TOWARDS INTEGRATED DYNAMIC REAL-TIME OPTIMIZATION AND CONTROL OF INDUSTRIAL PROCESSES*

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Abstract

This paper presents a two-level approach for integrating model based dynamic real-time optimization (D-RTO) and control of industrial processes, which is being developed in the INCOOP* project. In the presence of disturbances and changing parameters, a re-optimization at the D-RTO level may be necessary for optimal operation. A sensitivity based hybrid strategy is presented for triggering a D-RTO and quickly calculating feasible control updates. This avoids unnecessary re-optimizations. Results from dynamic optimization and sensitivity analysis of an industrial process are presented.

Keywords

dynamic real-time optimization (D-RTO), model predictive control (MPC), sensitivity analysis, ERP

Introduction

Plant operation is made up of decision-making tasks at different levels such as planning and scheduling, optimization and control. Increasing competition in the chemical industry requires a more agile plant operation in order to increase productivity under flexible operating conditions while decreasing the overall production cost (Backx et al., 1998). This demands integrated economic optimization of the overall plant operation. However, existing techniques such as stationary real-time optimization and linear MPC (Marlin, 2000) use steady-state and/or linear representations of a plant model. They are limited with respect to the achievable flexibility and economic benefit, especially when considering intentionally dynamic processes such as continuous processes with grade transitions and batch processes. In our philosophy, dynamics is at the core of plant operation. Systematic integration of model based dynamic optimization and control for an optimal plant operation is an open field of research, which is e.g. studied in the EU-funded project INCOOP*. In this paper we present a systematic approach, initially proposed by Kadam et al. (2002), for integrating dynamic real-time optimization (D-RTO) and model predictive control (MPC) for large-scale industrial processes. No application of integrated D-RTO and control to large-scale processes has been reported, so far. This work focuses on the interplay between D-RTO and MPC by proposing a new technique for triggering the D-RTO for a potential re-optimization and hence, an increase in the economic value of the dynamic operation.

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Two-level strategy of integrated D-RTO and control

The main objectives of a process optimization and control system are minimization of operating cost and a flexible and feasible operation even in the presence of various uncertainties or disturbances. Mathematically, the overall optimization problem can be written as:

$$
\begin{aligned}
&\min_{u,t_f} \Phi(x,u,t_0,t_f) \qquad \text{(P1)}\\
&s.t.\;\; 0 = f(\dot{x},x,u,d,t),\;\; x(t_0) = x_0\,,\\
&\qquad y = g(x,u,d,t),\\
&\qquad 0 \geq h(x,u,d);\, t \in [t_0,t_f].
\end{aligned}
$$

Φ denotes an economic objective function to be minimized on a time horizon $[t_0, t_f]$ corresponding to a certain campaign of process operation. *x(t)* denotes the system state with initial condition x_0, free operational variables *u(t)* and uncertain parameters *d(t)* which can be external disturbances (demand, product specification, prices), nominal process disturbances, model-plant mismatch and measurement noise. *f(.)* contains a DAE plant model, and *g(.)* maps the system states to the outputs *y(t)*. Operational constraints are collected in *h(.)*. Off-line solutions to problem P1 can be determined by standard techniques for dynamic optimization in case *d(t)* and x_0 are known.

Integrated framework of two-level strategy

In practical applications, an off-line solution of problem (P1) is not sufficient due to the uncertain parameters *d*(*t*) and unknown initial conditions x_0. Hence, successive re-optimizations of problem (P1) with updated models and initial conditions based on process measurements are required. This implies a closed loop D-RTO strategy that takes into account the information gathered from measurements at each sampling time.

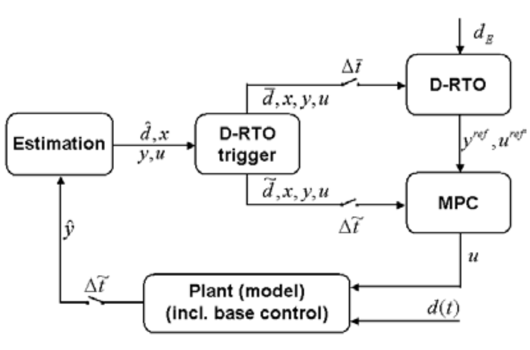

Figure 1: Closed-loop two-level strategy

However, the control relevant dynamics of typical processes will be too fast to enable real-time closed loop dynamic optimization because the current numerical techniques are not able to solve problem (P1) sufficiently fast on the sampling frequency for industrial-size applications involving large complex models. Besides these problems, incorporating various types of uncertainty/disturbances in the closed loop D-RTO strategy is not straightforward.

