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FEEDBACK CONTROL FOR OPTIMAL PROCESS OPERATION

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Abstract: Starting from the statement that the purpose of process control is to achieve optimal process operations and that optimal tracking of setpoints is in most cases only a means to this end, 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 on a finite horizon where the usual control specifications in terms of e.g. product purities enter as constraints and not as setpoints. 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.

Keywords: Process control, online optimization, predictive control, optimizing control, real-time optimization, finite horizon optimization, chromatography.

1. INTRODUCTION

From a process engineering point of view, the purpose of automatic feedback control (and that of manual control) is *not* primarily to keep some variables at their setpoints as well as possible or to nicely track setpoint changes but to operate the plant such that the net return is maximized in the presence of disturbances and while the model used for plant design does not represent the real process exactly so that an operating regime that was optimized for the plant model will not lead to an optimal operation of the real plant, exploiting the available measurements. This has been pointed out in a number of papers (e. g. Morari, et al., 1980, Narraway, et al., 1991, Narraway and Perkins, 1993, Zheng, et al., 1999, Skogestad, 2000) 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 setpoints or setpoint trajectories while assuring closed-loop stability. In chemical process control, however, good tracking of setpoints is mostly of interest for lower level control tasks. This is one reason why managers and process engineers often consider the choice and the tuning of controllers as a subordinate task, comparable to the procurement and maintenance of pumps or valves for a predefined purpose.

In their plenary lecture at ADCHEM 2000, Backx, Bosgra and Marquardt (2000) stressed the need for dynamic operations in the process industries in a increasingly marked-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 experience 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 1-layer approach (Zanin, et al., 2002) or full optimizing control (Rolandi and Romagnoli, 2005)).

First the idea to implement the optimal plant operation by conventional feedback control, termed "self-optimizing control", is discussed in Section 2. In highly automated plants, the goal of economically optimal operation is usually addressed by a two-layer structure (Marlin and Hrymak, 1997). 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 then characterized by setpoints for a set of controlled variables that are passed to lower-level controllers that keep the chosen variables as close to their setpoints as possible by manipulating the available degrees of freedom of the process within certain bounds. The two-layer structure has certain drawbacks. As the optimization is only performed intermittently, the adaptation of the operating conditions is slow. The manipulated variables cannot be kept at their constraints if they are used to reduce the variations of the controlled variables, thus the operating point cannot be at the constraints but some margin must be reserved for the feedback control layer. Thirdly, different models are used leading to inconsistencies. 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 numerical simulation and optimization algorithm 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 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 (2000) was outlined already in Morari, et al. (1980): 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. explicitly 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. Skogestad formulated the goal somewhat more modestly: to select the regulatory control structure of a process such that if the selected controlled variables are driven to suitably chosen setpoints, steady-state optimality of process operations is realized to the maximum extent possible. The selection is done with respect to the stationary process performance only, 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 setpoints 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 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 $\underline{d}$ $\underline{u}_{con}=f(\underline{y}_{set},\underline{d}_i)$ which is (implicitly) realized by regulating the chosen variables to their setpoints should be an approximation of the optimal input $\underline{u}_{opt}(\underline{d}_i)$. The application of this idea to the selection of control structures has been demonstrated in a number of application papers (Larsson, et al., 2001, 2003, Scharf and Engell, 2005).

The effect of feedback control on the profit function J in the presence of disturbances can be expressed as (Scharf and Engell, 2005)

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

The first term is the loss 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 than the second one, or if all terms are comparatively small, then a variation of the manipulated variables offers no advantage, and neither optimization nor feedback control are 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 setpoints should be performed rather than just regulation of the chosen variables to fixed pre-computed setpoints.

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

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

where $w(\underline{d})$ is the probability of the occurrence of the disturbance $\underline{d}$, 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 $\underline{u}_{con}$ may differ considerably from the desired values. This was discussed in a qualitative fashion by checking the sensitivity of the profit with respect to the controlled variables in (Skogestad, 2000). 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 $\underline{y}_{set}$ which is defined by the measurement errors (Scharf and Engell, 2005). For a disturbance scenario $\underline{d}_i$, the performance measure of a control structure is:

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

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 happen for small disturbances, as illustrated by Fig. 1 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. 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.

