



Feedback control for optimal process operation

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Abstract

In chemical process operation, the purpose of control is to achieve optimal process operation despite the presence of significant uncertainty about the plant behavior and disturbances. Tracking of set-points is often required for lower-level control loops, but on the process level in most cases this is not the primary concern and may even be counterproductive. In this paper, different approaches how to realize optimal process operation by feedback control are reviewed. The emphasis is on direct optimizing control by optimizing an economic cost criterion online over a finite horizon where the usual control specifications in terms of, e.g., product purities enter as constraints and not as set-points. The potential of this approach is demonstrated by its application to a complex process which combines reaction with chromatographic separation. Issues for further research are outlined in the final section.

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Contents

1. Introduction	204
2. Optimization by regulation (self-optimizing control)	204
3. Real-time optimization (RTO)	206
4. Reducing the gap between regulation and RTO	208
4.1. Frequent RTO	208
4.2. Integration of steady-state optimization into model-predictive control	208
4.3. Integration of nonlinear steady-state optimization in the linear MPC controller	209
5. Direct finite horizon optimizing control	210
5.1. General ideal	210
5.2. Case study: control of reactive simulated moving bed chromatographic processes	210
5.2.1. Process description	210
5.2.2. Control of SMB processes	211
5.2.3. Online optimizing control	211
5.2.4. The Hashimoto reactive SMB process	211
5.2.5. Optimizing controller application	212
5.3. Numerical aspects	213
6. Open issues	214
6.1. Modeling	214
6.2. Stability	215
6.3. State estimation	215

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6.4. Measurement-based optimization	215
6.5. Reliability and transparency	216
6.6. Effort vs. performance	216
7. Conclusions	216
Acknowledgements	216
References	217

1. Introduction

From a process engineering point of view, the purpose of automatic feedback control (and that of manual control as well) is *not* primarily to keep the controlled variables at their set-points as well as possible or to nicely track dynamic set-point changes, but to operate the plant such that the net return is maximized in the presence of disturbances and uncertainties, exploiting the available measurements. The model used for plant design will usually not represent the real process exactly so that an operating regime that was optimized for the plant model does not lead to an optimal operation of the real plant, but may even be infeasible. Feedback control, automatic or manual, is indispensable to handle the inaccuracies and uncertainties that are present in the design process, and to make full use of the capacity of the equipment. This has been pointed out in a number of papers (see e.g. [1–5]) but nonetheless almost all of the literature on automatic control and controller design for chemical processes is concerned with the task to make certain controlled variables track given set-points or set-point trajectories while assuring closed-loop stability. In chemical process control, however, good tracking of set-points is mostly of interest for lower-level control tasks. This contributes to the attitude of managers and process engineers to consider the choice and the tuning of controllers as a necessary but uninteresting task, comparable to the procurement and maintenance of pumps or valves for a predefined purpose, which should be performed as cheaply as possible.

In their plenary lecture at ADCHEM 2000, Backx et al. [6] stressed the need for dynamic operations in the process industries in an increasingly market-driven economy where plant operations are embedded in flexible supply chains striving at just-in-time production in order to maintain competitiveness. Minimizing operation cost while maintaining the desired product quality in such an environment is considerably harder than in a continuous production with infrequent changes, and this cannot be achieved solely by experienced operators and plant managers using their accumulated knowledge about the performance of the plant. Profitable agile operation calls for a new look on the integration of process control with process operations. In this contribution, we give a review of the state of the art in integrated process optimization and control of continuous processes and highlight the option of direct or online optimizing control (also called one-layer approach [7] or full optimizing control [8]).

First the idea to implement the optimal plant operation by conventional feedback control, termed “self-optimizing control” [5], is discussed in Section 2. In highly automated plants, the goal of an economically optimal operation is usually addressed by a two-layer structure [9] which is discussed in Section 3. On the upper layer, the operating point of the plant is optimized based upon a rigorous nonlinear stationary plant model (real-time optimization, RTO). The optimal operating point is characterized by set-points for a set of controlled variables that are passed to lower-level controllers that keep the chosen variables as close to these set-points as possible by manipulating the available degrees of freedom of the process within certain bounds. This two-layer structure has some drawbacks. As the optimization is only performed intermittently at a low sampling rate, the adaptation of the operating conditions is slow. Inconsistencies may arise from the use of different models on the different layers. These issues are partly addressed by schemes in which the economic optimization is integrated within a linear MPC controller on the lower level, as discussed in Section 4.

Recent progress in algorithms for numerical simulation and optimization enables to move from the two-layer architecture to direct online optimizing control. In this approach, the available degrees of freedom of the process are directly used to optimize an economic cost functional over a certain prediction horizon based upon a rigorous nonlinear dynamic process model. The regulation of quality parameters, which is usually formulated as a tracking or disturbance rejection problem, can be integrated into the optimization by means of additional constraints that have to be satisfied over the prediction horizon. The applicability of this integrated approach is demonstrated for the operation of simulated moving bed chromatographic processes. Finally, open issues and possible lines of future research are discussed.

2. Optimization by regulation (self-optimizing control)

The idea behind what was termed “self-optimizing control” by Skogestad [5] has been outlined already in [1]: a feedback control structure should have the property that the adjustments of the manipulated variables that are enforced by keeping some function of the measured variables constant are such that the process is operated at the economically optimal steady state in the presence of disturbances. Morari et al. [1] stated that the objective in the synthesis of a control structure is “to translate the economic

objectives into process control objectives”, a point of view that has thereafter found surprisingly little attention in the literature on control structure selection. A sub-goal in this “translation” is to select the regulatory control structure of a process such that steady-state optimality of process operations is realized to the maximum extent possible if the selected controlled variables are driven to suitably chosen set-points. In the approach described below, the selection is done solely with respect to the stationary process performance, the consideration of the dynamics of the controlled loops follows as a second step. This reflects that from a plant operations point of view, a control structure that yields nice transient responses and tight control of the selected variables may be useless or even counterproductive if keeping these variables at their set-points does not improve the economic performance of the process. The goal of the control structure selection is that in the steady state a similar performance is obtained as it would be realized by optimizing the stationary values of the operational degrees of freedom of the process for known disturbances and parameter variations. Thus the relation between the manipulated variables \underline{u} and the disturbances \underline{d}_i , $\underline{u}_{\text{con}} = f(\underline{y}_{\text{set}}, \underline{d}_i)$ which is (implicitly) realized by regulating the chosen variables to their set-points should be an approximation of the optimal input $\underline{u}_{\text{opt}}(\underline{d}_i)$. The application of this idea to the selection of control structures has been demonstrated in a number of application papers [10–12].

The effect of feedback control on the profit function J in the presence of disturbances can be expressed as [12]

$$\begin{aligned} \Delta J = & J(\underline{u}_{\text{nom}}, d = 0) - J(\underline{u}_{\text{nom}}, \underline{d}_i) \\ & + J(\underline{u}_{\text{nom}}, \underline{d}_i) - J(\underline{u}_{\text{opt}}, \underline{d}_i) + J(\underline{u}_{\text{opt}}, \underline{d}_i) - J(\underline{u}_{\text{con}}, \underline{d}_i). \end{aligned} \quad (1)$$

The first term is the loss due to disturbances that would be realized if the manipulated variables were fixed at their nominal values. The second term represents the effect of an optimal adaptation of the manipulated variables to the disturbance \underline{d}_i , and the third term is the difference of the optimal compensation of the disturbance and the compensation which is achieved by the chosen feedback control structure. If the first term in (1) is much larger (in absolute value) than the second one, or if all terms are relatively small, then a variation of the manipulated variables offers no advantage, and neither optimization nor feedback control is required for this disturbance. If the third term is not small compared to the attainable profit for optimized inputs for all possible regulating structures, then online optimization or an adaptation of the set-points should be performed rather than just regulation of the chosen variables to fixed pre-computed set-points.

Eq. (1) represents the loss (which may also be negative, i.e. a gain) of profit for one particular disturbance \underline{d}_i and a fixed control structure. The economic performance of a control structure can then be measured by

$$\Delta J = \int_{-d_{1,\text{max}}}^{d_{1,\text{max}}} \int_{-d_{n,\text{max}}}^{d_{n,\text{max}}} w(\underline{d}) (J(\underline{u}_{\text{nom}}, \underline{d}) - J(\underline{u}_{\text{con}}, \underline{d})) dd_1 \cdots dd_n, \quad (2)$$

where $w(\underline{d})$ is the probability of the occurrence of the disturbance vector \underline{d} , neglecting the effect of potential constraint violations. As feedback control is based on measurements, errors in the measurements of the controlled variables must be taken into account. A variable may be very suitable for regulatory control in the sense that the resulting inputs are a good approximation of the optimal inputs, but due to a large measurement error or a small sensitivity to changes in the inputs, the resulting values $\underline{u}_{\text{con}}$ may differ considerably from the desired values. This was considered in an approximative fashion by checking the sensitivity of the profit with respect to the controlled variables in [5]. An alternative is to consider the worst case control performance for regulation of the controlled variables to values in a range around the nominal set-point $\underline{y}_{\text{set}}$ which is defined by the measurement errors [12]. For a disturbance scenario \underline{d}_i , the performance measure of a control structure is

$$\begin{aligned} \min_{\underline{u}} & J(\underline{u}, \underline{d}_i, \underline{x}) \\ \text{s.t.} & \dot{\underline{x}} = \underline{f}(\underline{u}, \underline{d}_i, \underline{x}) = 0, \\ & \underline{y} = \underline{m}(\underline{x}) = \underline{M}(\underline{u}, \underline{d}_i), \\ & \underline{y}_{\text{set}} - \underline{e}_{\text{sensor}} \leq \underline{y} \leq \underline{y}_{\text{set}} + \underline{e}_{\text{sensor}}, \end{aligned} \quad (3)$$

where \underline{f} represents the plant dynamics. A regulatory control structure that yields a comparatively small value of the minimal profit is not able to guarantee the desired performance of the process in the presence of measurement errors and hence is not suitable. This formulation includes the practically relevant situation where closed-loop control leads to a worse result than keeping the manipulated variables constant at their nominal value. This will usually be the case for small disturbances, as illustrated by Fig. 1,

