Lehrstuhl für
Prozesstechnik
Prof. Dr.-Ing. W. Marquardt
RWTH Aachen

Technical Report LPT–2001–29

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J.V. Kadam[1], M. Schlegel[1], W. Marquardt[1], R.L. Tousain[2], D.H. v. Hessem[2], J. v.d. Berg[2], O.H. Bosgra[2]

Contribution to:
ESCAPE–12, The Hague, The Netherlands,
26–29.5.2002.

Published in:
J. Grievink, J. van Schijndel (Eds.): ”European Symposium on Computer Aided Process Engineering – 12”, Elsevier, 2002, 511–516.

[1] Lehrstuhl für Prozesstechnik
RWTH Aachen, D–52056 Aachen

[2] Systems and Control Group, Mech. Eng.
TU Delft, NL–2628 CD Delft

Enquiries should be addressed to:

Lehrstuhl für Prozesstechnik
RWTH Aachen
Templergraben 55
D–52056 Aachen

Tel.: +49 / 241 / 80 94668
Fax: +49 / 241 / 80 92326
E–Mail: secretary@lfpt.rwth–aachen.de

A Two-Level Strategy of Integrated Dynamic Optimization and Control of Industrial Processes – a Case Study*

J. V. Kadam[1], M. Schlegel[1], W. Marquardt[1],
R. L. Tousain[2], D. H. van Hessem[2], J. van den Berg[2] and O. H. Bosgra[2]

[1]Lehrstuhl für Prozesstechnik, RWTH Aachen,
Turmstr. 46, 52064 Aachen, Germany
[2]Systems and Control Group, Mech. Eng., TU Delft,
Mekelweg 2, 2628 CD Delft, The Netherlands

Abstract
This paper discusses a two-level strategy integrating dynamic trajectory optimization and control for the operation of chemical processes. The benefit of an online dynamic re-optimization of operational trajectories in case of disturbances is illustrated by a case study on a semi-batch reactive distillation process producing methyl acetate.

1. Introduction

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., 2000). This demands economic optimization of the plant operation. However, existing techniques such as stationary real time optimization and linear model predictive control (MPC) generally 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.

There is an evident need for model based process operation strategies which support the dynamic nonlinear behavior of production plants. More recent techniques such as dynamic trajectory optimization and nonlinear model predictive control (NMPC) are still subject to research, and often the size of the applicable process model is still a limiting factor. Moreover, the integration of model predictive control and dynamic optimization for an optimal plant operation is an open field of research, which is e.g. studied in the EU-funded project INCOOP*. Various strategies have been suggested to implement such an integration. In the so-called direct approach (Helbig et al., 2000) the two main tasks, economic trajectory optimization and control, are solved simultaneously repeti-

* This work has been funded by the European Commision under grant G1RD-CT-1999-00146 in the “INCOOP” project (www.lfpt.RWTH-Aachen.de/INCOOP). The authors gratefully acknowledge the fruitful discussions with all the INCOOP team members.

tively on each sample time of the process. This corresponds to a single-level optimal control strategy. However, for large-scale and highly nonlinear processes this approach is intractable e.g. due to computational limitations.

In this paper, we employ a vertical decomposition approach: Here, the problem is decomposed into an upper level dynamic trajectory (re-)optimization, and a lower level (nonlinear) MPC which drives the process along the current optimal trajectory determined on the upper level. The interaction between the two levels is a key issue for the feasibility of such a decomposition. Data from the plant processed by a suitable estimation procedure enables nonlinear model-based feedback which can be utilized for several purposes: The dynamic optimization needs not to be performed each sample time but instead depending upon the nature of external disturbances. The feasibility of this approach is shown by means of a case study.

2. Problem definition

The goal of an optimal process operation is to maximize profit. In the ideal case, a perfect model of the process exists, the initial state x_0 at the beginning of the operation is known exactly and the process is not disturbed. Then the associated optimal trajectories for the operational degrees of freedom can be determined entirely off-line through the solution of an optimal control problem (P1):

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

In this formulation, x denotes the system states with initial conditions x_0, u free operational variables and d given parameters. f contains the differential-algebraic process model, g maps the system state to the outputs y. Constraints such as path and endpoint constraints to be enforced are collected in h. Φ denotes an economic objective function to be minimized on the time horizon $[t_0, t_f]$ of the process operation. In principle, problem (P1) can be solved by standard techniques for dynamic optimization (e.g. Betts, 2001) to determine an optimal u and optionally the final time of operation t_f, e.g. in the case of batch operation or for minimizing transition time in continuous processes.

