path and endpoint) constraints are collected in $\bar{g}(\cdot) : \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_d} \to \mathbb{R}^{n_{\bar{g}}}$. Furthermore, uncertainties (e.g. uncertain model parameters, disturbances) are collected in the vector $d(t){\in}\mathbb{R}^{n_d}$. The elements of $d(t)$ can be either dependent on time or not. We consider here that a time-dependent uncertainty $d_i(t)$ (e.g. a drift in a reaction kinetic parameter) is parameterized by some expansion $d_i(t)=\sum_{k\in\mathcal{K}} c_{d_{i,k}}\phi_k(t)$, $i=1,\ldots,n_d$. The coefficients $[c_{d_{i,k}}]$ and other time-independent uncertain parameters are collected in a vector of uncertain parameters $p\in\mathbb{R}^{n_p}$ which is estimated along with the initial state x^j from past measurements.

The D-RTO problem (P) is solved numerically by a control vector parametrization (CVP) approach (Kraft, 1985). The dynamic optimization problem is converted into a nonlinear programming problem (NLP) by time-discretizing the controls u on the time horizon $[t_j, t_{f_j}]$ and using piecewise polynomial approximations. For the sake of simplicity, we consider a piecewise constant approximation $u_i(t_k)=c_{u_{i,k}}$, $k=1,\ldots,N$, $i=1,\ldots,n_u$, where N is the number of discretization intervals. Choosing the discretized controls $z := [c_{u_{i,k}}] \in \mathbb{R}^{n_z}, n_z = n_u \cdot N$, as the optimization variables, problem (P) can be transformed into the NLP

$$\min_z f(z,p) := \Phi(z,p) \qquad (\mathrm{P_D})$$
$$\text{s.t. } g(z,p) \geq 0.$$

The NLP problem is solved by employing an SQP algorithm. The objective function $f:\mathbb{R}^{n_z}\times\mathbb{R}^{n_p}\rightarrow\mathbb{R}$, constraints $g(\cdot):\mathbb{R}^{n_z}\times\mathbb{R}^{n_p}\rightarrow\mathbb{R}^{n_g}$, $n_g=n_{\bar{g}}\cdot N$, and their gradients are evaluated by a simultaneous integration of the DAE model and the sensitivity equation system for given z and p. We employ the dynamic optimization solver DyOS (2002) in this work.

3. SENSITIVITY ANALYSIS

3.1 Basic concepts

Let us consider the NLP ($\mathrm{P_D}$) for sensitivity analysis. The objective function $f(\cdot)$ and constraints $g(\cdot)$ are assumed to be at least twice continuously differentiable in z. The Lagrangian function of the constrained optimization problem ($\mathrm{P_D}$) is defined as $L(z,p,\lambda)=f(z,p)-\lambda^T g(z,p)$, where $\lambda\in\mathbb{R}^{n_g}$ is the vector of Lagrange multipliers. Let us consider z_0^*, λ_0^* as the *nominal*[2] *optimal solution* of problem ($\mathrm{P_D}$) corresponding to p_0. To simplify notation, the superscript * is omitted in the sequel. At the optimal solution, the constraints g are divided into the active constraints g^a and the inactive constraints g^{ina} of dimension n_g^a and $n_g - n_g^a$, respectively. The corresponding Lagrange multipliers λ_0 are divided accordingly into λ_0^a and λ_0^{ina}. The active constraint set is denoted by $\mathcal{G}_0$. The first order necessary conditions of optimality (NCO) are[3]:

[2] A nominal quantity $(\cdot)_0$ is evaluated at p_0.

