Model Requirements for Next Generation Integrated MPC and Dynamic Optimization

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Abstract

This paper outlines the requirements imposed upon models and modeling techniques applied for high performance model based control systems and model based optimizers for support of the operation of (chemical) processes. An overview is given of on-going developments in the area of integrated high performance model predictive control and model based dynamic optimization (INCOOP and IMPACT projects). To enable tight control of processes at given Cpk values and within imposed 6-sigma intervals on a variety of process variables, the models applied for control and for optimization have to be sufficiently accurate both as a function of frequency as well as a function of the time varying operating conditions. Requirements on the models are summarized. Modeling of relevant process behavior for control and optimization is a very significant cost factor in overall application development. Reduction of these costs by extensive use of a-priori knowledge and by integration of various modeling techniques is discussed.

Keywords

Model-based control, Dynamic optimization, Process modeling

Introduction

Industrial processes are subject to continuous improvement of performance with respect to yield, quality, flexibility and innovation. Market developments, legislation, social and environmental requirements have started to create a need for continuously better predictability of process performance and more flexible operation of the processes over the past two decades (García and Prett, 1986; Prett and Garcìa, 1988; Morari, 1988; Backx et al., 1998, 2000). Chemical Processing Industries are currently facing an enormous challenge: Within the next years they have to realize a turnaround in their financial performance to remain attractive for capital investors.

Gradual decline of the productivity of invested capital over the past three decades has become a major point of concern of the chemical processing industries. The financial performance of many companies belonging to the Chemical Processing Industries is lagging economic developments of the market, which makes it hard to compete with industries that do better than average like for example the Information and Communication Technology oriented industries.

The relatively poor performance of the Chemical Processing Industries may be explained from the hesitation of industry to adapt to and anticipate fast changes in the market. Fast developments of new markets, stimulated by rapidly adopted microelectronic and information technology developments, have created a complete turnaround of the market. The market has turned from a regional, mainly supply driven market into a worldwide, demand driven market over the past 15 years. Many of the processing industries and the Chemical Processing Industries in particular did not yet follow this turnaround and are still mainly organized to predominantly produce in a supply driven way. Latest developments of computing, modeling and control technologies of the past decade offer a great opportunity however to quickly realize the changes from the technical side. Organizational adaptations have to be made accordingly though.

Wide application of model based control and optimization technology in chemical process industries is hampered until now by the following limitations of current state-of-the-art technologies:

- Costs of application development are (too) high in relation to direct return on the investments that have to be made for the development of these applications
- Most of the currently applied MPC technologies in industry are based on the use of process models for prediction and control that approximate process dynamics in a linear, time invariant way. Chemical plants are often producing a mix of products with different specifications, which involves transitions between different operating points with corresponding different process dynamics in each of these operating points related to the non-linearities in process behavior
- Performance of state-of-the art MPC technologies in terms of their capabilities to reduce variances of critical process variables and product parameters is restricted by limitations in the models applied for prediction and for control to cover the whole frequency range at which the process is operated. This limitation stems from the techniques and procedures applied for process testing, process identification and model validation
- Extensive (re-)use of available information and knowledge on dynamic process behavior is one of the ways to significantly reduce costs of application

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development related to process testing and the engineering effort involved. State-of-the-art technologies hardly support this.
- Currently applied techniques for (closed loop) model based optimization of plant performance use first principles based steady state models. Consistency of these models with the models obtained from process identification and applied inside the model predictive control systems is not guaranteed. As a consequence the performance of the systems is restricted to satisfy robustness requirements over the applicable operating envelope.
- Currently applied techniques for (closed loop) model based optimization of plant performance are limited to steady state only, which implies that they don't support transitions between various operating points and adequate response to plant upsets.

This paper discusses developments that overcome the obstacles summarized above. These developments are done in the context of two development projects: IMPACT and INCOOP. The IMPACT project (Eureka project with label 2063) has the objective of developing dedicated model based control and transition optimization techniques for various types of PE/PP polymer manufacturing processes. The INCOOP project (EC funded 5th framework) focuses on the integration of non-linear high performance model based control and dynamic plant optimization.