3. Decomposition of dynamic optimization and control

The fact that the assumptions stated above are not fulfilled prevents an off-line solution of problem (P1) from being sufficient in any practical application. This is mainly due to model uncertainty and time-varying external disturbances $d(t)$ and unknown initial conditions x_0. To cope with this situation, a successive re-optimization of problem (P1) with updated models and initial conditions based on process measurements is required. However, the control relevant dynamics of typical processes will be too fast to enable real-time closed loop dynamic optimization. This is because current numerical techniques are not able to solve the problem (P1) for industrial-size applications involving large models sufficiently fast on the sample frequency and given small prediction horizon. High sampling frequency generally demands shorter prediction horizons and this might cause feasibility problems as well.

Alternatively, instead of solving (P1) directly, we consider a hierarchical decomposition. The two level strategy decomposes the problem into an upper level economic optimization problem (P2a) and a lower level control problem (P2a), as shown in Figure 1.

(P2a)

$$
\begin{aligned}
&\min_{u^{ref},t_{fi}} \overline{\Phi}(\bar{x},u^{ref},t_0,t_f)\\
&s.t.\ \ 0=\bar{f}(\dot{\bar{x}},\bar{x},u^{ref},\bar{d},\bar{t}),\ \ \bar{x}(t_{0i})=\bar{x}_{0i}\\
&\quad y^{ref}=\bar{g}(\bar{x},u^{ref},\bar{d},\bar{t})\\
&\quad 0\ge \bar{h}(\bar{x},u^{ref},\bar{d})\\
&\quad \bar{t}\in[\bar{t}_{0i},\bar{t}_{fi}]\\
&\quad \bar{t}_{0i+1}=\bar{t}_{0i}+\Delta\bar{t},\quad \bar{t}_{fi+1}=\bar{t}_{fi}+\Delta\bar{t}
\end{aligned}
$$

(P2b)

$$
\begin{aligned}
&\min_{u}\sum_i (y_i-y^{ref})^T Q(y_i-y^{ref})+(u_i-u^{ref})^T R(u_i-u^{ref})\\
&\qquad\qquad +(\tilde{x}_N-\bar{x}_N)^T P(\tilde{x}_N-\bar{x}_N)\\
&s.t.\ \ 0=\tilde{f}(\dot{\tilde{x}},\tilde{x},u,\tilde{d},\tilde{t}),\ \ \tilde{x}(t_{0i})=\tilde{x}_{0i}\\
&\quad y=\tilde{g}(\tilde{x},u,\tilde{d},\tilde{t})\\
&\quad 0\ge \tilde{h}(\tilde{x},u,\tilde{d})\\
&\quad \tilde{t}\in[\tilde{t}_{0i},\tilde{t}_{fi}]\\
&\quad \tilde{t}_{0i+1}=\tilde{t}_{0i}+\Delta\tilde{t},\quad \tilde{t}_{fi+1}=\tilde{t}_{fi}+\Delta\tilde{t}
\end{aligned}
$$

The former is a dynamic real-time optimization (D-RTO) problem, which determines trajectories u^{ref}, y^{ref} for all relevant process variables such that an economical objective function $\overline{\Phi}$ 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 $\overline{\Phi}$. The problem is repetitively solved on the rest of the entire time horizon on a sample time $\Delta\bar{t}$ for an update of the previous reference trajectories. The sample time has to be sufficiently large to capture the slow process dynamics, yet small enough to make flexible economic optimization possible. The re-optimization may not be necessary at each optimization sample time, instead it can be done based on the disturbance dynamics. The process model $\bar{f}$ used for the optimization has to have sufficient prediction quality and should cover a wide range of process dynamics.