[3] $(\cdot)_z = \frac{\partial(\cdot)}{\partial z}$, $(\cdot)_{zz} = \frac{\partial^2(.)}{\partial z^2}$, $(.)_{zp} = \frac{\partial^2(.)}{\partial z\partial p}$

$$L_z(z_0,p_0,\lambda_0)=0, \qquad (\mathrm{NCO})$$
$$g_i^a(z_0,p_0)=0;\ \lambda_{0,i}^a>0;\ i=1,\ldots n_g^a\in\mathcal{G}_0,$$
$$g_j^{ina}(z_0,p_0)>0;\ \lambda_{0,j}^{ina}=0;\ j=1,\ldots n_g^{ina}\notin\mathcal{G}_0.$$

Let the NCO and the strong second order sufficient conditions (SSC) be satisfied at z_0 and λ_0. Further, the active constraint gradients g_z^a are linearly independent. Also, assume that the active constraint set $\mathcal{G}$ at the changed parameter value $p=p_0+\Delta p$ is the same as $\mathcal{G}_0$. With these assumptions, Fiacco (1983) proved that the functions $z=z(p)$ and $\lambda^a=\lambda^a(p)$ are at least once differentiable in p. In the vicinity of p_0, the *parametric sensitivities* $z_p := \frac{dz}{dp}$ and $\lambda_p^a := \frac{d\lambda^a}{dp}$ of the optimal solution can be calculated by differentiating the NCO with respect to z, λ^a and p. The resultant linear equation system (Fiacco, 1983) to be solved is

$$\begin{bmatrix} L_{zz}(\cdot) & -g_z^{a,T}(\cdot) \\ g_z^a(\cdot) & 0 \end{bmatrix}\begin{bmatrix} z_p \\ \lambda_p^a \end{bmatrix} = -\begin{bmatrix} L_{zp}(\cdot) \\ g_p^a(\cdot) \end{bmatrix} \qquad (1)$$

where all the functions are evaluated at z_0, p_0, λ_0. A first order update due to a perturbation Δp can thus be calculated from a Taylor expansion as

$$\Delta z := z(p) - z_0 = z_p(p_0)\Delta p, \qquad (2a)$$
$$\Delta\lambda^a := \lambda^a(p) - \lambda_0^a = \lambda_p^a(p_0)\Delta p, \qquad (2b)$$
$$\Delta\lambda^{ina} := \lambda^{ina}(p) - \lambda_0^{ina} = 0. \qquad (2c)$$

In order to solve equation (1), we need first order partial derivatives of the constraint functions g_z, g_p and second order partial derivatives of the Lagrange function L_{zz}, L_{zp}. This computation requires a significant effort which can be prohibitive for large-scale problems. Finite difference formulae or automatic differentiation (Nocedal and Wright, 1999) can be used to provide sufficiently accurate second order derivatives.

3.2 The case of a changing active set

For a moderate perturbation Δp, the active constraint set $\mathcal{G}(p)$ can change. It is unknown a-priori whether such a change actually occurs. At the new optimal solution $z(p_0+\Delta p)$, some of the nominally active constraints $g^a(z_0,p_0)$ or the nominally inactive constraints $g^{ina}(z_0,p_0)$ can become inactive or active. Therefore, equation (1) is reformulated as the QP problem (Ganesh and Biegler, 1987)

$$\min_{\Delta z}\ 0.5\Delta z^T L_{zz}(\cdot)\Delta z \qquad (3a)$$
$$+\Delta p^T L_{zp}^T(\cdot)\Delta z + f_z^T(\cdot)\Delta z$$
$$\text{s.t. } g_z(\cdot)\Delta z \geq -g_p(\cdot)\Delta p - g(\cdot), \qquad (3b)$$

where all the functions are evaluated at z_0, p_0, λ_0. The solution of this QP problem, the updates Δz and new Lagrange multipliers $\bar{\lambda}=\lambda(p_0+\Delta p)$, corresponds to taking a Newton step (not necessarily full) of Δz from z_0 of problem ($\mathrm{P_D}$) while respecting all inequality constraints to first order. The solution also detects a new active set

$\bar{\mathcal{G}} := \mathcal{G}(p_0 + \Delta p)$ which is a better estimate of the true active set. Note that the updates always satisfy all constraints to first order, which cannot be guaranteed for the solution of the sensitivity equation system (1) due to the potential changes in the active set. If the active set does not change, the solutions of problems (3) and (1) are the same.