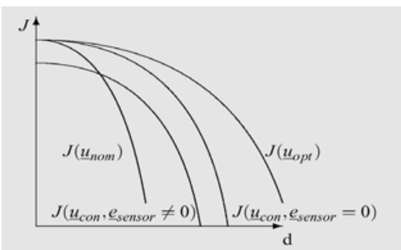

Figure 1: Schematic representation of the influence of a disturbance on the profit for different control approaches in the presence of measurement errors

Application studies have shown that the profit loss that is obtained by using regulation instead of steady-state optimization can be quite low for suitably chosen control structures. E.g., in (Larsson, et al., 2001) a performance loss of less than 5% is reported for the Tennessee Eastman benchmark problem (Downs and Vogel, 1993). The above analysis and subsequent control structure selection so far are limited to disturbances or variations of the plant behavior that persist over a very large horizon compared to the plant dynamics. The inclusion of disturbances with a higher bandwidth is an open issue.

3. REAL-TIME OPTIMIZATION (RTO)

The established approach to create a link between regulatory control and optimization of the economics of the unit or the plant under control is *real-time optimization* (RTO) (see e. g. Marlin and Hrymak, 1997, and the references therein). An RTO system is a model-based, upper-level control system operated in closed-loop that provides setpoints 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 Figure 2. Its hierarchical structure follows the ideas put forward already in the 1970's (Findeisen, et al., 1980).

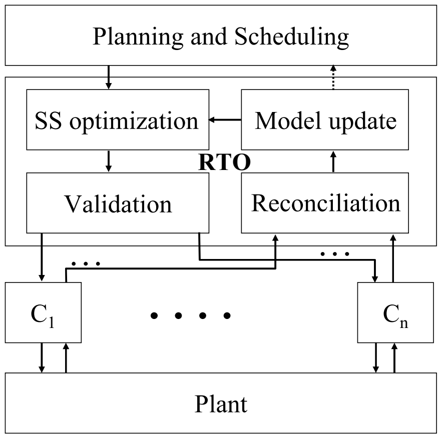

Figure 2: Elements of real-time optimization (RTO)

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 that optimize an economic cost function while meeting the technical constraints of the process and the economic constraints imposed by the plant management system. These values are then filtered by a supervisory system (which often includes the plant operators) (e. g. checked for plausibility, mapped to ramp changes, clipped to avoid large changes) (Miletic and Marlin, 1996) 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). The implementation of the optimal steady states by linear model predictive controllers was discussed in detail in (Rao and Rawlings, 1999).

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 to 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 to handle different speeds of response and to structure the system into smaller modules. This separation of concerns from a management point of view may be misunderstood that the process control layer is a necessary piece of equipment to run the process but the RTO system and the plant management system help to earn money. Consequently, the control system is just a part of the cost and any "luxury" on this layer should be avoided.

In (Forbes and Marlin, 1996, Zhang and Forbes, 2000), 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 setpoints 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 setpoints.

The last factor advocates a filtering of the changes before they are applied to the real plant to avoid inefficient moves (Miletic and Marlin, 1998, Zhang et al., 2001). The issue of model fidelity was discussed in detail in (Zhang and Forbes, 2000, Yip and Marlin, 2004). 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 the absolute value is not critical (Forbes, et al., 1994, Forbes and Marlin, 1995). 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 (2003) made the very interesting proposal to include the effect of set-point changes on the accuracy of the parameter estimates into the RTO optimization. Nonetheless, plant-model mismatch will always be an important issue. Cheng and Zafiriou (2000) proposed a modification of an SQP optimization algorithm (Zhou, et al., 1997) for steady-state optimization on the RTO layer such that the available measurement information is taken into account when the search direction and the step size are computed. In this fashion, 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 (Forbes, et al., 1994). Their algorithm avoids the need to determine gradients of the cost function and of the constraints by perturbations of the input to the real plant (and hence long periods of sub-optimal operation) as required by the algorithms proposed by Roberts and co-workers (Roberts 1979, Brdys, et al., 1987, Zhang and Roberts, 1990).

Duvall and Riggs (2000) 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 setpoint selection affects the production rate and/or operating costs*". In particular, they argue that the operators would most likely know which variables should be kept at their bounds but will not be able to optimize setpoints within their admitted ranges according to the disturbances encountered. This practically results in the same comparison as assuming that a "self-optimizing" regulatory control scheme according to Skogestad (2000) is used on the lower level.