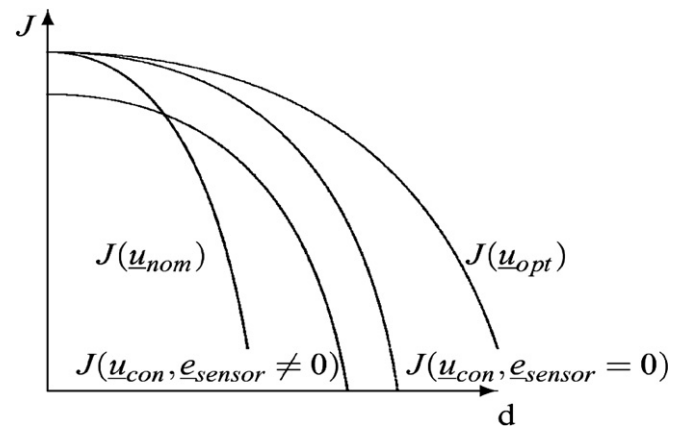


Fig. 1. Schematic representation of the influence of a disturbance on the profit for different control approaches in the presence of measurement errors. $J(\underline{u}_{\text{nom}})$: performance for nominal inputs, $J(\underline{u}_{\text{opt}})$: performance for optimal inputs, $J(\underline{u}_{\text{con}})$: performance under feedback control with and without measurement errors.

where the effect of disturbances of different magnitudes on the performance of a process is illustrated for fixed nominal inputs, optimized inputs, and feedback control with and without measurement errors. For small disturbances, keeping the controlled inputs at their set-points is better than reacting to disturbed measurements of y . It is therefore important to include scenarios with small disturbances and not only those with very large ones into the set of disturbances that are considered in the analysis of the self-optimizing capacity of a control structure.

Application studies have shown that the profit loss that is incurred by using regulation to fixed set-points instead of steady-state optimization can be quite low for well-chosen control structures. For example in [10] a performance loss of less than 5% is reported for the Tennessee Eastman benchmark problem [13].

The analysis described above and the control structure selection process that follows from it so far are limited to disturbances or variations of the plant behavior that persist over a very large period of time compared to the plant dynamics. The inclusion of disturbances with a higher bandwidth into the analysis as well as the integration with the dynamic aspects of control structure selection is still an open issue.

3. Real-time optimization (RTO)

A well-established approach to create a link between regulatory control and optimization of the economics of the unit or of the plant under control is *real-time optimization* (RTO) (see e.g. [9], and the references therein). An RTO system is a model based, upper-level control system that is operated in closed loop and provides set-points to the lower-level control systems in order to maintain the process operation as close as possible to the economic optimum. The general structure of an RTO system is shown in Fig. 2. Its hierarchical structure follows the ideas put forward already in the 1970s, e.g. by Findeisen, et al. [14].

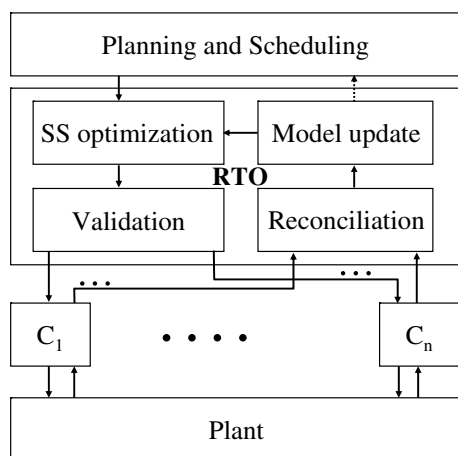


Fig. 2. Hierarchical control structure with real-time optimization (RTO), $C_1 \dots C_n$ denote the local regulatory controllers.

The planning and scheduling system provides production goals (e.g. demands of products, quality parameters), parameters of the cost function (e.g. prices of products, raw materials, energy costs) and constraints (e.g. availability of raw materials), and the process control layer provides plant data on the actual values of all relevant variables of the process. This data is first analyzed for stationarity of the process and, if a stationary situation is confirmed, reconciled using material and energy balances to compensate for systematic measurement errors. The reconciled plant data is used to compute a new set of model parameters (including unmeasured external inputs) such that the plant model represents the plant as accurately as possible at the current (stationary) operating point. Then new values for critical state variables of the plant are computed which optimize an economic cost function while meeting the constraints imposed by the equipment, the product specifications, and safety and environmental regulations as well as the economic constraints imposed by the plant management system. These values are filtered by a supervisory system (which usually includes the plant operators) (e.g. checked for plausibility, mapped to ramp changes, clipped to avoid large changes, etc. [15]) and forwarded to the process control layer which uses these values as set-points and implements appropriate moves of the operational degrees of freedom (manipulated variables). For a discussion of the implementation of the optimal steady states by linear model-predictive controllers see the paper by Rao and Rawlings [16].

As the RTO system employs a stationary process model and the optimization is only performed if the plant is approximately in a steady state, the time between successive RTO steps must be large enough for the plant to reach a new steady state after the last commanded move. Thus the sampling period must be several times the largest time-constant of the controlled process. Reported sampling times are usually on the order of magnitude of several (4–8) hours or once per day.

The introduction of an RTO system provides a clear separation of concerns and of time-scales between the RTO system and the process control system. The RTO system optimizes the plant economics on a medium time-scale (shifts to days) while the control system provides tracking and disturbance rejection on shorter time-scales from seconds to hours. Often the control system is again divided into separate layers in order to handle different speeds of responses and to structure the system into smaller modules. This separation of concerns however may be misunderstood by the plant management leading to the erroneous conclusion that dynamics do not matter and that the hard- and software on the process control layer is a necessary piece of equipment that is necessary to run the process but it is the RTO system that helps to earn money.

In [17,18], a performance metric for RTO systems, called design cost, was introduced where the profit obtained by the use of the RTO system is compared to an estimate of the theoretical profit obtained from a hypothetical

delay-free static optimization and immediate implementation of the optimal set-points without concern for the plant dynamics. The cost function consists of three parts:

- the loss in the transient period before the layered system consisting of the RTO system and the process control layer has reached a new steady state,
- the loss due to model errors in the steady state,
- the loss due to the propagation of stochastic measurement errors to the optimized set-points.

The last contribution to the loss calls for a filtering of the changes before they are applied to the real plant to avoid inefficient moves [19,20]. The issue of model fidelity was discussed in detail in [18,21]. In general, the use of a rigorous model is recommended. Adequacy of a model requires that the gradient and the curvature of the profit function are described precisely whereas its absolute value is not critical [22,23]. As parameter estimation is a core part of an RTO system, the commanded set-point changes have an influence on the model accuracy and hence on the closeness to the true optimum. Yip and Marlin [24] made the very interesting proposal to include the effect of set-point changes on the accuracy of the parameter estimates into the RTO optimization.

The issue of (steady-state or iterative) optimization with inaccurate models has been addressed since long in the literature. Roberts and co-workers proposed several algorithms that combine parameter re-estimation with the use of empirical gradients obtained from small perturbations of the plant operation to account for structural plant-model mismatch [25–27]. Cheng and Zafriou [28] proposed a modification of the FFSQ optimization algorithm [29] for steady-state optimization on the RTO layer such that the observed plant performance is taken into account when the search direction and the step size are computed but avoids the use of empirical gradients. Convergence to the optimum can be assured even for considerable structural plant-model mismatch, resulting from the use of simplified process models that do not satisfy the conditions for a sufficiently accurate model as formulated in [22].

Compared to running a plant with fixed set-points for the regulatory control layer, the introduction of the RTO layer significantly increases the complexity of the control system and causes additional costs in design, implementation and maintenance. Thus the question arises, whether it pays off or not. Duvall and Riggs [30], in the evaluation of the performance of their RTO scheme for the Tennessee Eastman Challenge Problem pointed out: “*RTO profit should be compared to optimal, knowledgeable operator control of the process to determine the true benefits of RTO. Plant operators, through daily control of the process, understand how process set-point selection affects the production rate and/or operating costs*”. In particular, they state that the operators would most likely know which variables should be kept at their bounds but they will not be able to optimize set-points within their admitted ranges according to the disturbances

encountered. This comparison therefore is quite similar to the comparison with a well chosen, “self-optimizing” regulatory control structure without RTO. In the example, a significant improvement by RTO was found.

Quoting the famous Dutch soccer player and coach Johan Cruyff, “*every advantage is also a disadvantage*”. The advantage of the RTO/MPC structure is that it provides a clear separation between the tasks of the control and the optimization layer. This separation is performed with respect to time-scales as well as to models. Rigorous nonlinear models are used only on the steady-state optimization layer. Such models nowadays are often available from the plant design phase, so the additional effort to develop the model sometimes is not very high. The control algorithms are based upon linear models (or no models at all if conventional controllers are tuned in simulations or on-site) which can be determined from plant data. As pointed out by, e.g., Backx et al. [6] and Sequeira et al. [31] this implies however that the models on the optimization layer and on the control layer will in general not be fully consistent, in particular their steady-state gains may differ.

The main disadvantage of the RTO approach is the delay of the optimization which is inevitably encountered because of the steady-state assumption. After the occurrence of a disturbance the optimization has to be delayed until the controlled plant has settled into a new steady state. To detect whether the plant is in a steady state itself is not a simple task (see e.g. [32]).

Suppose a step disturbance occurs in some unmeasured external input to the plant. Then first the control system will regulate the plant (to the extent possible) to the set-points that were computed before the disturbance occurred. After all control loops have settled, the RTO optimizer can be started, and after the results have been computed (which may also require a considerable amount of time, depending on the complexity of the model used) and validated, the control layer can start to regulate the plant to the new set-points. Thus it will take several times the settling time of the control layer to drive the plant to the new optimized mode of operation. In the first phase, the control system will try hard to maintain the previously optimal operating conditions even if without fixing the controlled variables to their set-points the operation of the plant would have been more profitable. If the disturbance persists for one sampling period of the RTO system plus one settling time of the regulatory layer, it can be estimated that the use of the RTO system on the average recovers about half of the difference between the profit obtained by the regulatory system alone (with fixed set-points) and an online-optimizing controller that implements the optimal set-points within the settling time of the regulatory control layer. The combined RTO/regulatory control structure will work satisfactorily for infrequent step changes of feeds, product specifications or product quantities but it will provide no benefit for changes that occur at time scales below the RTO sampling period.