To solve the overall optimization problem, we propose a two-level strategy which can be extended to consider the supply chain optimization as part of the complete problem. The problem is composed of an upper level economic optimization problem (D-RTO)

$$
\begin{aligned}
&\min_{u^{ref},t_{f_i}} \bar{\Phi}(\bar{x},u^{ref},t_0,t_{f_i}) \qquad \text{(P2a)}\\
&s.t.\;\; 0 = \bar{f}(\dot{\bar{x}},\bar{x},u^{ref},\bar{d},\bar{t}),\; \bar{x}(t_{0_i}) = \bar{x}_{0_i}\\
&\quad y^{ref} = \bar{g}(\bar{x},u^{ref},\bar{d},\bar{t})\\
&\qquad 0 \geq \bar{h}(\bar{x},u^{ref},\bar{d})\\
&\qquad \bar{t} \in [\bar{t}_{0_i},\bar{t}_{f_i}];\; \bar{t}_{0_{i+1}} = \bar{t}_{0_i} + \Delta\bar{t},\; \bar{t}_{f_{i+1}} = \bar{t}_{f_i} + \Delta\bar{t}
\end{aligned}
$$

and a lower level control problem (MPC)

$$
\begin{aligned}
&\min_{u} \int_{\tilde{t}_{0_j}}^{\tilde{t}_{f_j}} (y-y^{ref})^T Q (y-y^{ref}) + (u-u^{ref})^T R (u-u^{ref}) d\tau \qquad \text{(P2b)}\\
&\qquad\qquad + (\tilde{x}_N - \bar{x}_N)^T P (\tilde{x}_N - \bar{x}_N)\\
&s.t.\;\; 0 = \tilde{f}(\dot{\tilde{x}},\tilde{x},u,\tilde{d},\tilde{t}),\; \tilde{x}(t_{0_j}) = \tilde{x}_{0_j}\\
&\qquad y = \tilde{g}(\tilde{x},u,\tilde{d},\tilde{t})\\
&\qquad 0 \geq \tilde{h}(\tilde{x},u,\tilde{d})\\
&\qquad \tilde{t} \in [\tilde{t}_{0_j},\tilde{t}_{f_j}];\; \tilde{t}_{0_{j+1}} = \tilde{t}_{0_j} + \Delta\tilde{t},\; \tilde{t}_{f_{j+1}} = \tilde{t}_{f_j} + \Delta\tilde{t}\,.
\end{aligned}
$$

The two different time-scales present in the problem formulation, $\bar{t}$ in the i^{th} D-RTO and $\tilde{t}$ in the j^{th} MPC problem with corresponding sampling times $\Delta\bar{t}$ and $\Delta\tilde{t}$ respectively, are shown in Figure 2. As given in Figure 1, the D-RTO problem (P2a) determines optimal trajectories u^{ref}, y^{ref} for all relevant process variables such that an economical objective function $\bar{\Phi}$ is minimized and constraints $\bar{h}$ are satisfied. Only economic objectives such as maximization of production or minimization of process operation time are considered in $\bar{\Phi}$. The process model $\bar{f}$ used for the optimization has to have sufficient prediction quality and should cover a wide range of process dynamics. Hence, a fundamental process model is a natural candidate. For closed loop D-RTO, the problem is repetitively solved on the rest of the entire time horizon $[\bar{t}_{0_i},\bar{t}_{f_i}]$ with sampling frequency $\Delta\bar{t} \neq const$ for an update of the previous reference trajectories (see Figure 2). The sampling time has to be sufficiently large to capture the slow process dynamics, yet small enough to make flexible economic optimization possible. Re-optimization is not necessary at each sampling time $\tilde{t}_{0_j}$, rather, based on the disturbance dynamics.

The MPC problem (P2b) is then solved in a conventional delta-mode to track the optimal reference trajectories (see Figure 1) in a strict operational envelope computed on the D-RTO level. This envelope is a small region around the reference trajectories u^{ref}. The MPC sampling time $\Delta\tilde{t}$ has to be significantly smaller than the D-RTO sampling time $\Delta\bar{t}$ to handle the fast, control relevant process dynamics. One requirement for the process model $\tilde{f}$ used on the MPC level, which might be different from the model $\bar{f}$ (albeit derived from it) used on the D-RTO level, is that it has to be simple enough, such that the problem (P2b) can be solved in the available computation time $\Delta\tilde{t}$. A good prediction quality of $\tilde{f}$ is required for the shorter time horizon $[\tilde{t}_{0_j}, \tilde{t}_{f_j}]$ of (P2b). The initial conditions $\bar{x}_{0_i}, \tilde{x}_{0_j}$ and disturbances $\bar{d}$, $\tilde{d}$ for D-RTO and MPC are estimated from process measurements by a suitable estimation procedure such as an extended Kalman filter (EKF).