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 is not very high. The control algorithms are based upon linear models (or no models at all if conventional controllers are tuned on-site) which can be determined from plant data. As pointed out by e. g. (Backx, et al., 2000), (Sequeira et al., 2002) 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 will 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. Jiang, et al., 2003).

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 setpoints 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 setpoints. 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 setpoints 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, 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 setpoints) and an online-optimizing controller that implements the optimal setpoints 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 (1997) listed several areas for improvement of RTO systems. Two important ones are addressed in the remainder of this paper: the integration with the process control layer, and the extension to unsteady-state 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 of RTO to work with rather long sampling periods, several authors have proposed schemes that work with smaller sampling times on the optimizing layer. E.g., Sequeira et al. (2002) propose to change the set-points for the regulatory layer in much shorter intervals (in the case study presented 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 convincing, however the approach suffers from neglecting the dynamic aspects. This concerns two aspects: the interaction of the set-point change with the regulatory control layer and the assumption that a steady-state optimization performed at an instationary operating point yields the right move of the set-points. In the same line of thinking, Basak, et al. (2002) discussed an on-line 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 hours 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.

The fast sampling approach is similar to gain scheduling control because 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. It shares the potential of stability problems with gain scheduling controllers that usually can only be avoided if "slow", quasi-stationary set-point changes are realized (Shamma and Athans, 1992, Lawrence and Rugh, 1995).

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

The so-called LP-MPC and QP-MPC two-stage MPC structures that are frequently used in industry to narrow the gap between the low-frequency nonlinear steady-state optimization performed on the RTO layer and the relatively fast MPC layer (Morshedi, et al., 1985, Brosilow and Zhao, 1988, Yousfi and Tournier, 1991, Muske, 1997, Sorensen and Cutler, 1998, Nath and Alzein, 2000) were analyzed by Ying and Joseph (1999). The task of the upper MPC layer is to compute the setpoints (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 (see Fig. 3). This structure addresses the following issues:

- A faster change of the setpoints after the occurrence of disturbances is realized;
- 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 infrequent setpoint 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.

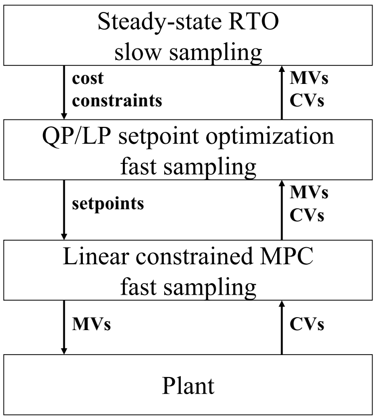

Figure 3: Two-layer MPC with setpoint optimization

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 DMC or QDMC controller that determine the steady-state behavior of the controller (setpoints of the regulated variables, targets of the manipulated variables, weights on the deviations of the regulated variables from the setpoints 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., 2000). In the parameter optimization, a full nonlinear steady-state plant model is used. Note that this optimization is only performed once (off-line), whereas 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 setpoints and to a controller that controls the plant to fixed pre-computed purity setpoints (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 setpoints, 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. (2000, 2002) reported the formulation, solution and industrial implementation of a combined MPC/optimizing control scheme for an FCC unit. The plant has 7 manipulated inputs and 6 controlled variables. The economic cost used 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. The economic objective value is computed using a nonlinear steady-state process model. As only the first move of the controller is implemented, a penalty term is added that penalizes the deviation of the first values of the manipulated variables from their final values within the control horizon. Several variants for this penalty term are investigated. The different components of the cost function are weighted such that the economic criterion and the MPC part have a similar influence on the values of the overall cost.

This combined optimizing/MPC controller was implemented and tested at a real plant with a sampling rate of 1 minute, a control horizon of 2 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 setpoints 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 setpoints for a linear MPC scheme in terms of dynamic response. A similar control scheme was experimentally validated in (Costa, et al., 2005).

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 are reported in particular in polymerization processes (Qin and Badgewell, 2003, Bartusiak, 2005, Naidoo, et al., 2005). 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 setpoints that implies a safety margin between these setpoints 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 setpoints 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 inevitably 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 largely reduces the need for tuning of the weights in less explicit formulations. In contrast, Exxon's technology for NMPC employs a combination of criteria that represent reference tracking, operating cost and control moves (Bartusiak, 2005).