On the lower level, an MPC problem (P2b) is solved in such a way that the process variables track the optimal reference trajectories in a strict operation envelope computed on the D-RTO level. The operation envelope, especially for controls u, is a small region around the reference trajectories; thus the MPC is referred to as delta mode MPC. The MPC sample time $\Delta\tilde{t}$ has to be significantly smaller than the D-RTO sample time $\Delta\bar{t}$, since it has 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 $\bar{f}$ used on the D-RTO level, is that it has to be simple enough, such that problem (P2b) can be solved sufficiently fast. A good prediction quality of $\tilde{f}$ is required for the shorter time horizon $[\tilde{t}_{0i},\tilde{t}_{fi}]$ of (P2b). The initial conditions $\bar{x}_{0i},\tilde{x}_{0i}$ 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).

A proper separation of disturbances on different time scales is crucial for the decomposition of control and optimization, since the actions on both levels are induced by some

kind of disturbance. Besides physical disturbances acting on the process directly, changing external conditions such as market and environmental conditions also can be viewed as disturbances, because they require an update of reference trajectories for the optimal process operation. For example, it is conceivable that prices or product specification requirements change during the process operation. The production should then be adapted to the new situation, which can be done by a re-optimization of the process operation. The estimator (cf. Figure 1) estimates disturbances for which disturbance models have been added to the process model. The time-scale separation decomposes slowly varying or persistent from stochastic disturbances with time constants smaller than the prediction horizon of the MPC. The decision for a possible re-optimization is based on a disturbance sensitivity analysis of the optimal reference trajectories. A re-optimization is started only if persistent disturbances have been detected and have high sensitivities. On the lower level, both types of disturbances are used in the nonlinear prediction of the process. Persistent disturbances are taken up as a bias on the corresponding variables in the MPC, whereas stochastic disturbances are accounted for via the disturbance models added to the process dynamics. In this fashion the MPC problem (P2b) can be solved to obtain the updated control moves (cf. Lee and Ricker, 1994).
The structure in Figure 1 differs from the one suggested by Helbig et al. (2000): The sequence of estimation and time-scale separation is reversed. Both alternatives seem to have their merits and need to be investigated in the future.

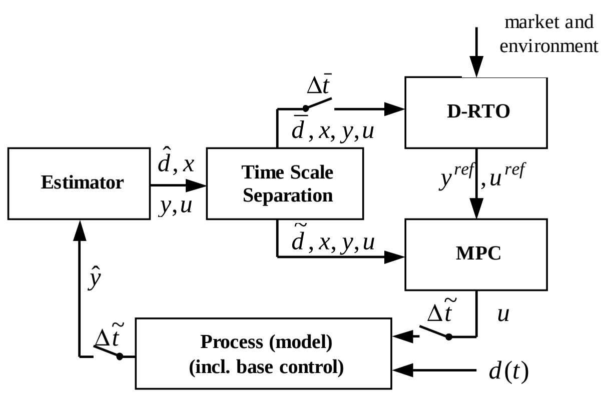

Figure 1. Vertical decomposition of dynamic optimization and model predictive control

4. Case study

The concept introduced above has been implemented in prototype software tools and applied to an industrial-size test example. Details on the numerical algorithms used in the different modules are beyond the scope of this paper. The process studied is a semi-batch reactive distillation process producing methyl acetate (MA) by esterification of acetic acid (AC) with methanol (MT) and byproduct water (W) (cf. continuous process described e.g. in Agreda et al., 1990). The process is started up with pure MT in the batch still and AC as a side feed stream. A gPROMS (gPROMS, 2001) model with 74 differential and 743 algebraic equations has been developed for this process. The dynamic optimization problems (P2a) have been solved using the optimizer ADOPT (Schlegel et al., 2001). The objective is to maximize the amount of product (MA) for a fixed batch time of 4 hours (optimum, found by an off-line optimization with free final time) under strict enforcement of product purity of 0.95. The operational degrees of freedom are the reflux ratio and the reboiler vapor stream. Optimal profiles calculated by an off-line optimization run are shown in Figure 2 and 3 (solid lines) for the nominal case without disturbances.