Marlin and Hrymak [9] listed several areas for improvement of RTO systems. Two important ones are also addressed in the remainder of this paper: the integration with the process control layer, and the extension to dynamic operation. They pointed out that instead of sending set-points to the control layer, an ideal RTO system should output a design (i.e. tuning parameters or even a choice of the control structure) of the control system that leads to an optimized performance under the current long-term operating conditions.

4. Reducing the gap between regulation and RTO

4.1. Frequent RTO

As a consequence of the drawback that RTO is applied with rather long sampling periods, several authors have proposed schemes that use smaller sampling times on the optimizing layer. For example, Sequeira et al. [31] proposed to change the set-points for the regulatory layer in much shorter intervals (in the case study presented they used 1/50 of the settling time of the plant) and to perform a “real-time evolution” of the set-points by heuristic search (used here to reduce the computation time) based upon the stationary process model and the available measurements. To avoid overshooting behavior, the steps of the decision variables are bounded in each step. In the example shown, this scheme outperforms steady-state RTO with regulatory control especially for non-stationary disturbances and in the first phase after a disturbance occurs, which is not too surprising. The idea that a “step in the right direction” should be better than to wait until the process has settled to a new steady state is certainly convincing, however the approach suffers from neglecting the dynamics of the plant. Basak et al. [33] discussed an online optimizing control scheme for a complex crude distillation unit. They proposed to perform a steady-state optimization of the unit for an economic cost function under constraints on the product properties with respect to the operational degrees of freedom and a model parameter update at a sampling rate of 1–2 h and to apply the computed manipulated values directly to the plant. If the update of the manipulated variables is based solely on information on the plant inputs and the economics, such a scheme will react to disturbances only via the model parameter update. If dynamic variables enter the optimization, the resulting dynamics of the controlled plant will be unpredictable from the stationary behavior. The idea to perform updates of the operating point using a stationary model more frequently than every few settling times of the plant but to limit the size of the changes that are applied to the plant such that quasi-stationary transients are realized is also used in industrial practice. This leads to the implementation of the optimal set-point changes by ramps rather than steps or, in other terms, of a nonlinear integral controller, causing slow moves of the overall system.

If a fast sampling RTO scheme is used, it will, at least for very short sampling times, interact with the regulatory

control layer causing uncontrolled effects because the separation of the time scales does no longer hold. The assumption that a steady-state optimization performed at an instationary operating point yields the right move of the set-points is similar to the basic idea of gain scheduling control. In both cases, a projection of the actual dynamic state on a corresponding stationary point that is defined by the values of the measured, actuated or demanded variables during transients is performed and the control move is computed under the (in principle wrong) assumption that the plant actually is in this steady state. Fast sampling RTO thus shares the potential of stability problems with gain scheduling controllers which usually can only be avoided if “slow”, quasi-stationary set-point changes are realized (see e.g. [34,35]).

4.2. Integration of steady-state optimization into model-predictive control

In order to narrow the gap between the low frequency nonlinear steady-state optimization performed on the RTO layer and the relatively fast linear MPC layer, the so-called LP-MPC and QP-MPC two-stage MPC structures are frequently used in industry [36–41]. A detailed analysis of their properties was given by Ying and Joseph [42]. The extended structure is shown in Fig. 3.

The task of the upper MPC layer is to compute the set-points (targets) both for the controlled variables and for the manipulated inputs for the lower MPC layer by solving a constrained linear or quadratic optimization problem, using information from the RTO layer and from the MPC layer. The optimization is performed with the same sampling period as the lower-level MPC controller. At each sampling instant, the minimization

$$\min_{y_{\text{set}}, u_{\text{set}}} [(y_{\text{set}} - y^*)^T C_y (y_{\text{set}} - y^*) + (u_{\text{set}} - u^*)^T C_u (u_{\text{set}} - u^*) + c_y (y_{\text{set}} - y^*) + c_u (u_{\text{set}} - u^*)] \quad (4)$$

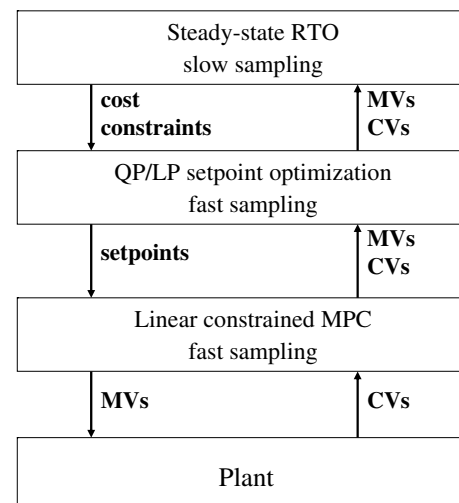


Fig. 3. Two-layer MPC with set-point optimization.

$$\begin{aligned}
\text{Subject to } y_{\text{set}} &= A_S u_{\text{set}} + d(k), \\
d(k) &= d(k-1) + \Delta(k), \\
y_{\text{min}} &\leq y_{\text{set}} \leq y_{\text{max}}, \\
u_{\text{min}} &\leq u_{\text{set}} \leq u_{\text{max}}
\end{aligned} \tag{5}$$

is performed.

The steady-state gain A_S and the disturbance estimate are provided by the MPC layer whereas the nominal set-points y^* and u^* are provided by the RTO layer. This structure addresses the following issues:

- A faster change of the set-points after the occurrence of disturbances is realized;
- The inconsistency of the nonlinear steady-state model on the RTO layer and the linear steady-state model used on the MPC layer is reduced;
- Large set-point changes that may drive the linear controllers unstable are avoided;
- The distribution of the offsets from the desired targets that are realized by the MPC controller is explicitly controlled and optimized.

The plant model and the disturbance estimate used on the intermediate optimization layer is the same as that used (and eventually updated) on the MPC layer, thus avoiding inconsistencies, whereas the weights in the cost function and the linear constraints are chosen such that they approximate the nonlinear cost function and the constraints on the RTO layer around the present operating point. As long as this approximation is good, optimal operations are ensured.

A simpler approach to the integration of steady-state optimization and model-predictive control is to optimize those tuning parameters of a dynamic matrix controller (DMC) or a QDMC controller that determine the steady-state behavior of the controller (set-points of the regulated variables, targets of the manipulated variables, weights on the deviations of the regulated variables from the set-points and on the deviations of the of the manipulated variables from the targets) such that the profit obtained is maximized over a number of disturbance scenarios as proposed by Kassidas et al. [43]. In the parameter optimization, a full nonlinear steady-state plant model is used. Note that this optimization is only performed once (off-line), and only the usual computations of the DMC or QDMC controller moves employing linear plant models have to be performed online. The approach was compared to rigorous steady-state optimization (similar to what a RTO layer working together with a zero-offset controller would yield) of the purity set-points and to a controller that controls the plant to fixed pre-computed purity set-points (also optimized over the various disturbance scenarios) for a simple distillation example. The optimization approach led to a considerable variation of the controlled outputs over the different scenarios, while when the process is regulated to fixed set-points, this variation is mapped to the manipulated

variables. The optimally tuned DMC controller implements a compromise between these extremes and realizes about 70% of the average additional profit that results for rigorous optimization. Even better results can be expected for examples where the optimal operation is mostly determined by the constraints.

4.3. Integration of nonlinear steady-state optimization in the linear MPC controller

Zanin et al. [7,44] reported the formulation, solution and industrial implementation of a combined MPC/optimizing control scheme for a fluidized-bed catalytic cracker, FCC. The plant has seven manipulated inputs and six controlled variables. The economic criterion is the amount of LPG produced. The optimization problem that is solved in each controller sampling period is formulated in a mixed manner: range control MPC with a fixed linear plant model (imposing soft constraints on the controlled variables by a quadratic penalty term that only becomes active when the constraints are violated) plus a quadratic control move penalty plus an economic objective that depends on the values of the manipulated inputs at the end of the control horizon:

$$\begin{aligned}
\min_{\Delta u(k+i); i=0, \dots, m-1} & \sum_{j=1}^p \|W_1(y(k+j) - r)\|_2^2 + \sum_{i=0}^{m-1} \|W_2 \Delta u(k+i)\|_2^2 \\
& + W_3 f_{\text{eco}}(u(k+m-1)) + \|W_4(u(k+m-1) \\
& - u(k-1) - \Delta u(k))\|_2^2 + W_5 [f_{\text{eco}}(u(k+m-1), y(k+\infty)) \\
& - f_{\text{eco}}(u(k), y'(k+\infty))]^2.
\end{aligned} \tag{6}$$

The value of the economic objective f_{eco} is computed using a nonlinear steady-state process model. As only the first move of the controller is implemented, penalty terms are added that penalize the deviation of the first values of the manipulated variables from their final values within the control horizon in order to prevent that the economically optimal control move is always “shifted to infinity”. Several variants for this penalty term were investigated. The different components of the cost function were weighted such that the economic criterion and the MPC part have a similar influence on the values of the overall cost.

This combined optimizing/LMPC controller was implemented and tested at a real Petrobras FCC with a sampling rate of 1 min, a control horizon of two steps and a prediction horizon of 20 steps. An impressive performance is reported, both in terms of the economic performance and of the smoothness of the transients, pushing the process to its limits. The integrated control scheme performed substantially better than the conventional scheme where the operators chose set-points based on their experiences that were then implemented by a conventional MPC scheme. The final weights of the different contributions to the cost function were determined by experiments. Simulations also showed that the one-layer approach compared favorably to

a two-layer approach in which the economic optimization provided set-points for a linear MPC scheme in terms of dynamic response. Nonetheless, the optimizing controller was not implemented in daily operation. The reasons will be discussed below. A similar control scheme was experimentally validated in [45] for a paste dryer.