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., 2000) and Johansen and Sbarbaro (2005) for blending processes and by (Busch, et al., 2005) for a waste-water treatment plant.

5.2 Case Study: Control of reactive simulated moving bed chromatographic processes

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 the 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 the batch mode, the adsorbent is not used efficiently and it 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 (Broughton 1961). It is gaining increasing attention in industry due to its advantages in terms of productivity and solvent consumption (Guest 1997, Juza, et al. 2000). 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 outlet lines by one column in the direction of the liquid flow (see Fig. 4).

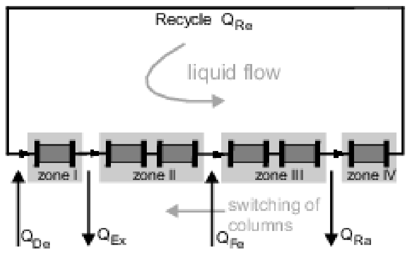

Figure 4: Simulated Moving Bed principle

After a startup phase, SMB processes reach a 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 columns plotted for different time instants within a switching period.

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 (Engell and Toumi 2005, Toumi and Engell, 2005).

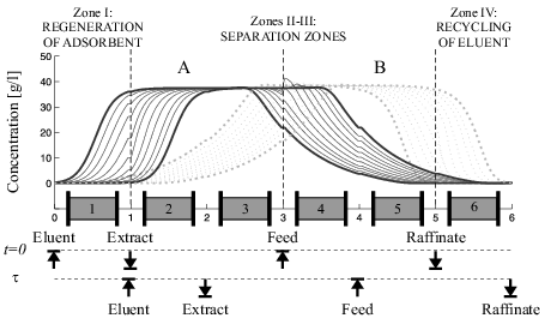

Figure 5: Concentration profiles of an SMB process

Klatt, et al. (2002) 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 optimisation based on a rigorous process model. The model parameters are adapted based on online measurements. The low-level control task is to keep the process near the optimal cyclic steady state despite disturbances, plant degradation and plant/model mismatch by controlling the front positions. 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 (Klatt, et al., 2002, Wang, et al., 2003). 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. Thus an additional purity controller is required, and the overall scheme becomes quite complex without actually ensuring optimality.

Online optimizing control. As the progress in efficient numerical simulation and optimization enabled a dynamic optimization of the process within one switching period, Toumi and Engell (2004a) proposed a direct finite horizon optimizing control scheme that employs the same rigorous nonlinear process model that is used for process optimization and applied it to a 3-zones reactive SMB process for glucose isomerisation (Toumi and Engell 2004a,b) The key feature of this approach is that the production cost is minimised on-line over a finite horizon while the product purities are considered as constraints, thus a real online optimisation of all operational degrees of freedom is performed, and there is no tracking of any precomputed setpoints or reference trajectories. In (Toumi, et al. 2005), this control concept was extended to the more complex processes VARI*COL* (Ludemann-Homburger, et al., 2000 Toumi, et al., 2003) and PowerFeed (Kearney and Hieb 1992) 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 of Toumi, et al. (2004a,b), 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., 2004a, Erdem, et al., 2004b, Abel, et al., 2005). 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 (Natarajan and Lee, 2000) the switching period is kept fixed although it has a considerable influence on the process performance.

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, 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, this 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 (Borren and Fricke, 2005). However, for reactions of the type A <=> B, a uniform catalyst distribution in the SMBR promotes the backward reaction near the product outlet which is detrimental to the productivity, further, 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 (Hashimoto, et al., 1983) 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 separately and the reactors can constantly be placed in 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.