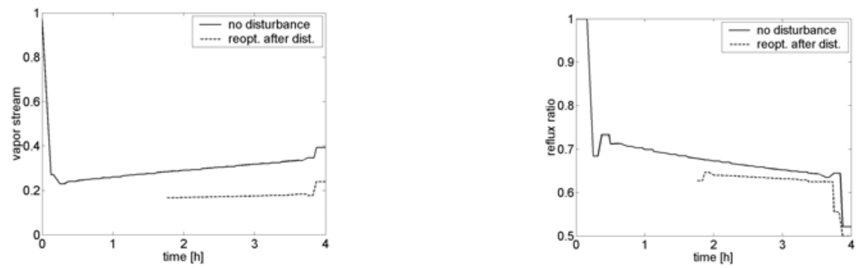

Figure 2. Control profiles for the nominal case and with re-optimization.

The disturbance scenario considered in our study is a drop of 50% in the feed rate of the side stream, which occurs before 1.75 hours. This is a persistent disturbance which is directly measurable and effects the product significantly. The analysis of the sensitivity of the optimal solution to the disturbance has shown that the nominal optimal trajectories need not to be updated for disturbance values less than 25% and these are handled at the MPC level. This decision making strategy for considering re-optimization or MPC at a current sample time subject to disturbances is proven to be suitable for this case study. However, further research is needed in this area.

The performance of the two level strategy is compared with using NMPC, delta mode MPC only and open loop operation. The product quality and the amount of product obtained using the above control strategies are depicted in Figure 3. If the original optimal trajectories would be followed (open-loop strategy) further, the disturbance prevents the required product quality of 0.95 to be met (* line in Figure 3) and leads to economic losses for this batch. A delta mode MPC that enforces a strict operation envelope around the reference trajectories and an NMPC without considering such an envelope are applied separately. The results depicted in Figure 3 (dash-dotted and dotted line resp.) show that these approaches are not economically viable (produces off-spec and less amount of product) for the given disturbance scenario.

The two level strategy of integrated dynamic optimization and control is then applied to the problem. A delta-mode MPC (constraints on control actions) is employed as a lower level MPC. The disturbance is recognized and a re-optimization of the trajectories is started (triggered by the sensitivity-based strategy). The new optimal operational trajectories are determined in order to meet the desired requirements. The re-optimization, which takes the changed state of the process due to the disturbance into account leads to changed optimal control profiles (Figure 2 -dashed lines). The profiles in Figure 3, left (dashed line) show that the product quality of 0.95 is met in the closed loop operation. Figure 3, right (dashed line) shows that more amount of on-spec product is produced. Thus the two level strategy guaranties an economical feasible operation which is not guaranteed by the NMPC. Note that a rigorous nonlinear model is used at the MPC level which is the best option that can be considered.

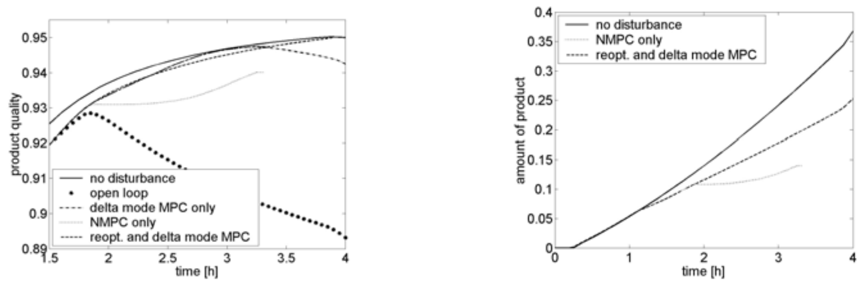

Figure 3. Product quality and amount of product

5. Conclusion

In this paper it has been explained that a more flexible plant operation to cope with changing market and operating conditions can be achieved by a systematic integration of dynamic optimization and model predictive control techniques. A vertical decomposition appears to be a viable strategy, which guaranties overall feasibility that might not be possible by an MPC only. With the help of a simulation study the benefit of the two level strategy, especially the dynamic re-optimization during the operation has been illustrated. Future research work in this area is required on a rigorous strategy for the separation of time scales, the relation of the process models used on the different levels, the choice of appropriate numerical algorithms on the different levels, etc.

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