5. Direct finite horizon optimizing control

5.1. General ideal

For demanding applications, the replacement of linear MPC controllers by nonlinear model-predictive control is a promising option and industrial applications have been reported in particular in polymerization processes [46–49]. If nonlinear model-based control is used to implement optimal set-points or optimal trajectories at a plant, it is only a small step to replace the traditional quadratic cost criterion that penalizes the deviations of the controlled variables from the reference values and the input variations by an economic criterion. Constraints on outputs (e.g. strict product specifications) as well as process limitations can then be included directly in the optimization problem. This approach has several advantages over a combined steady-state optimization/linear MPC scheme:

- Fast reaction to disturbances, no waiting for the plant to reach a steady state is required;
- Regulation of constrained variables to set-points which implies a safety margin between these set-points and the constraints is avoided, the exact constraints can be implemented for measured variables and only the model error has to be taken into account for unmeasured constrained variables;
- Over-regulation is avoided, no variables are forced to fixed set-points and all degrees of freedom can be used to optimize process performance;
- No inconsistency arises from the use of different models on different layers;
- Economic goals and process constraints do not have to be mapped to a control cost whereby economic optimality is lost and tuning is difficult;
- The overall scheme is structurally simple.

An important point in favor of using an economic cost criterion and formulating restrictions of the process and the product properties as constraints is that this reduces the need for tuning of the weights in less explicit formulations. Exxon's technology for NMPC employs a combination of criteria that represent reference tracking, operating cost and control moves [48].

In the next section, it will be demonstrated that direct online optimizing control can successfully be applied to control problems that are hard to tackle by conventional control techniques. Other application studies have been reported, e.g. by Singh et al. [50] and Johansen and Sbar-

baro [51] for blending processes and by Busch et al. [52] for a waste-water treatment plant.

5.2. Case study: control of reactive simulated moving bed chromatographic processes

5.2.1. Process description

Chromatographic separations are a widespread separation technology in the fine chemicals, nutrients and pharmaceutical industry. Chromatography is applied for difficult separation tasks, in particular if the volatilities of the components are similar or if the valuable components are sensitive to thermal stress. The separation of enantiomers (molecules that are mirror images of each other) is an example where chromatography is the method of choice. The standard chromatographic process is a batch separation where pulses of the mixture that has to be separated are injected into a chromatographic column followed by the injection of pure solvent. The components travel through the column at different speeds and can be collected at the end of the column in different purified fractions. In batch mode, the adsorbent is not used efficiently and the process usually leads to highly diluted products.

The goal of a continuous operation of chromatographic separations with a counter-current movement of the solid phase and the liquid phase led to the development of the simulated moving bed (SMB) process by Broughton, [53]. It is gaining increasing attention in industry due to its advantages in terms of productivity and solvent consumption [54,55]. An SMB process consists of several chromatographic columns connected in series which constitute a closed loop. An effective counter-current movement of the solid phase relative to the liquid phase is achieved by periodically and simultaneously moving the inlet and the outlet lines by one column in the direction of the liquid flow (see Fig. 4).

After a start-up phase, SMB processes reach a periodic or cyclic steady state (CSS). The length of a cycle is equal to the duration of a switching period times the number of columns, but relative to the port positions, the profiles are repeated every switching period. Fig. 5 shows the concentration profiles of a binary separation along the col-

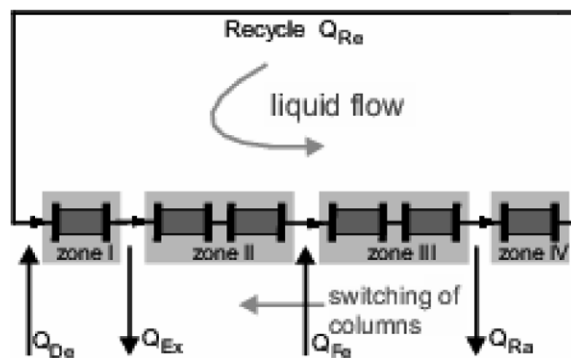


Fig. 4. Simulated moving bed principle.

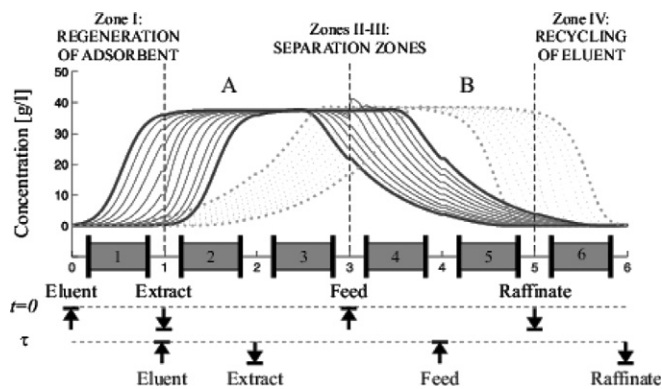


Fig. 5. Concentration profiles of an SMB process. The figure shows the concentration profiles at different instances during one switching period. At the end of the period, the ports are switched.

umns plotted for different time instants within a switching period.

5.2.2. Control of SMB processes

Classical feedback control strategies are not directly applicable to SMB processes due to their mixed discrete and continuous dynamics, spatially distributed state variables with steep slopes, and slow and strongly nonlinear responses of the concentrations profiles to changes of the operating parameters. A summary of different approaches to control of SMB processes can be found in [56,57].

Klatt et al. [58] proposed a two-layer control architecture similar to the RTO/MPC scheme where the optimal operating trajectory is calculated at a low sampling rate by dynamic optimization based on a rigorous process model. The model parameters are adapted using online measurements. The low level control task is to keep the concentrations in the columns near the values at the optimal cyclic steady state despite disturbances, plant degradation and plant/model mismatch. This is achieved by controlling the positions of the four concentration fronts in the process. The controller is based on input/output models that are identified using simulation data produced by the rigorous process model near the optimal cyclic steady state [58,59]. A disadvantage of this two-layer concept is that keeping the front positions at the values obtained from the rigorous optimization does not guarantee the product purities if structural plant/model mismatch occurs. To ensure the specified product purities, an additional purity controller is required, and the overall scheme becomes quite complex without actually ensuring optimal operation because the lower-level controllers change the optimized inputs in a suboptimal fashion.

5.2.3. Online optimizing control

As the progress in efficient numerical simulation and optimization enabled a dynamic optimization of an SMB-process within one switching period, a direct finite horizon optimizing control scheme that employs the same rigorous nonlinear process model that is used for process

optimization in the two-layer structure was proposed and applied to a 3-zones reactive SMB process for glucose isomerization [60,61]. The key feature of this approach is that the production cost is minimized online over a finite horizon while the product purities are considered as constraints, thus a real online optimization of all operational degrees of freedom is performed, and there is no tracking of pre-computed set-points or reference trajectories. In [62], this control concept was extended to the more complex processes VARICOL [63,64] and PowerFeed [65] where the ports are switched asynchronously and the flow rates are varied in the subintervals of the switching period. These process variants offer an even larger number of degrees of freedom that can be used for the optimization of the process economics while satisfying the required product purities. In the optimizing control scheme proposed in [60,61], the states of the process model are determined by forward simulation starting from measurements in the recycle stream and in the product streams.

A different optimization-based approach to the control of SMB processes was proposed by Erdem et al., [66–68]. In their work, a moving horizon online optimization is performed based on a linear reduced-order model that is obtained from linearizing a rigorous model around the periodic steady state. The state variables of the model are estimated by a Kalman Filter that processes the product concentration measurements. Due to the use of repetitive MPC [69] where the sampling time is equal to the switching time, the switching period has to be kept fixed which may cause a loss of performance compared to the optimization of all available degrees of freedom.

5.2.4. The Hashimoto reactive SMB process

The integration of chemical reactions into chromatographic separations offers the potential to improve the conversion of equilibrium limited reactions. By the simultaneous removal of the products from the reaction zone, the reaction equilibrium is shifted to the side of the products. This combination of reaction and chromatographic separation can be achieved by packing the columns of the SMB process uniformly with adsorbent and catalyst, which leads to the reactive SMB (SMBR) process. The SMBR process can be advantageous in terms of higher productivity in comparison to a sequential arrangement of reaction and separation units [70]. However, for equilibrium reactions of the type $A \leftrightarrow B$, a uniform catalyst distribution in the SMBR promotes the backward reaction near the product outlet which is detrimental to the productivity. Further on, the renewal of deactivated catalyst is difficult when it is mixed with adsorbent pellets, and the same operating conditions must be chosen for separation and reaction what may lead to either suboptimal reaction or suboptimal separation. The Hashimoto SMB process [71,72] overcomes the disadvantages of the SMBR by performing separation and reaction in separate units that contain only adsorbent or only catalyst. In this configuration, the conditions for reaction and for separation can be chosen

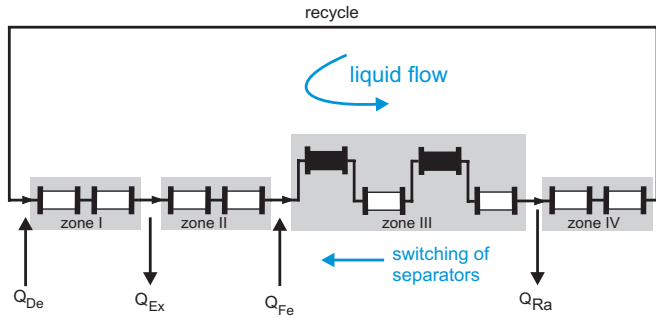


Fig. 6. Four-zone Hashimoto reactive SMB process. White: separation units, black: reactor units.

separately and the reactors can constantly be placed in some of the separation zones of the SMB process by appropriate switching. The structure of a Hashimoto SMB process is shown in Fig. 6. The dynamics of this class of processes is highly complex.