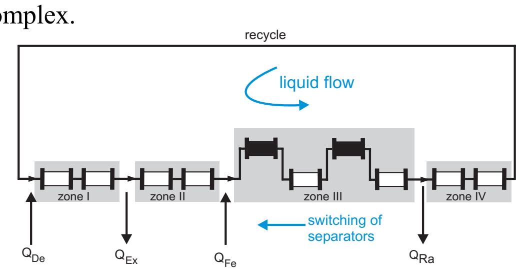

Figure 6: Four-zones Hashimoto SMB process

Optimizing controller application. The example process considered in (Küpper and Engell, 2005) is the racemization of *Tröger's Base (TB)* in combination with chromatographic separation for the production of *TB-* that is used for the treatment of cardiovascular diseases. 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 Tröger's Base system is described by an adsorption isotherm that is of multi component Langmuir type:

$$q_i = \frac{H_i c_{p,i}}{1 + \sum_k b_{i,k} c_{p,k}} \text{, k = +, - .} \tag{4}$$

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-zones Hashimoto process with 8 chromatographic columns, 2 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_D for a constant feed flow and a given purity requirement of 99% 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 averaged over the prediction horizon leaves the plant in the extract product stream, an additional productivity requirement was added. The resulting mathematical formulation of the optimization problem is:

$$\min_{\beta_I, \beta_{II}, \beta_{III}, \beta_{IV}} \sum_{i=1}^{H_P} Q_i + \Delta\beta \, R \, \Delta\beta$$

$$s.t. \quad \begin{cases} \tilde{x}_{smb}^{k} = x_{smb}^{k} + \int_{t=0}^{\tau} f_{smb}(x_{smb}(t, u_{smb}(t), p))dt \\ x_{smb}^{k+1} = P\tilde{x}_{smb}^{k}, \end{cases}$$

$$\frac{\sum_i^{H_{P1}} Pur_{Ex,i}}{H_{P1}} \geq (Pur_{Ex,\min} - \Delta Pur_{Ex}) \tag{5}$$

$$\frac{\sum_i^{H_{P1}} m_{Ex,i}}{H_{P1}} \geq 0.7 m_{Fe} - \Delta m_{Ex}$$

$$Q_I \leq Q_{\max}$$

$$Q_{De}, Q_{Ex}, Q_{Fe}, Q_{\mathrm{Re}} \geq 0,$$

where the purity error and the mass error are calculated according to

$$\begin{aligned} \Delta Pur_{Ex} &= Pur_{Ex,plant,i-1} - Pur_{Ex,\mathrm{model},i-1}, \\ \Delta m_{Ex} &= m_{Ex,plant,i-1} - m_{Ex,\mathrm{model},i-1}. \end{aligned} \tag{6}$$

The model of the plant consists of rigorous dynamic models of the individual columns of the plant, the node equations and the port switching. The chromatographic columns are described accurately by the general rate model (Guichon, et al., 1994) 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 pdes are discretized using a Galerkin approach on finite elements for the bulk phase and orthogonal collocation for the particle phase (Gu, 1995). The reactors consist of 3 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 FFSQP (Zhou, et al., 1997) 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 8 because the optimizer performs this number of iterations within one cycle of the process (8 switching periods), as required for online control.

In the simulation scenario, an exponential decrease of the catalyst activity was assumed that occurs in the case of a disturbance in the heating system. A model/plant mismatch was introduced by disturbing the initial Henry coefficients H_A and H_B of the model by +10% and -15%. The parameters of the controller are displayed in Table 1.

Table 1: Controller parameters

Sampling time		8 periods = 1 cycle
Prediction horizon	H_P	6 cycles
Control horizon	H_C	1 cycle
Regularization	R	[0.3 0.3 0.3 0.3]
Controller start		72^{nd} period
Estimator start		72^{nd} period

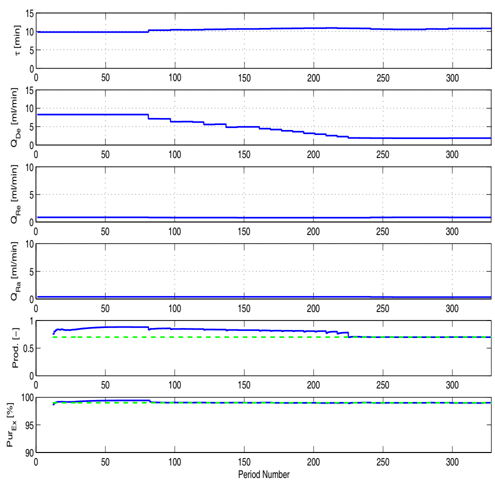

Figure 7: Simulation of the optimizing controller of the Hashimoto reactive SMB process

The performance of the controller is illustrated by Fig. 7. The controller manages to keep the purity and the productivity above their lower limits, while it improves the economical operation of the plant by reducing the solvent consumption. As reported in (Toumi and Engell, 2004a,b) the optimizing controller has been implemented at a medium scale commercial SMB plant using a PLC-based process control system and an additional PC for optimization and parameter estimation.