Note that only an economic objective is handled at the D-RTO level, while disturbance rejection is accounted for on the MPC level. Consequently, any soft constraints (e.g. product quality on short time horizon) can be moved to the D-RTO level. The process models ($\bar{f}$, $\tilde{f}$) used at each level should be consistent; e.g. a linear time variant model along the reference trajectories determined by linearization of the D-RTO model and subsequent model reduction at each sampling time can be used at the MPC level.

D-RTO trigger: Sensitivity based approach

At $\tilde{t}_{0_j}$ state and disturbance estimates $(\hat{x}_{0_j}, \hat{d}_j)$ are available. As the process may have disturbed from the reference trajectories, updated control profiles need to be applied for the future time horizon. As shown in Figure 1 updates can be done by again solving the D-RTO problem which is computationally expensive. The updated solution and the predicted benefits (objective function) may not be significantly different from the reference solution. Hence, a trigger strategy is embedded into the two-level strategy in Figure 1 to trigger a D-RTO solution only if necessary, otherwise it provides quick linear updates of u^{ref}, y^{ref}. D-RTO trigger is based on disturbance sensitivity analysis. The schematic of D-RTO trigger is given in Figure 2.

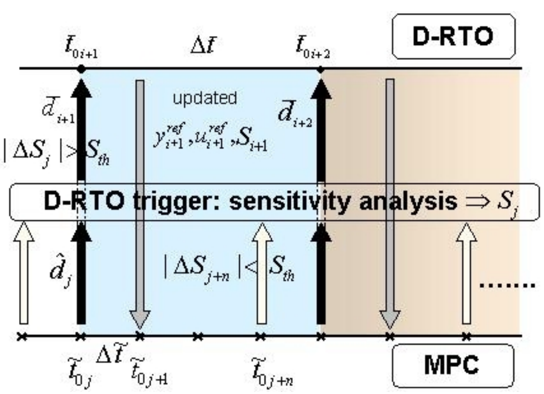

Figure 2: Schematic of D-RTO trigger

An optimal solution u_i^{ref} is available at the nominal disturbance values $\bar{d}_i$ from the previous optimization at $\bar{t}_{0_i}$. At each sampling time $\tilde{t}_{0_j}$ Lagrange function sensitivities $S_j = dL_j / d\hat{d}_j \big|_{\tilde{t}_{0j}}$, $L_j = \bar{\Phi}(u_i^{ref}, \hat{d}_j) + \mu_i^T h(u_i^{ref}, \hat{d}_j)$ are calculated. Here, L_j is a scalar computed at sampling time $\tilde{t}_{0_j}$; S_j is a vector, i.e. the derivative of L_j w. r. t. all components of $\hat{d}_j$. Similarly, S_i are the sensitivities to the disturbances $\bar{d}_i$ at the previous optimal solution. Simultaneously, the parametric sensitivities U_j of controls w. r. t. $\hat{d}_j$ and the possibly changed active constraint set are calculated by solving a QP problem (Kadam and Marquardt, 2002a). As shown in Figure 2 if the change in sensitivities ($\Delta S_j = S_j - S_i$) and Lagrange functions ($\Delta L_j = L_j - L_i$) are larger than a threshold value S_{th} and the active constraint set is changed, a re-optimization has to be done. This signifies that the linear approximation of L as $\Delta L_j = S_i^T(\hat{d}_j - \bar{d}_i)$ is not valid anymore and the re-optimized solution may be different. The trigger criteria mentioned above can be tested in very little computation time. If the criteria is not met, just a linear update of the solution based on already computed sensitivities U_j would be sufficient (cf. Büskens and Maurer, 2001). The threshold value S_{th} is determined by doing off-line simulations of the problem. By employing this strategy, a re-optimization is started only if persistent disturbances have been detected, and if they have high impact on L with possible constraints activation or de-activation. The computation of the second kind of sensitivity U_j computed at $\tilde{t}_{0_j}$ uses second order information (Hessian of the Lagrange function; so far computed by using a finite difference technique) for *optimal updates* and only first order information for *feasible updates*.

Application of two-level strategy to industrial processes

In the INCOOP project two continuous industrial processes are being considered for benchmarking of the proposed two-level strategy. A prototype software platform has been developed, which consists of the dynamic optimizer ADOPT and its extension for MPC problems, an EKF routine, process models in gPROMS and an INCA-OPC server for a flexible data communication between different applications and a plant. The algorithmic details of each module are beyond the scope of this paper.