5.2.5. Optimizing controller application

The example application that will briefly be described in the sequel is the racemization of *Tröger's Base* (TB) in combination with a chromatographic separation in order to produce of the enantiomer TB – that is used for the treatment of cardiovascular diseases. More details can be found in [73,74]. The solvent is an equimolar mixture of acetic acid that acts as the catalyst for the reaction and 2-propanole that increases the solubility of the mixture. The adsorption of the Tröger's Base system to the solid phase can be described by an adsorption isotherm that is of multi-component Langmuir type:

$$q_i = \frac{H_i c_{p,i}}{1 + \sum_k b_{i,k} c_{p,k}}, \quad k = +, -. \quad (7)$$

Here $c_{p,i}$ denotes the concentration of component i in the pores of the particle phase and q_i the adsorbed fraction. The reaction takes place in plug flow reactors that are operated at 80 °C whereby the catalyst is thermally activated. In the chromatographic columns that have a temperature of 25 °C the catalyst is virtually deactivated. In the simulation run shown below, a four-zone Hashimoto process with eight chromatographic columns, two reactors, and a column distribution as shown in Fig. 6 is considered. The objective of the optimizing controller is to minimize the solvent consumption Q_{De} for a constant feed flow and a given purity requirement in the presence of a plant/model mismatch. The inevitable mismatch between the model and the behavior of the real plant is taken into account by feedback of the difference of the predicted and the measured product purities. A regularization term is added to the objective function to obtain smooth trajectories of the input variables. The controller has to respect the purity requirement for the extract flow which is averaged over the prediction horizon, the dynamics of the Hashimoto SMB model and the maximal flow rate in zone I due to limited pump capacities. In order to guarantee that at least

70% of the mass of the components fed to the plant leaves the plant in the extract product stream (averaged over the prediction horizon), an additional productivity requirement was added. The resulting mathematical formulation of the optimization problem is

$$\begin{aligned} \min_{\beta_I, \beta_{II}, \beta_{III}, \beta_{IV}} & \sum_{i=1}^{H_P} Q_{De_i} + \Delta\beta_i R \Delta\beta_i \\ \text{s.t.} & \begin{cases} \tilde{x}_{\text{smb}}^k = x_{\text{smb}}^k + \int_{t=0}^{\tau} f_{\text{smb}}(x_{\text{smb}}(t), \beta(t)) dt, \\ x_{\text{smb}}^{k+1} = P \tilde{x}_{\text{smb}}^k, \end{cases} \\ & \frac{\sum_i^{H_P} \text{Pur}_{\text{EX},i}}{H_P} \geq (\text{Pur}_{\text{EX},\text{min}} - \Delta\text{Pur}_{\text{EX}}), \quad (8) \\ & \frac{\sum_i^{H_P} m_{\text{EX},i}}{H_P} \geq 0.7 m_{\text{Fe}} - \Delta m_{\text{EX}}, \\ & Q_I \leq Q_{\text{max}}, \\ & Q_{De}, Q_{Ex}, Q_{Fe}, Q_{Re} \geq 0, \end{aligned}$$

where the purity error $\Delta\text{Pur}_{\text{EX}}$ and the mass error Δm_{EX} are calculated according to

$$\begin{aligned} \Delta\text{Pur}_{\text{EX}} &= \text{Pur}_{\text{EX},\text{plant},i-1} - \text{Pur}_{\text{EX},\text{model},i-1}, \\ \Delta m_{\text{EX}} &= m_{\text{EX},\text{plant},i-1} - m_{\text{EX},\text{model},i-1}. \end{aligned} \quad (9)$$

The model of the plant consists of rigorous dynamic models of the individual columns of the plant and the node equations (represented by the function f_{smb}) and the port switching (represented by the permutation matrix P). The degrees of freedom of the optimization problems are the transformed flow rates β_I – β_{IV} in the four zones of the process which depend on the ratios of the flow rates of the liquid phase in the zones to the effective solid flow rate that is defined by the switching period τ [58]. H_P denotes the prediction horizon. The chromatographic columns are described by the general rate model [75] which accounts for all important effects of a radially homogeneous column, i.e. mass transfer between the liquid and the solid phase, pore diffusion, and axial dispersion. The partial differential equations are discretized using a Galerkin approach on finite elements for the bulk phase and orthogonal collocation for the particle phase [76]. The reactors consist of three columns in series. Each column is discretized into 12 elements, yielding an overall model with 1400 dynamic states. For the solution of the optimization problem, the feasible path solver FFSQ [29] is applied. It first searches for a feasible operating point and then minimizes the objective function. The number of iterations of the SQP solver was limited to 5 because the optimizer can perform at least this number of iterations within one cycle of the process (eight switching periods), as required for online control. If convergence is not achieved within five iterations, the best feasible solution obtained is applied.

In the simulation scenario, a model/plant mismatch was introduced by disturbing the initial Henry coefficients H_+ and H_- of the model by +5% and –4%. The parameters of the controller are displayed in Table 1.

Table 1

Controller parameters	
Sampling time	1 cycle = 8 periods
Prediction horizon, H_P	5 cycles = 40 periods
Control horizon, H_C	1 cycle = 8 periods
Regularization, R	[0.7 0.7 0.7 0.7]
Number of finite elements per column	12
Model order	1400

The performance of the controller is illustrated by Fig. 7. The controller manages to track the purity reference and to keep the productivity above its lower limits, while it improves the economical operation of the plant by reducing the solvent consumption. The optimizing controller has been implemented at a medium scale SMB plant using a PLC-based process control system and an additional PC for optimization and parameter estimation [102]. A photograph of the setup is shown in Fig. 8. The reactors are in a heated bath on top of the SMB plant. An experimental result where a significant disturbance – a pump failure – occurred exactly when the controller was switched on is shown in Fig. 9.

5.3. Numerical aspects

In the example described above, a relatively simple numerical approach using direct simulation, computation of the gradients by perturbation and a feasible path SQP algorithm for the computation of the optimal controls



Fig. 8. Experimental SMB-plant with external reactors (in the heated bath on the top, left).

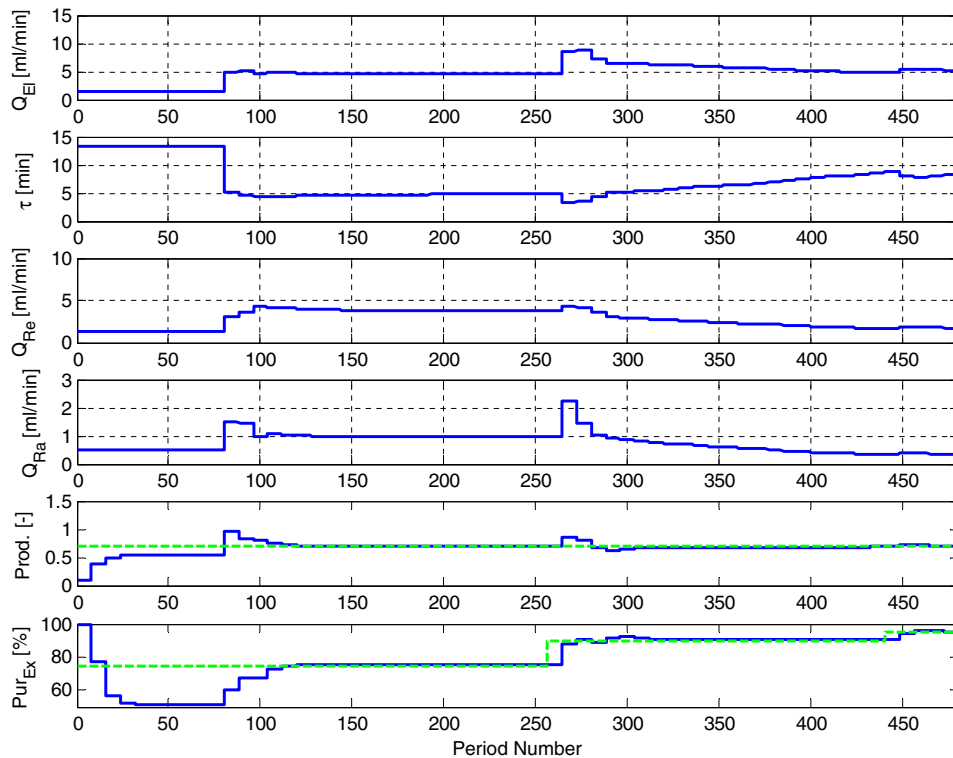


Fig. 7. Simulation of the optimizing controller of the Hashimoto reactive SMB process. The controller was started at period 80. τ denotes the switching period, Prod the productivity. The dashed lines represent the set-points.

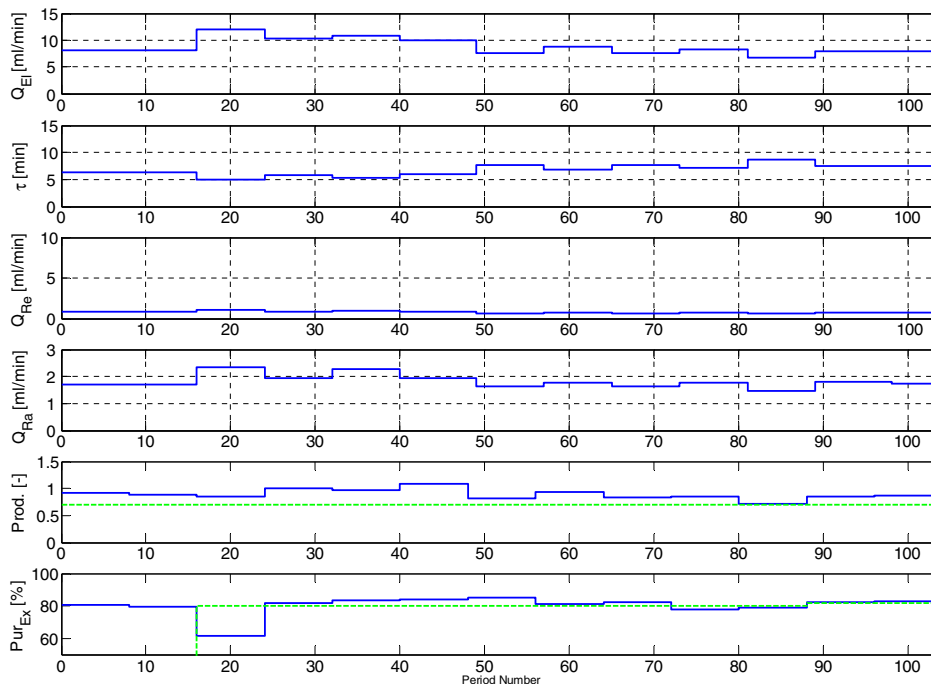


Fig. 9. Experimental result with the optimizing controller – the controller was started at period 17 and a pump failure occurred during periods 17–24 [102].

was used. By using more advanced numerical techniques, much shorter computation times can be realized. Diehl et al. [77] proposed a scheme for the solution of nonlinear model-predictive control problems with large plant models where the multiple shooting method [78] with a tailored SQP algorithm is used and only one iteration of the SQP-problem is performed in each sampling interval. Moreover, the steps performed in the algorithm are ordered such that a new output is computed fast immediately after a new measurement have become available and the remainder of the computations is done thereafter, thus reducing the reaction time to disturbances considerably. A further improvement of the speed of the solution of the optimization problem is presented in [79]. The maximum time needed for the solution of a quadratic NMPC problem for a distillation column modeled by a rigorous DAE model of order $106 + 159$ and prediction and control horizons of 36 sampling intervals is reported to be less than 20 s for a Pentium 4 computer. Diehl et al. [80] proved convergence of the real-time iteration scheme to the optimal solution for general cost functions.