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 was used. By using more advanced numerical techniques, much shorter computation times can be realized. Diehl, et al. (2002) proposed a scheme for the solution of nonlinear model-predictive control problems with large plant models where the multiple shooting method (Bock and Plitt, 1984) 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 became 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 (Schäfer, et al., 2006). 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. (2005) 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 were similar progress has been reported (e. g. Biegler, et al., 2002, Grossmann and Biegler, 2004). Jockenhövel, et. al. (2003) 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 long prediction horizons.

6. OPEN ISSUES

Modeling. In a direct optimizing control approach accurate dynamic nonlinear process models are needed. While nonlinear steady-state models are nowadays available for control purposes for many processes because they are 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 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 effect the behavior only on time scales much longer than the prediction horizon or shorter than the sampling time of the controller. However, the appropriate simplification of nonlinear models still is an unresolved problem (Lee, 2000, Marquardt, 2002). The alternative to use black-box or grey-box models as proposed frequently in nonlinear model-predictive control (e.g. Draeger and Engell, 1995, Wang, et al., 2003, Camacho and Bordons, 2005) does not seem appropriate for optimizing control with performance requirements formulated as constraints.

Stability. Optimization of a cost function over a finite horizon in general neither assures optimality of the complete trajectory nor stability of the closed-loop system. Closed-loop stability has been addressed extensively in the theoretical research in nonlinear model-predictive control. There is a pronounced difference in the attention that practitioners and researchers pay to this issue – practitioners will usually tend to say that if suffices to choose sufficiently long prediction and control horizons which, for stable plants, will work indeed. Nonetheless, the theoretical discussion has led to a clear understanding of what is required to ascertain 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 stage cost 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 (Chen and Allgöwer, 1998, Mayne, et al, 2000). If the stage cost is an economic cost function, bounded cost will in general not ensure boundedness of the difference of the states to the equilibrium state because economic cost functions often involve only few process variables, mostly inputs and mass flows leaving the physical system. Moreover, there is no fixed equilibrium state.

An optimizing control algorithm with guaranteed stability in principle can be designed if in addition to the direct optimizing controller a steady-state optimization is performed to determine the desired terminal state. Then 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 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 will 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 (Nagy, et al., 2005). The constraint on the terminal state has to be computed for each update of the optimal terminal state what is computationally demanding but should be feasible on the steady-state optimization layer. By the choice of the weighting terms, a compromise 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 can be established. 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 goals as well as the models used are consistent in this structure.

An alternative approach to guaranteeing stability of an optimizing controller is applied in (Johansen and Sbarbaro, 2005) to a linear process with a static nonlinearity at the output, based on an augmented control Lyapunov function.

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 (Jang, et al., 1986, Muske and Rawlings, 1994, Rao, et al., 2000). Parameter estimation can be included in this formulation. Experience with the application of moving horizon state estimation however still is quite limited to date. Simpler and computationally less demanding schemes as the constrained extended Kalman filter (CEKF) may provide a comparable performance (Gesthuisen, et al., 2001). 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.

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 and 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 (Roberts 1979, Brdys, et al., 1987). As shown by Tatjewski (2002), optimality can be achieved without parameter update and for structural plant-model mismatch 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 (Gao and Engell, 2005) and should be explored in the continuous case as well. An alternative to implement measurement-based optimization is to formulate the optimization problem (partly) as the tracking of necessary conditions which are robust against model mismatch (Srinivasan, et al., 2002, Chatzidoukas, et al., 2005, Kadam, et al., 2005).

Reliability and transparency. As discussed above, relatively large nonlinear dynamic optimization problems can be solved in real-time nowadays, so this issue does not prohibit the application of a direct optimizing control scheme to complex units. A practically very important 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 setpoints by the operators may be feasible, they can hardly act as filters in direct optimizing control of complex units. 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 should 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 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 reactions and enable comparisons with their intuitive strategies are believed to be essential for practical success.

Effort vs. performance. Of course, the complexity of the control scheme has to be traded against the gain in performance. 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 appropriate. In a more dynamic situation or for complex nonlinear multivariable plants, the direct optimizing control idea should be explored. As for an 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.

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