Section 2 of the paper first outlines requirements imposed upon process operation in accordance with market requirements. In section 3 these requirements on process operation are translated to requirements on the models that are applied for control and optimization. Section 4 focuses on the dynamic operation of plants and the additional impact on models applied for the support of such operation. Section 5 discusses model requirements and modeling approaches for high performance model based process control. Section 6 shows some preliminary results on a PE polymer manufacturing process. Final remarks and conclusions are given in section 7

Requirements on Process Operations

The main requirement on process operation is: To produce products that meet specifications in the requested volume at the right time and at minimum cost in accordance with an imposed schedule respecting operational and legal permit constraints. The optimization of process performance involves fulfilling these requirements the best possible way. Realization of the requirements implies that the optimization has both to exploit the technical capabilities of the process and to use freedom in process operation to achieve economic optimization without taking too much risk on unplanned process shutdowns. As a consequence the optimization has to blend the functionality of current generation economic optimizers, which generally do not consider process dynamics with state-of-the-art technology from the field of dynamic optimization, which, however, usually does not concentrate on economic problems, but rather on control-oriented problems. A dynamic 'Money Conservation Law' is developed to integrate both worlds. The objective function V is written as a sum of profit made along a trajectory and a capital inventory term (Van der Schot, 1998):

$$\max V = \max \int_{t_0}^{t_f} EUR_{revenues}(t) - EUR_{expenses}(t)\,dt + EUR_{inventory}\Big|_{t_0}^{t_f} \quad (1)$$

This trajectory gives the recipe for an optimal transition between operating conditions or for the optimum path to recover from encountered disturbances in a certain operating point. It comes down to maximizing the added value of the process over a fixed time horizon $[t_0, t_f]$. In this, we define the Euro flows (€ /hr) as the product of physical flows (kg/hr) and product prices (€ /kg). These prices will depend on product quality and on market conditions. The product quality is governed by process operation and can be simulated by a rigorous dynamic model of the (chemical) process. This model can be included in the overall optimization as a set of equality constraints.

The functions $\Phi(x(t), u(t))$ and $\Psi(x(t_f), u(t_f))$, that link process manipulations $u(t)$ and process states $x(t)$ to performance measures in the applied criterion function (cf. Equation 2) related to this optimization problem, essentially consist of two separate components:
- a smooth non-linear part related to the process transfer characteristics obtained from the DAE model described by the equality constraints in Equation 2. This model connects manipulated variables and disturbances to process outputs,
- a highly non-linear part that connects product properties to market values of these products.

$$\max_{u(t)} \quad V = \int_0^{t_f} \Phi(x(t), u(t))\,dt + \Psi(x(t_f), u(t_f)) \quad (2)$$

subject to

$$0 = f(\dot{x}(t), x(t), u(t))$$
$$0 \le c(x(t), u(t))$$

The first component—the one that describes the process transfer characteristics—has a high complexity due to the process mechanisms involved. The second part has limited complexity but involves discontinuous functions, which are very nasty from an optimization viewpoint. This is due to the fact that products within high quality specifications have a high, market determined fixed value. Products that meet looser specifications generally have a lower, also market determined, fixed value. Off-spec products have an even lower value that even may be negative (cf. Van der Schot et al., 1999). The market values of products relate to specified ranges for a selected group of product properties. Products with properties in the specified intervals all have the same value. The product value changes as soon as one or more of the product properties exceed the specified tolerances for these parameters.

Operation of the process is subject to operating constraints on process inputs, process outputs and/or rates of change of these variables. Both performance and robustness of the control systems directly relate to the quality and accuracy of the models used as prediction models in the control systems. The problem to be solved in order to enable process operation as outlined, is to get models that satisfy the following conditions (cf. De Moor and Berckmans, 1996; Jacobsen et al., 1991; Johansen and Foss, 1995; Johansen, 1996; Kemna and Mellichamp, 1995; Lindskog and Ljung, 1995; Ljung et al., 1991; Rivera and Gaikwad, 1995; Skogestad et al., 1991; Tsen and Wong, 1995; Tulleken, 1993; Wei and Lee, 1996):

- describe all process dynamics that are relevant for model predictive control and dynamic optimization of the process in accordance with given specifications
- cover the full operating envelope of the process consisting of specified operating points and transition trajectories between these operating points covered by process optimization