An alternative to the multiple shooting approach is to apply full discretization techniques where similar progress has been reported [81,82]. Jockenhövel et al. [83] reported the application of conventional NMPC with a quadratic cost criterion to the Tennessee Eastman challenge problem with 30 dynamic and 149 algebraic states, 11 control variables, several constraints on state variables, and control and prediction horizons of 60 steps. Using full discretization and an interior point method, a reliable solution well within the sampling time of 100 s is achieved. It can thus be concluded that online optimizing control is computationally

feasible nowadays for models with several hundred state variables and for sufficiently long prediction horizons. The complexity of rigorous models no longer is a strong reason not to employ them in optimization-based control schemes.

6. Open issues

6.1. Modeling

In a direct optimizing control approach accurate dynamic nonlinear process models are needed. While nonlinear steady-state models are nowadays available for many processes because they are created and used extensively in the process design phase, there is still a considerable effort required to formulate, implement and validate nonlinear dynamic process models. The recent trend towards the use of training simulators may partly alleviate this problem. Training simulators are increasingly ordered together with new plants and are available before the real plant starts production. The models inside the training simulator represent the plant dynamics faithfully even for states far away from the nominal operating regime (e.g. during start-up and shut-down) and can be used also for optimization purposes. Such rigorous models may however include too much detail from a control point of view. It does not seem to be necessary to include dynamic phenomena that affect the behavior only on time scales much longer than the prediction horizon or shorter than the sampling time of the controller. The appropriate simplification of nonlinear models still is an unresolved problem [84,85]. The alternative approach to use black-box or grey-box models as

proposed frequently in nonlinear model-predictive control [59,86–88] may be effective for regulatory control where the model only has to capture the essential dynamic features of the plant, but seems to be less suitable for optimizing control where the optimal plant performance is aimed at and hence the best stationary values of the inputs and of the controlled variables have to be computed accurately by the controller.

6.2. Stability

Optimization of a cost function over a finite horizon in general neither assures optimality of the complete trajectory beyond this horizon nor stability of the closed-loop system. Closed-loop stability has been addressed extensively in the theoretical research in nonlinear model-predictive control. The theoretical discussion has led to a clear understanding of what is required to ascertain the stability of a nonlinear model-predictive control scheme and clearly pointed out the deficiencies of less sophisticated schemes. Stability results so far have been proven for regulatory NMPC where stability means convergence to the desired equilibrium point. Stability can be assured by proper choice of the cost function within the prediction horizon and the addition of a cost on the terminal state and the restriction of the terminal state to a suitable set [89,90]. If the cost function within the prediction horizon is an economic cost function, a bounded cost over the horizon will however in general not ensure boundedness of the deviation of the state vector from an equilibrium state because economic cost functions often involve only very few process variables, mostly input streams and mass flows leaving the physical system. Moreover, in direct optimizing control there is no fixed equilibrium state.

A possible approach towards optimizing control with guaranteed stability is to compute the optimal steady state online first and then the optimal moves over the control horizon. In this case, the cost function can be extended by a terminal cost that penalizes the distance of the state at the end of the prediction horizon from the optimal steady state and – if necessary by a (small) quadratic penalty term on the deviation of the state (or of suitable outputs) from the terminal state within the prediction horizon. If a suitable constraint on the terminal state is added, this should provide a stabilizing control scheme. It has been demonstrated recently that algorithms of this type are computationally feasible even for very large nonlinear plant models [91]. By the choice of the weighting terms, a compromise can be established between optimizing process performance over a limited horizon at a fast sampling rate and long-term performance under the assumption that no major disturbance occurs in the future. This leads to a hierarchical scheme similar to the RTO/MPC scheme where the upper layer provides the terminal state and the terminal region and the lower layer now is “cost-conscious” and no longer purely regulatory. In contrast to the RTO/MPC-scheme, the optimization criteria as

well as the models used on both layers are consistent in this structure.

An alternative approach to guaranteeing stability of an optimizing controller was applied in [51] to a linear process with a static nonlinearity at the output, based on an augmented control Lyapunov function.

6.3. State estimation

For the computation of economically optimal process trajectories based upon a rigorous nonlinear process model, the state variables of the process at the beginning of the prediction horizon must be known. As not all states will be measured in a practical application, state estimation is a key ingredient of a directly optimizing controller. The state estimation problem is of the same complexity as the optimization problem, unless simple approaches as predicting the state by simulation of a process model are employed. The natural approach is to formulate the state estimation problem also as an optimization problem on a moving horizon [92–94]. The estimation of some important but variable or unknown model parameters can be included in this formulation. A control scheme where NMPC is combined with moving horizon estimation has recently been realized in [95]. But still experience with the application of moving horizon state estimation is quite limited to date. Simpler and computationally less demanding schemes as the constrained extended Kalman filter (CEKF) may provide a comparable performance and are more easy to implement (but not easier to tune) [48,96]. As accurate state estimation is at least as critical for the performance of the closed-loop system as the exact tuning of the optimizer, more attention should be paid to the investigation of the performance of state estimation schemes in realistic situations with non-negligible model-plant mismatch.

6.4. Measurement-based optimization

In the scheme described in Section 5, feedback of the measured variables is only realized via the updates of the state and of the parameters and by a bias term in the formulation of the constraints and possibly in the cost criterion. As discussed in the Section on RTO, a near-optimal solution requires that the gradients provided by the model and the second derivatives are accurate. However in such a scheme there is no feedback present to establish optimality despite the presence of model errors. This can be addressed by the solution of a modified optimization problem [25,26] or by taking the presence of model errors into account in the local search [28]. As shown by Tatjewski, [97], optimality can be achieved in the presence of structural or parametric plant-model mismatch even without parameter updating by correcting the optimization criterion based on gradient information derived from the available measurements. This idea was extended to handling constraints and applied to batch chromatography in [98] and might be explored in the continuous case as well. An alternative way

to implement measurement-based optimization is to formulate the optimization problem (partly) as the tracking of necessary conditions of optimality which are robust against model mismatch [99–101].

6.5. Reliability and transparency

As discussed above, relatively large nonlinear dynamic optimization problems can nowadays be solved in real-time, so this issue does no longer prohibit the application of a direct optimizing control scheme to complex units. A practically very important limiting issue however is that of reliability and transparency. It is hard, if not impossible to rule out that a nonlinear optimizer does not provide a solution which at least satisfies the constraints and gives a reasonable performance. While for RTO an inspection of the commanded set-points by the operators usually will be feasible, this is less likely in a dynamic situation. Hence automatic result filters are necessary as well as a backup scheme that stabilizes the process in the case where the result of the optimization is not considered safe. But the operators will still have to supervise the operation of the plant, so a control scheme with optimizing control must be structured into modules which are not too complex. The concept of adding a cost term that represents steady-state optimality as described above provides a possible solution for the dynamic online optimization of larger complexes based on decentralized optimizing control of smaller units. The co-ordination of the units is performed by the steady-state real-time optimization that sends the desired terminal states plus adequate penalty terms to the lower-level controls. These penalty terms must reflect the sensitivity of the global optimum with respect to local deviations, i.e. how an economic gain on the local level within the optimization horizon is traded against a global loss due to not steering the plant to the globally optimal steady state. Still, acceptance by the operators and plant managers will be a major challenge. Good interfaces to the operators that display the predicted moves and the predicted reaction of the plant and enable comparisons with their intuitive strategies are believed to be essential for practical success.

6.6. Effort vs. performance

The gain in performance by a more sophisticated control scheme always has to be traded against the increase in cost due to the complexity of the control scheme – a complex scheme will not only cause cost for its implementation but it will need more maintenance by better qualified people than a simple one. If a carefully chosen standard regulatory control layer leads to a close-to-optimal operation, there is no need for optimizing control. If the disturbances that affect profitability and cannot be handled well by the regulatory layer (in terms of economic performance) are slow, the combination of regulatory control and RTO is sufficient. In a more dynamic situation or for complex nonlinear multivariable plants, the idea of direct optimiz-

ing control should be explored and implemented if significant gains can be realized in simulations. Similar to any NMPC controller that is designed for reference tracking, a successful implementation will require careful engineering such that as many uncertainties as possible are compensated by simple feedback controllers and only the key dynamic variables are handled by the optimizing controller based on a rigorous model of the essential dynamics and of the stationary relations of the plant without too much detail.

7. Conclusions

This survey paper points out that process control should be seen as a means to optimize plant operations rather than to just track pre-computed set-points. Appropriate selection of the control structure and real-time optimization (RTO) provide significant contributions to plant profitability. Recent progress in numerical optimization algorithms as well as in NMPC theory and technology has rendered the application of online dynamic optimization based upon rigorous models to complex plants feasible. Using an economic cost function in the MPC computations instead of a function that penalizes the distance to the desired set-points or trajectories which are assumed as given and fixed offers new exiting possibilities. Several application studies have already demonstrated the feasibility and the potential of this approach. Industrial implementations will continue to require a considerable engineering effort in particular because of the issues of robustness and transparency. The structuring of a control system in hierarchical layers and subsystems of reduced complexity will remain a key ingredient of solutions which are accepted in industrial practice, but the distribution of the functionalities between the layers can be re-thought due to the possibilities of direct optimizing control.