For computing L_{zz} and L_{zp}, an estimate of the true active set $\mathcal{G}$ and the corresponding Lagrange multipliers λ have to be known a-priori. One can use the nominal active set $\mathcal{G}_0$ as an initial guess and iterate as detailed below. Moreover, the Lagrange function is non-differentiable in z, p at a point where the active set changes. We assume strict complementary, e.g. $\bar{\lambda}(g_0(z_0, p_0) + g_z(z_0, p_0)\Delta z + g_p(z_0, p_0)\Delta p) = 0$, at any solution of QP (3). With this assumption, non-differentiability does not pose any difficulty in computing solutions of the QP problem, since the second-order derivatives are computed using a fixed active set. Again, note that Δz, $\bar{\lambda}$ and $\bar{\mathcal{G}}$ are feasible with respect to the linearized constraints (3), albeit the true active set may be different. Better optimal solution updates can be calculated by solving the QP problem iteratively to account for a change of the active set. The iterative strategy is as follows:

(1) By using a finite difference formula, compute $f_{zz}, g_{zz}, f_{zp}, g_{zp}$ at the nominal optimal solution z_0 corresponding to p_0.
(2) If the NLP (P_D) is nonlinear in p calculate f_z, g_z and g_p at z_0 and the changed uncertain parameter value $p{=}p_0{+}\Delta p$ by doing a sensitivity integration to account for the perturbation Δp; and assign $\Delta p{:=}0$.
(3) Initialize iteration $k{:=}0$, $z_k{:=}z_0$ $\lambda_k{:=}[\lambda_0^a, 0]$, $\mathcal{G}_k{:=}\mathcal{G}_0$.
(4) Assemble L_{zz} and L_{zp} from the pre-computed $f_{zz}, g_{zz}, f_{zp}, g_{zp}$ using λ_k and $\mathcal{G}_k$.
(5) Solve QP (3) to obtain Δz_k, z_k, $\bar{\lambda}_k$ and $\bar{\mathcal{G}}_k$.
(6) Set $\lambda_{k+1} = \bar{\lambda}_k$, $\mathcal{G}_{k+1} := \bar{\mathcal{G}}_k$, and $k := k+1$. If the active set is changed go back to step (4).
(7) Calculate g, f_z, g_z and g_p by doing a sensitivity integration for the updated solution z_k from steps (4)-(6) and p from step (2). If still $g(z_k, p) < 0$ go back to step (3).
(8) Declare that optimal updates $z = z_k$, $\lambda = \lambda_k$ and $\mathcal{G} := \mathcal{G}_k$ have been calculated.

The reduced Hessian strategy of Ganesh and Biegler (1987) can be employed to efficiently solve QP (3). For a given range of uncertainty, the accuracy of the updates is usually acceptable.

4. FAST UPDATE AND D-RTO TRIGGER

It is assumed that the perturbations Δp are measured or estimated without time delay, and a perfect controller is available to reject disturbances that are not considered in p, and which affect during the current sample interval. *Fast updates* of the controls are calculated as

$$z(p) = z_0 + \Delta z \text{ i.e. } u(t) = u_0 + \Delta u(t) \quad (4)$$

with Δz being the solution of QP (3). Output and state trajectories are updated by integrating the DAE model in p for the updated control.

The *optimality error of the updated inputs* $z(p)$ is defined here as residuals

$$\epsilon_{opt} = \frac{\|L_z(z, p, \lambda)\|_\infty}{\|\lambda\|_2}; \epsilon_{infs} = \frac{\|g(z, p)\|_\infty}{\|z\|_2}. \quad (5)$$

It is comprised of the error in the Lagrange sensitivity (ϵ_{opt}) and the nonlinear constraint infeasibility (ϵ_{infs}), which quantify optimality and feasibility of the updated controls with respect to uncertainty. Note that any changed active constraint set is taken into account in this calculation. We define τ_{opt}, τ_{infs} as a maximum allowable optimality error given by a controller. If the *D-RTO trigger criteria*, $\epsilon_{opt}{>}\tau_{opt}$ and $\epsilon_{infs}{>}\tau_{infs}$, are met a re-optimization is triggered to get a new set of optimal control and output trajectories.