Model Requirements

In order to get sets of models that accurately reflect all control relevant dynamics of the process in all selected operating points of a real plant, extensive plant tests are required, if traditional model predictive control (MPC) system design methodologies are applied. Traditional MPC design techniques based upon the application of system identification techniques require testing of the process in each operating point. The tests involve persistent excitation of all relevant process dynamics with sufficient energy and during a sufficiently long time to ensure good identification results (Ljung, 1987; Ljung and Söderström, 1983). The duration of a plant test is governed by the time to steady state (T_{ss}) of the unit that is tested, by the number of process inputs that have to be tested (N_{inp}) and by the type of test signals applied. A system identification related plant test typically takes a time T_{test} in the range given by (3) for each operating point that needs to be tested, if model quality has to be ensured.

$$3 \cdot Int(\frac{N_{inp}}{5} + 1) \cdot T_{ss} \leq T_{test} \leq 5 \cdot N_{inp} \cdot T_{ss} \qquad (3)$$

The type of test signals applied governs the actual required time for plant testing. The effort involved in plant testing makes application of this approach to processes operated in a broad range of operating points, or to processes operated in specific operating points for a relatively short time compared to the dynamic response times of the process, economically or even technically unfeasible. Many of the slow dynamics, which to a large extent are related to physical phenomena like e.g. material transport, residence times, warming up and cooling down of huge heat capacities with restricted energy flows, etc. can be modeled quite accurately using first principles based modeling techniques. Often these dynamics also don't vary much even under operating condition changes. Relative fast dynamics related to local physical, chemical, biological phenomena frequently are hard to be modeled accurately using first principles modeling techniques. Examples of such hard to model phenomena are for example flows through complex piping systems, turbulent flows around a valve, inhomogenity in mixtures in reactor tanks, specific reaction complexes (e.g. polymerization, cracking, ...), kinetics in complex chemical reaction systems, metabolisms of biomass, etc. The use of validated, first principle model based dynamic process simulators that accurately reflect the slow process dynamics as a reference for the design of the model predictive control system may overcome the problem of the required long plant tests for process identification in each operating point. Relatively short dedicated plant tests at well-selected operating conditions may be applied to accurately model the relevant fast dynamics using traditional process identification techniques. A combination of both modeling approaches in a heuristic way to model all relevant dynamics for process control may be a feasible way to solve the problem. The specific assumption made here is that a high fidelity, first principles based, dynamic process model covers the main process mechanisms that govern the low frequency transfer characteristics of the process over a sufficiently large operating range covering all relevant operating conditions (Backx, 1999).

Model based or model predictive process control in combination with trajectory optimization to find optimum dynamic transition paths can contribute to meeting the new needs on high performance plant operation. These technologies make extensive use of available knowledge on the dynamic behavior of processes for continuously driving the process to desired operating and performance conditions. Model predictive control enables revision of the control strategy on a sample-by-sample-basis using latest information on the status of the plant and its environment. The knowledge of process behavior is represented in the form of a mathematical model that describes the process dynamics, which are relevant for control. This model is explicitly used in the controller for predicting future process responses to past input manipulations and measured disturbances and to calculate best future input manipulations that satisfy the control objectives. The model is assumed to reflect all significant dynamic properties of process input/output behavior. It furthermore has to enable simulation of the future process outputs on the basis of known past process inputs within a pre-specified operating envelope of the process with limited inaccuracy and uncertainty (Cutler and Ramaker, 1980; Muske and Rawlings, 1993; Froisy, 1994; Qin and Badgwell, 1997; Richalet, 1997).

Dynamic Operation of Processes

Process operation has to become fully dynamic in stead of quasi-steady-state to meet the market requirements described in section 1. Processes in this respect have to be viewed as dynamically operated elements of a supply chain. This supply chain is composed of severa,l mutually interacting processes (Backx et al., 1998). The total supply chain has to meet the requirements of the market. As a consequence specific processes have to be operated in a way that production and products can easily be adapted to the changing and highly fluctuating market demand. Ideally a plant has to be controlled in such a way that production can follow market demand to the extent that 'Just-in-time' production at specifications might be feasible thus minimizing stocks of finished products and intermediates and enabling maximum capital productivity. The consequence of operating plants this way is that processes need to be operated under conditions that are fully synchronized with demand despite a wide range of dynamic effects that govern production behavior. Several sources of dynamics may be discriminated in this respect that all contribute to the overall dynamic behavior of a production plant:

- Marketplace dynamics
- Ecosphere dynamics
- Macro scale plant dynamics
- Meso scale unit process dynamics
- Micro scale reaction dynamics

The *marketplace* dynamics are characterized by long cycles. The cyclic behavior of the market place typically ranges from months to many years. The actual dynamic behavior is affected by various types of discrete events, which cause relatively fast (days to weeks time-frame) fluctuations in the market conditions. Examples of such events are feedstock (or utilities) availability, product demand as well as the prices for both feedstock and product. The market behavior is largely unpredictable due the large number of influencing factors, which are mostly unknown. It is a major disturbance that has to be coped with.