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References

- [1] M. Morari, G. Stephanopoulos, Y. Arkun, Studies in the synthesis of control structures for chemical processes, Part I, *AIChE J.* 26 (1980) 220–232.
- [2] L.T. Narraway, J.D. Perkins, G.W. Barton, Interaction between process design and process control: economic analysis of process dynamics, *J. Process Control* 1 (1991) 243–250.
- [3] L.T. Narraway, J.D. Perkins, Selection of process control structure based on linear dynamic economics, *Ind. Eng. Chem. Res.* 32 (1993) 2681–2692.
- [4] A. Zheng, R.V. Mahajannam, J.M. Douglas, Hierarchical procedure for plantwide control system synthesis, *AIChE J.* 45 (1999) 1255–1265.
- [5] S. Skogestad, Plantwide control: the search for the self-optimizing control structure, *J. Process Control* 10 (2000) 487–507.
- [6] T. Backx, O. Bosgra, W. Marquardt, Integration of model predictive control and optimization of processes, in: *Proceedings of IFAC Symposium ADCHEM, Pisa, 2000*, pp. 249–260.
- [7] A.C. Zanin, M. Tvrzka de Gouvea, D. Odloak, Integrating real-time optimization into the model predictive controller of the FCC system, *Contr. Eng. Pract.* 10 (2002) 819–831.
- [8] P.A. Rolandi, J.A. Romagnoli, A framework for online full optimizing control of chemical processes, in: *Proceedings of ESCAPE 15, Elsevier, 2005*, pp. 1315–1320.
- [9] T.E. Marlin, A.N. Hrymak, Real-time operations optimization of continuous processes, in: *Proceedings of CPC V, AIChE Symposium Series, vol. 93, 1997*, pp. 156–164.
- [10] T. Larsson, K. Hestetun, E. Hovland, S. Skogestad, Self-optimizing control of a large-scale plant: the Tennessee Eastman process, *Ind. Eng. Chem. Res.* 40 (2001) 4889–4901.
- [11] T. Larsson, S. Govatsmark, S. Skogestad, Control structure selection for reactor, separator, and recycle processes, *Ind. Eng. Chem. Res.* 42 (2003) 1225–1234.
- [12] S. Engell, T. Scharf, M. Völker, A methodology for control structure selection based on rigorous process models, in: *16th IFAC World Congress, Tu-E14-TO/6, 2005*.
- [13] J.J. Downs, E.F. Vogel, A plant-wide industrial process control problem, *Comp. Chem. Eng.* 17 (1993) 245–255.
- [14] W. Findeisen, F.N. Bailey, M. Brdys, K. Malinowski, P. Wozniak, A. Wozniak, *Control and Coordination in Hierarchical Systems*, John Wiley, New York, 1980.
- [15] I. Miletic, T.E. Marlin, Results analysis for real-time optimization (RTO): deciding when to change the plant operation, *Comp. Chem. Eng.* 20 (1996) 1077.
- [16] C.V. Rao, J.B. Rawlings, Steady states and constraints in model predictive control, *AIChE J.* 45 (1999) 1266–1278.
- [17] J.F. Forbes, T.E. Marlin, Design cost: a systematic approach to technology selection for model-based real-time optimization systems, *Comp. Chem. Eng.* 20 (1996) 717–734.
- [18] Y. Zhang, J.F. Forbes, Extended design cost: a performance criterion for real-time optimization systems, *Comp. Chem. Eng.* 24 (2000) 1829–1841.
- [19] I. Miletic, T.E. Marlin, On-line statistical results analysis in real-time operations optimization, *Ind. Eng. Chem. Res.* 37 (1998) 3670–3684.
- [20] Y. Zhang, D. Nadler, J.F. Forbes, Results analysis for trust constrained real-time optimization, *J. Process Control* 11 (2001) 329–341.
- [21] W.S. Yip, T.E. Marlin, The effect of model fidelity on real-time optimization performance, *Comp. Chem. Eng.* 28 (2004) 267–280.
- [22] J.F. Forbes, T.E. Marlin, J. MacGregor, Model selection criteria for economics-based optimizing control, *Comp. Chem. Eng.* 18 (1994) 497–510.
- [23] J.F. Forbes, T.E. Marlin, Model accuracy for economic optimizing controllers: the bias update case, *Ind. Eng. Chem. Fund.* 33 (1995) 1919–1929.
- [24] W.S. Yip, T.E. Marlin, Designing plant experiments for real-time optimization systems, *Contr. Eng. Pract.* 11 (2003) 837–845.
- [25] P.D. Roberts, An algorithm for steady-state system optimization and parameter estimation, *Int. J. Syst. Sci.* 10 (1979) 719–734.
- [26] M. Brdys, J.E. Ellis, P.D. Roberts, Augmented integrated system optimization and parameter estimation technique: derivation, optimality and convergence, *Proc. IEE* 134 (1987) 201–209.
- [27] H. Zhang, P.D. Roberts, On-line steady-state optimization of nonlinear constrained processes with slow dynamics, *Trans. Inst. Meas. Contr.* 12 (1990) 251–261.
- [28] J.H. Cheng, E. Zafriou, Robust model-based iterative feedback optimization of steady-state plant operations, *Ind. Eng. Chem. Res.* 39 (2000) 4215–4227.
- [29] J. Zhou, A. Tits, C. Lawrence, *User's Guide for FFSQ, Version 3.7.*, University of Maryland, 1997.
- [30] P.M. Duvall, J.B. Riggs, On-line optimization of the Tennessee Eastman challenge problem, *J. Process Control* 10 (2000) 19–33.
- [31] E. Sequeira, M. Graells, L. Puigjaner, Real-time evolution of online optimization of continuous processes, *Ind. Eng. Chem. Res.* 41 (2002) 1815–1825.
- [32] T. Jiang, B. Chen, X. He, P. Stuart, Application of steady-state detection method based on wavelet transform, *Comp. Chem. Eng.* 27 (2003) 569–578.
- [33] K. Basak, K.S. Abhilash, S. Ganguly, D.N. Saraf, On-line optimization of a crude distillation unit with constraints on product properties, *Ind. Eng. Chem. Res.* 41 (2002) 1557–1568.
- [34] J.S. Shamma, M. Athans, Gain scheduling: potential hazards and possible remedies, *IEEE Control Systems Magazine* 12 (3) (1992) 101–107.
- [35] D.A. Lawrence, W.J. Rugh, Gain scheduling dynamic linear controllers for a nonlinear plant, *Automatica* 31 (1995) 381–390.
- [36] A.M. Morshedi, C.R. Cutler, T.A. Skrovaneck, Optimal solution of dynamic matrix control with linear programming techniques, *Proc. Am. Control Conf.* 208 (1985).
- [37] C. Brosilow, G.Q. Zhao, A linear programming approach to constrained multivariable process control, *Contr. Dyn. Syst.* 27 (1988) 141.
- [38] C. Yousfi, R. Tournier, Steady-state optimization inside model predictive control, *Proc. Am. Control Conf.* 1866 (1991).
- [39] K.R. Muske, Steady-state target optimization in linear model predictive control, *Proc. Am. Control Conf.* 3597 (1997).
- [40] R.C. Sorensen, C.R. Cutler, LP integrates economics into dynamic matrix control, *Hydrocarbon Process.* 9 (1998) 57–65.
- [41] R. Nath, Z. Alzein, On-line dynamic optimization of olefins plants, *Comp. Chem. Eng.* 24 (2000) 533–538.
- [42] Ch. M. Jing, B. Joseph, Performance and stability analysis of LP-MPC and QP-MPC cascade control systems, *AIChE J.* 45 (7) (1999) 1521–1534.
- [43] A. Kassidas, J. Patry, T. Marlin, Integration of process and controller models for the design of self-optimizing control, *Comp. Chem. Eng.* 24 (2000) 2589–2602.
- [44] A.C. Zanin, M. Tvrzka de Gouvea, D. Odloak, Industrial implementation of a real-time optimization strategy for maximizing production of LPG in a FCC unit, *Comp. Chem. Eng.* 24 (2000) 525–531.
- [45] C.E.S. Costa, F.B. Freire, N.A. Correa, J.T. Freire, R.G. Correa, Two-layer real-time optimization of the drying of pastes in a spouted bed: experimental implementation, in: *16th IFAC World Congress, Prague, 2005, Paper Fr-M06-TO/6*.
- [46] S.J. Qin, T. Badgewell, A survey of industrial model predictive control technology, *Contr. Eng. Pract.* 11 (2003) 733–764.
- [47] B.A. Foss, T.S. Schei, Putting nonlinear model predictive control into use. *Preprints International Workshop on Assessment and Future Directions of NMPC, Freudenstadt, 255–262*.
- [48] R.D. Bartusiak, NMPC: a platform for optimal control of feed- or product-flexible manufacturing, *Preprints International Workshop on Assessment and Future Directions of NMPC, Freudenstadt, 2005, pp. 3–14*.
- [49] K. Naidoo, J. Guiver, P. Turner, M. Keenan, M. Harmse, Experiences with nonlinear MPC in polymer manufacturing,