The fast update (counter j) and D-RTO trigger (counter i) are embedded in the two-level strategy shown in Figure 1(right). The iterative algorithm is as follows: [4]

(1) Set counter $i{:=}1$ and counter $j{:=}1$;
(2) Solve the upper level D-RTO (P) on $t{\in}[0, t_{f_j}]$ to obtain the **reference solution** z^i_{ref}, λ^i_{ref}, $y^i_{ref}(t)$ computed at p_0. Assign $z^j_{ref}{=}z^i_{ref}$, $y^j_{ref} = y^i_{ref}$ as the reference trajectories for the lower level control and fast update. Compute L^j_{zz}, L^j_{zp} by finite differences.
(3) **for** $j = 2, N$ (number of sample intervals) **do**
  (a) At t_j, implement the control $u^{j-1}(t_{j-1})$ and get the **measurements** y^j and **estimates** $\hat{x}^j, \hat{d}^j$ to update p^j.
  (b) Reduce the time horizon for a batch operation by $\Delta\tilde{t}$ i.e. $t_j{=}t_{j-1}{+}\Delta\tilde{t}$, $t_{f_j}{=}t_{f_{j-1}}$. On the reduced horizon, **assemble** the shifted reference discretized controls $\bar{z}^j_{ref}$, $\bar{\lambda}^j_{ref}$ L^j_{zz}, L^j_{zp} from the corresponding quantities z^{j-1}_{ref}, λ^{j-1}_{ref}, $L^{j-1}_{zz}, L^{j-1}_{zp}$ on the previous horizon $[t_{j-1}, t_{f_{j-1}}]$. Evaluate the constraints g^j and sensitivities f^j_z, g^j_z for the controls $\bar{z}^j_{ref}$, estimated parameters p^j and states $\hat{x}^j$ by doing a sensitivity integration.
  (c) **Fast update:** Solve QP (3) to obtain Δz^j,λ^j and $\mathcal{G}^j$. Calculate the updated controls $z^j_{ref}{=}\bar{z}^j_{ref}{+}\Delta z^j$ and the Lagrange multipliers $\lambda^j_{ref}{=}\lambda^j$. Compute

[4] A reference quantity $(\cdot)_{ref}$ is any currently available quantity to be updated, and which is evolved through the previous fast updates and any rigorous re-optimizations.

y_{ref}^j by doing one integration of the DAE model for the updated control.

(d) Compute the optimality error (ϵ_{opt}, ϵ_{infs}) of the updated controls and check the **D-RTO trigger** criteria:
if ($\epsilon_{opt}>\tau_{opt}$) and ($\epsilon_{infs}>\tau_{infs}$)
trigger a re-optimization and solve D-RTO (P) (set $i{:=}i{+}1$) to get new optimal references $z_{ref}^j = u_{ref}^j, y_{ref}^j, \lambda^j$.

(4) **end for**; batch operation completed.

5. ILLUSTRATIVE EXAMPLE

A semi-batch reactor is considered here, which is derived from the continuous Williams-Otto benchmark reactor described by Forbes (1994). 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 reactions are exothermic, the heat produced has to be removed from the cooling jacket by manipulating the cooling water temperature. A detailed dynamic process model and its parameters are given elsewhere (Kadam and Marquardt, 2003). 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) should be respected. $F_{B_{in}}$ and T_w are the control variables. For this illustration the reactor is run for a fixed batch time of 1000 sec.