The dynamics of the ecosphere also shows cycles of different time scales. Typical examples of these *ecosphere* dynamics are the sometimes very rapidly changing weather conditions (e.g. a rain shower, a thunderstorm, a clouded sunny day, ...), the fast day-night patterns or the several orders of magnitude slower seasonal cycles with different temperature, humidity, waste water requirements and cooling water conditions. Like market behavior also ecosphere behavior is largely unpredictable. It generally has a large impact on actual process performance. Due to this large influence on actual process behavior it has to be compensated by control systems and optimizers.

The mix of unit processes that together form the plant determines *plant dynamics*. The dynamic behavior of the plant is governed both by the dynamics of each of the unit processes and by the dynamics related to recycles (e.g. recovery and re-use of materials, waste water, ...) and integration (e.g. heat integration, cooling water, ...). These dynamics may span several decades ranging from minutes to several days. As an example a Cracker plant like an Ethylene plant may be mentioned. This plant consists of reactors with dynamics in the minute range as well as distillation columns with dynamics that can range up to a day. Heat integration may cause such a plant to show dynamic behavior spanning days up to weeks.

Unit process dynamics normally span a few decades on a time scale. The actual unit process dynamics highly depend upon the type of unit process and may range from sub-seconds to days. Forming processes (e.g. Steel rolling, Extrusion of Polymers, glass forming, ...) are examples of processes showing sub-second to minute dynamics. Fluidized bed or slurry loop polyethylene and polypropylene reactors, high purity ethylene and propylene distillation columns and glass melting tanks are examples of unit processes with dynamics that may range from several hours up to one or even more days.

Reaction dynamics are usually very fast. They can span several decades of a time scale as well, but often they are in the micro second to second range.

All these overlapping dynamics together form the dynamics that have to be handled by the systems that are applied for operation of the plant. Adequate control of this wide range of dynamics is crucial to meet both flexibility requirements and quality requirements of products in accordance with continuously changing market demand.

The effect of adequate control of a wide range of dynamics in relation to product quality at the unit process level is shown in Figure 1. The bandwidth of the closed loop system determines the reduction in variance due to disturbances of the controlled variables. The reduction in variance that will be achieved by the control system can be estimated by calculating the frequency dependant reduction of the power spectral density (PSD) of the con-