- Preprints International Workshop on Assessment and Future Directions of NMPC, Freudenstadt, 2005, pp. 335–345.
- [50] A. Singh, J.F. Forbes, P.J. Vermeer, S.S. Woo, Model-based real-time optimization of automotive gasoline blending operations, *J. Process Control* 10 (2000) 43–58.
- [51] T.A. Johansen, D. Sbarbaro, Lyapunov-based optimizing control of nonlinear blending processes, *IEEE Trans. Control Syst. Technol.* 13 (4) (2005) 631–638.
- [52] J. Busch, M. Santos, J. Oldenburg, A. Cruse, W. Marquardt, A framework for the mixed integer dynamic optimization of waste water treatment plants using scenario-dependent optimal control, in: *Proceedings of ESCAPE 15*, Elsevier, 2005, pp. 955–960.
- [53] D. Broughton, C. Gerhold, Continuous sorption process employing fixed bed of sorbent and moving inlets and outlets, US Patent 2985586, 1961.
- [54] D.W. Guest, Evaluation of simulated moving bed chromatography for pharmaceutical process development, *J. Chromatogr. A* 760 (1997) 159–162.
- [55] M. Juza, M. Mazzotti, M. Morbidelli, Simulated moving-bed chromatography and its application to chirotechnology, *Trends Biotechnol.* 18 (2000) 108–118.
- [56] S. Engell, A. Toumi, Optimization and control of chromatography, *Comp. Chem. Eng.* 29 (2005) 1243–1252.
- [57] A. Toumi, S. Engell, Advanced control of simulated moving bed processes, in: H. Schmidt-Traub (Ed.), *Preparative Chromatography*, Wiley-WCH, Weinheim, 2005, pp. 401–416 (Chapter 9).
- [58] K.-U. Klatt, F. Hanisch, G. Dünnebier, S. Engell, Model-based optimization and control of chromatographic processes, *J. Process Control* 24 (2000) 1119–1126.
- [59] C. Wang, K.-U. Klatt, G. Dünnebier, S. Engell, F. Hanisch, Neural network-based identification of SMB chromatographic processes, *Contr. Eng. Pract.* 11 (2003) 949–959.
- [60] A. Toumi, S. Engell, Optimal operation and control of a reactive simulated moving bed process, *Preprints IFAC Symposium ADCHEM*, Hong Kong, 2004, pp. 243–248.
- [61] A. Toumi, S. Engell, Optimization-based control of a reactive simulated moving bed process for glucose isomerization, *Chem. Eng. Sci.* 59 (2004) 3777–3792.
- [62] A. Toumi, M. Diehl, S. Engell, H.G. Bock, J.P. Schlöder, Finite horizon optimizing of control advanced SMB chromatographic processes, in: *16th IFAC World Congress*, Fr-M06-TO/2, 2005.
- [63] O. Ludemann-Hombourger, R.M. Nicoud, The VARICOL process: a new multicolumn continuous separation process, *Separat. Sci. Technol.* 35 (2000) 1829–1862.
- [64] A. Toumi, S. Engell, O. Ludemann-Hombourger, R.M. Nicoud, M. Bailly, Optimization of simulated moving bed and Varicol processes, *J. Chromatogr. A* 1006 (1–2) (2003) 15–31.
- [65] M. Kearney, K. Hieb, Time variable simulated moving bed process, US Patent 5,102,553, 1992.
- [66] G. Erdem, S. Abel, M. Morari, M. Mazzotti, M. Morbidelli, Automatic control of simulated moving beds. Part I: Linear isotherms, *Ind. Eng. Chem. Res.* 43 (2004) 405–421.
- [67] G. Erdem, S. Abel, M. Morari, M. Mazzotti, M. Morbidelli, Automatic control of simulated moving beds. Part II: Nonlinear isotherms, *Ind. Eng. Chem. Res.* 43 (2004) 3895–3907.
- [68] S. Abel, G. Erdem, M. Amanullah, M. Morari, M. Mazzotti, M. Morbidelli, Optimizing control of simulated moving beds-experimental implementation, *J. Chromatogr. A* 1092 (1) (2005) 2–16.
- [69] S. Natarajan, J.H. Lee, Repetitive model predictive control applied to a simulated moving bed chromatography system, *Comp. Chem. Eng.* 24 (2000) 1127–1133.
- [70] T. Borren, J. Fricke, Chromatographic reactors, in: H. Schmidt-Traub (Ed.), *Preparative Chromatography*, Wiley-WCH, Weinheim, 2005, pp. 371–400 (Chapter 8).
- [71] T. Borren, J. Fricke, H. Schmidt-Traub, Reactive liquid chromatography, in: H. Schmidt-Traub, A. Gorak (Eds.), *Integrated Reaction and Separation Operations*, Springer, 2006 (Chapter 5).
- [72] K. Hashimoto, S. Adachi, H. Noujima, Y. Ueda, A new process combining adsorption and enzyme reaction for producing higher-fructose syrup, *J. Biotechnol. Bioeng.* 25 (1983) 2371–2393.
- [73] A. Küpper, S. Engell, Nonlinear model predictive control of the Hashimoto simulated moving bed process, in: *International Workshop on Assessment and Future Directions of NMPC*, Freudenstadt, 2005.
- [74] A. Küpper, A. Toumi, S. Engell, Optimization and control of reactive chromatographic processes, in: H. Schmidt-Traub, A. Gorak (Eds.), *Integrated Reaction and Separation Operations*, Springer, 2006, 2006 (Chapter 7).
- [75] G. Guiochon, S. Golshan-Shirazi, A. Katti, *Fundamentals of Preparative and Nonlinear Chromatography*, Academic Press, Boston, 1994.
- [76] T. Gu, *Mathematical Modelling and Scale Up of Liquid Chromatography*, Springer, New York, 1995.
- [77] M. Diehl, H.G. Bock, J.P. Schlöder, Z. Nagy, F. Allgöwer, Real-time optimization and nonlinear model predictive control of processes governed by differential-algebraic equations, *J. Proc. Contr.* 12 (2002) 577–585.
- [78] H.G. Bock, K.J. Plitt, A multiple shooting algorithm for direct solution of optimal control problems, in: *Proceedings of 9th IFAC World Congress*, Pergamon Press, Oxford, 1984, pp. 243–247.
- [79] A. Schäfer, P. Kühl, M. Diehl, J.P. Schlöder, H.G. Bock, Fast reduced multiple shooting methods for nonlinear model predictive control, *Chem. Eng. Process.*, submitted for publication.
- [80] M. Diehl, H.G. Bock, J.P. Schlöder, A real-time iteration scheme for nonlinear optimization in optimal feedback control, *SIAM J. Control Optim.* 43 (2005) 1714–1736.
- [81] L.T. Biegler, A.M. Cervantes, A. Wächter, Advances in simultaneous strategies for dynamic process optimization, *Chem. Eng. Sci.* 57 (2002) 575–593.
- [82] I.E. Grossmann, L.T. Biegler, Future perspective on optimization, *Comp. Chem. Eng.* 28 (2004) 1193–1218.
- [83] T. Jockenhövel, L.T. Biegler, A. Wächter, Dynamic optimization of the Tennessee Eastman process using the OptControlCentre, *Comp. Chem. Eng.* 27 (2003) 1513–1531.
- [84] J.H. Lee, Modeling and identification in nonlinear model predictive control, in: F. Allgöwer, A. Zheng (Eds.), *Nonlinear Model Predictive Control*, Birkhäuser, 2000, pp. 269–293.
- [85] W. Marquardt, Nonlinear model reduction for optimization based control of transient chemical processes, in: J.B. Rawlings, B.A. Ogunnaike, J.W. Eaton (Eds.), *Proceedings of the 6th International Conference of Chemical Process Control*, AIChE Symposium Series 326, vol. 98, 2002, pp. 12–42.
- [86] A. Draeger, S. Engell, Nonlinear model predictive control using neural net plant models, in: R. Berber (Ed.), *Methods of Model Based Process Control*, Kluwer Academic Publishers, 1995, pp. 627–639.
- [87] B.A. Foss, T.A. Johansen, A.V. Sørensen, Nonlinear predictive control using local models – applied to a batch process, *Control Eng. Practice* 3 (1995) 389–396.
- [88] E.F. Camacho, C. Bordons, Nonlinear model predictive control: an introductory survey, *Preprints International Workshop on Assessment and Future Directions of NMPC*, Freudenstadt, 2005, pp. 15–30.
- [89] H. Chen, F. Allgöwer, A quasi-infinite horizon nonlinear model predictive control scheme with guaranteed stability, *Automatica* 14 (1998) 1205–1217.
- [90] D.Q. Mayne, J.B. Rawlings, C.V. Rao, P.O.M. Scokaert, Constrained model predictive control: stability and optimality, *Automatica* 36 (2000) 789–814.
- [91] R. Roman, Z.K. Nagy, F. Allgöwer, S.P. Agachi, Dynamic modeling and nonlinear model predictive control of a fluid catalytic cracking unit, in: *Proceedings of ESCAPE 15*, Elsevier, 2005, pp. 1363–1368.
- [92] S.-S. Jang, B. Joseph, H. Mukai, Comparison of two approaches to online parameter and state estimation of nonlinear systems, *Ind. Eng. Chem. Proc. Des. Develop.* 25 (1986) 809–814.

- [93] K.R. Muske, J.B. Rawlings, Nonlinear moving horizon state estimation, in: R. Berber (Ed.), *Methods of Model Based Process Control*, Kluwer Academic Publishers, 1995, pp. 349–365.
- [94] C.V. Rao, J.B. Rawlings, D.Q. Mayne, Constrained state estimation for nonlinear discrete-time systems, *IEEE Trans. AC* 48 (2003) 246–258.
- [95] M. Diehl, P. Kühn, H.G. Bock, J.P. Schlöder, B. Mahn, J. Kallrath, Combined nonlinear model predictive control and moving horizon estimation for a copolymerization process, in: *Proc. ESCAPE 16/PSE 2006, Computer-Aided Chemical Engineering*, vol. 21B, Elsevier, 2006, pp. 1527–1532.
- [96] R. Gesthuisen, K.-U. Klatt, S. Engell, Optimization-based state estimation – a comparative study for the batch polycondensation of PET, in: *Proceedings of ECC 2001 Porto*, 2001, pp. 1062–1067.
- [97] P. Tatjewski, Iterative optimizing set-point control – the basic principle redesigned, in: *15th IFAC World Congress, Barcelona*, 2002, Paper T-Th-E16-3.
- [98] W. Gao, S. Engell, Iterative set-point optimisation of batch chromatography, *Comp. Chem. Eng.* 29 (2005) 1401–1410.
- [99] B. Srinivasan, D. Bonvin, E. Visser, S. Palanki, Dynamic optimization of batch processes II. Role of measurements in handling uncertainty, *Comp. Chem. Eng.* 27 (2002) 27–44.
- [100] C. Chatzidoukas, C. Kiparissides, B. Srinivasan, D. Bonvin, Optimisation of grade transitions in an industrial gas-phase olefin polymerization fluidized bed reactor via NCO tracking, in: *16th IFAC World Congress, Prague, 2005*, Paper Mo-A06-TO/2.
- [101] J.V. Kadam, M. Schlegel, B. Srinivasan, D. Bonvin, W. Marquardt, Dynamic real-time optimization: from off-line numerical solution to measurement-based implementation. in: *16th IFAC World Congress, Prague, 2005*, Paper Fr-M06-TO/1.
- [102] A. Küpper, S. Engell, Optimizing control of the Hashimoto SMB process: experimental application, in: *IFAC Symposium DYCOPS 2007*, submitted for publication.