The operational objective is to maximize the yield of the main products at the end of batch. The dynamic optimization problem reads as

$$\max_{F_{B_{in}}(t), T_w(t)} \Phi(t_f) = c_p n_p(t_f) + c_e n_e(t_f) \qquad (6)$$

s.t. *process model*, and

$$0 \le F_{B_{in}}(t) \le 5.784 \frac{\text{kg}}{\text{sec}},\ V(t_f) \le 5\ \text{m}^3,$$
$$20 \le T_w(t) \le 100\ ^\circ\text{C},\ 60 \le T_r(t) \le 90\ ^\circ\text{C}.$$

The initial reactor temperature $T_{r,0}$ and feed temperature T_{in} are fixed at their nominally optimal values of 60 °C and 35 °C, respectively, calculated by off-line optimization. A disturbance ΔT_{in} affects the feed temperature at, say, t=250 sec during batch operation. It is assumed to be measured directly. Further, 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}. This parameter is assumed to be estimated on-line. We collect T_{in} and b_1 in the vector of uncertain parameters p. The two-level D-RTO strategy is applied in closed-loop in the presence of the aforementioned uncertainty and disturbance.

Problem (6) is solved by employing DyOS (2002) to obtain a reference solution. Each control profile is time-discretized and approximated as piecewise constant function on 32 equidistant intervals to transform problem (6) into the NLP (P_D). The nominal optimal control and constraint profiles are depicted in Figure 2 by bold lines. These

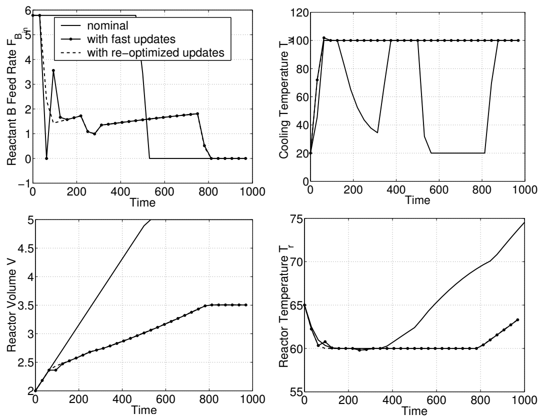

Fig. 2. Nominal and closed-loop simulation profiles of control and constraint variables: Δb_1=+10% and ΔT_{in}=−10 °C at t=250 sec

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 hold-up* (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.

Two cases of uncertainty and disturbances are considered: a) Δb_1=+10% and ΔT_{in}=−10 °C at t=250 sec, and b) Δb_1=−25% and ΔT_{in}=−10 °C at t=250 sec. The algorithm of the two-level strategy with the fast update and D-RTO trigger described in Section 4 and Figure 1 (right) is applied in closed-loop. The closed-loop control and constraint profiles are shown in Figure 2 and 3 for the cases a) and b), respectively. The profiles shown by dash-dotted lines depict the response of the fast update and D-RTO trigger strategy. Moreover, the profiles shown by dashed lines depict the response of repetitive re-optimizations i.e. the single level D-RTO strategy (Figure (1)). When the algorithm is employed, only once a re-optimization was triggered at t=125 sec in case a) and none in case b). It can be observed in the figures that the closed-loop updated solution is almost identical to the true optimal solution (depicted by dashed lines) using the fast update strategy with only a minimum number of re-

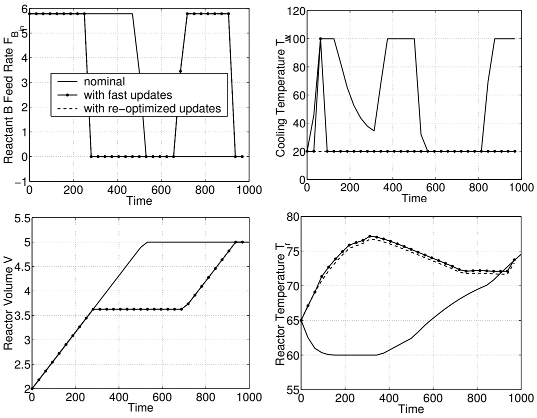

Fig. 3. Nominal and closed-loop simulation profiles of control and constraint variables: Δb_1=−25% and ΔT_{in}=−10 ℃ at t=250 sec

optimizations triggered. Note that the structure of the true optimal solution is drastically different from that of the nominal solution. Most interestingly, in case b), $F_{B_{in}}$ 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, and the batch operation is optimized in real-time. The computational time of one iterate of the D-RTO trigger integrated two-level strategy is approximately 15 sec. It is significantly smaller than approximately 60 sec required for a re-optimization which is warm-started with the nominal solution.