Problem description and optimization results

The process considered here is a continuous polymerization reactor with a subsequent separation unit and monomer recycle, which produces different grades of a polymer. Frequent production rate and grade changes are common. An optimal grade change operation from polymer grade A to B is considered. Objective of the grade change operation is to minimize the off-spec polymer production and the transition time with operational constraints on reactor temperature, monomer and catalyst feed rate and the polymer content in the reactor, etc. and a subsequent steady state operation corresponding to grade B after the transition. Besides the presence of uncertainties due to unknown reaction parameters, catalyst activity etc., the process is operated at an open loop unstable operating point. Thus the optimization-control problem is a challenging one. A detailed process model consisting of about 2000

DAEs has been developed. Two reaction parameters are considered here, which are believed to be, however uncertain, varying by ± 5% of their nominal value.

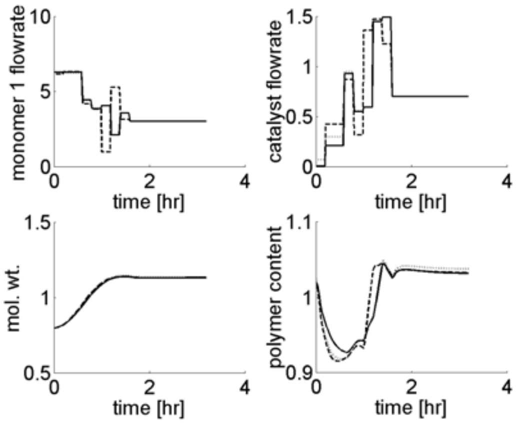

Figure 3: Dynamic optimization results and feasible updates due to a change in parameter 1

The two-level strategy has not yet been completely applied to this industrial case. Here, we present results from the dynamic optimization and D-RTO trigger problems. The optimization problem is solved at time t_0. The open loop scaled nominal optimal profiles are shown in Figure 3 as bold line. The objective of the D-RTO trigger is to decide if a re-optimization is required or a linear feasible update using the sensitivity information is sufficient.

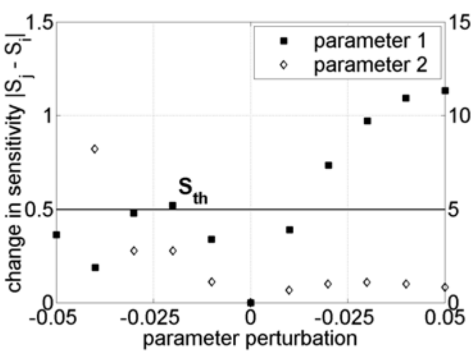

Figure 4: Lagrange function sensitivities

The parameters are randomly perturbed between their bounds in the simulated plant. They are assumed to be estimated in a real-time application of the strategy as $\hat{d}_j$. As discussed in the previous section, sensitivities of the Lagrange function S_j and the parametric sensitivities U_j (with and without 2nd order Lagrange function information) of the controls with respect to the disturbances (the two reaction parameters) along with active set changes are calculated. Scaled absolute changes in sensitivities at different disturbance parameter values are plotted in Figure 4. The changes in sensitivities are not uniformly distributed; especially, those with respect to parameter 2 are larger than S_{th} in the negative direction. Even for small parameter changes active set change has been observed. However, feasible linear updates shown as dotted line in Figure 3, are possible for up to changes of +4% in parameter 1 and –3% parameter 2. The QP Hessian matrix is observed to be indefinite when using second order information (its accuracy depends upon finite difference perturbation and integration tolerance) at the above mentioned parameter changes. This problem needs further consideration. The re-optimized profiles depicted as dash-dashed line steer to the desired grade, in contrast to the feasible-only updates. The sensitivity based strategy adaptively triggers optimization, which is a critical part of the two-level strategy.

Conclusion and future perspective

A systematic approach has been proposed for an integrated D-RTO and control of industrial processes. The two-level strategy distinguishes economic and control objectives and solves the problem on different time scales. This allows to consider different but consistent models and sets of constraints at each level. The D-RTO problem is not solved frequently, but triggered only if potential economic benefits are sensed. A sensitivity analysis based strategy has been formulated for a potential re-optimization and feasible updates, albeit sub-optimal. Some of the techniques are already presented by other research groups although in bits and pieces. We have shown here the value of a hybrid approach using these techniques in an integrated framework. The proposed two-level approach is viable for industrial processes and can guarantee overall feasibility (end point product specifications), that may not be achievable with nonlinear MPC. Only few representative results are shown in the paper. Full implementation of the two-level approach to industrial processes is underway.

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