6. CONCLUSIONS

A novel solution update and D-RTO trigger strategy are developed for providing real-times updates and initiating a rigorous re-optimization when necessary. These techniques are integrated into a closed-loop two-level D-RTO strategy. With a case-study, it is pointed out that the nominally active constraints set can drastically change with perturbations in uncertain parameters. Hence, in such cases, parametric sensitivity based input update techniques that assume a constant active set (Büskens and Maurer, 2002) are not applicable. Changed active sets due to perturbations are detected, and first order updates are calculated by solution of a D-RTO problem consistent QP subproblem. Furthermore, the accuracy of closed-loop updates is acceptable. The two-level approach with the D-RTO trigger is shown to be quite effective in rejecting a large range of uncertainty in model parameters, and process disturbances. The closed-loop updated solution is almost identical to the true optimal solution corresponding to a perturbation in uncertain parameters. Moreover, when the accuracy of fast updates is not acceptable, the D-RTO trigger handles uncertainty by triggering a rigorous re-optimization.

REFERENCES

Backx, T., O. Bosgra and W. Marquardt (1998). Towards intentional dynamics in supply chain conscious process operation. In: *FOCAPO 98, Snowbird, Utah.* www.lpt.rwth-aachen.de/Publication/Techreport/1998/LPT-1998-25.html.

Binder, T., L. Blank, W. Dahmen and W. Marquardt (2002). *Online Optimization of Large Scale Systems.* Chap. Multiscale concepts for moving horizon optimization, pp. 341–361. Springer.

Büskens, C. and H. Maurer (2002). *Online Optimization of Large Scale Systems.* Chap. Sensitivity analysis and real-time optimization of parametric nonlinear-programming problems, pp. 3–16. Springer.

Diehl, M., H.G. Bock, J.P. Schloder, R. Findeisen, Z. Nagy and F. Allgower (2002). Real-time optimization and nonlinear model predictive control of processes governed by differential-algebraic equations. *Journal of Process Control* **12**(4), 577–585.

DyOS (2002). *DyOS User Manual, Release 2.1.* Lehrstuhl für Prozesstechnik, RWTH Aachen University. Aachen, Germany.

Fiacco, A. V. (1983). *Introduction to Sensitivity and Stability Analysis in Nonlinear Programming.* Academic Press, New York.

Forbes, J. Fraser (1994). Model structure and adjustable parameter selection for operations optimizations. PhD thesis. McMaster University.

Ganesh, N. and L. T. Biegler (1987). A reduced Hessian strategy for sensitivity analysis of optimal flowsheets. *AICHE J.* **33**(2), 282–296.

Kadam, J. V. and W. Marquardt (2003). A strategy for update of dynamic optimization solution in the presence of uncertainty. Technical report. Lehrstuhl für Prozesstechnik, RWTH Aachen University.

Kadam, J. V., W. Marquardt, M. Schlegel, R.L. Tousain, D.H. van Hessem, J. van den Berg and O. H. Bosgra (2002). A two-level strategy of integrated optimization and control of industrial processes: a case study. In: *European Symposium on Computer Aided Process Engineering - 12* (J. Grievink and J. v. Schijndel, Eds.). Elsevier. pp. 511–516.

Kraft, D. (1985). On converting optimal control problems into nonlinear programming problems. *Comput. Math. Prog.* **15**, 261–280.

Nocedal, J. and S.J. Wright (1999). *Numerical Optimization.* Springer-Verlag.