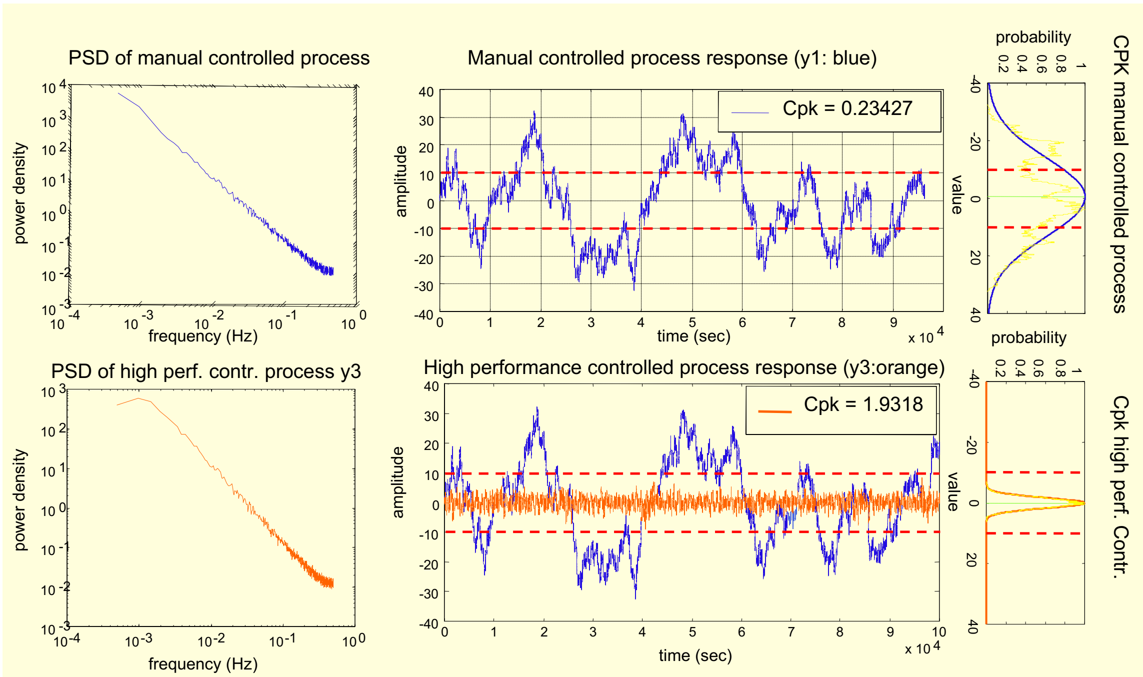

Figure 1: Bandwidth of a 'quasi-steady-state' (q.s.s.) control system and a 'High Performance' control system in relation to performance.

trolled variables Y(f) by closed loop control. Application of the theorem of Parceval (e.g. Papoulis, 1984) gives a direct estimate of the variance reduction achieved by the control system:

$$\sigma_{cl}^2 = \frac{\Phi_{yy}|_{cl}}{\Phi_{yy}|_{ol}} \cdot \sigma_{ol}^2 = \frac{\frac{1}{2\pi}\int_{-\infty}^{\infty}|Y_{cl}(f)|^2\,df}{\frac{1}{2\pi}\int_{-\infty}^{\infty}|Y_{ol}(f)|^2\,df} \cdot \sigma_{ol}^2 = \frac{1}{2\pi}\int_{-\infty}^{\infty}|Y_{cl}(f)|^2\,df \quad (4)$$

$\Phi_{yy}|_c l$ and $\Phi_{yy}|_o l$ respectively denote the closed loop and open loop power spectral densities of the controlled signal. The closed loop control system acts as a high-pass filter with a cut-off frequency determined by the bandwidth of the control system to reject output disturbances.

Process Modeling for High Performance Model Based Process Control

High performance process operation requires fully reproducible and predictable control of process units both during steady operation in a selected operating point as well as during transition between different operating points. This implies the need for models that accurately describe process dynamics over a frequency range that exceeds the intended bandwidth of the control system. As is shown in Figure 1 this bandwidth is governing the performance that can be achieved. Also for close tracking of transition trajectories a large bandwidth control system is necessary to enable high performance disturbance rejection during transition and to make fast transitions possible. The accuracy requirements on the models applied for control are fully dictated by:

- the bandwidth of the control system,
- the disturbance characteristics (amplitude ranges or probability density functions, frequency contents) of the variables that need to be controlled
- the process transfer characteristics (bandwidth of process transfers in relation to the bandwidth of the disturbances) over the operating envelope that needs to be handled by the control system

The bandwidth of the control system and the bandwidth of the model are linked by the role of the model in model predictive and model based control systems:

> *The model is assumed to accurately predict process output behavior thus minimizing the closed loop gain and providing an accurate estimate of the actual output disturbance (cf. Figure 2).*

From the frequency point on where the model looses accuracy in describing the process transfer behavior, the model predictive control system turns from a primarily feedforward driving control system into a classic (multivariable) feedback controller. This feedback controller

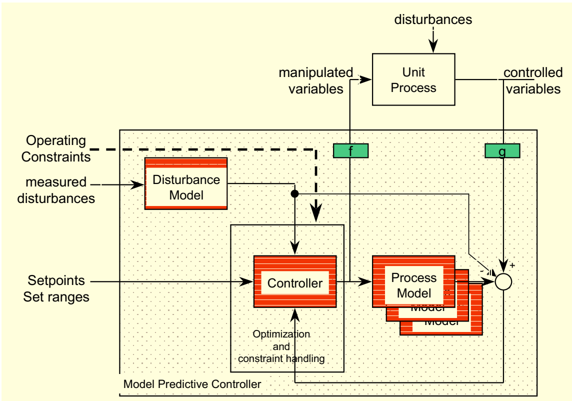

Figure 2: Structure of a model predictive control system.

has all the well known difficulties with stability and performance and is hard to tune (Rosenbrock, 1970; MacFarlane, 1979). Therefore the control system is tuned to not give any control performance any more in this frequency range in most industrial applications. As a consequence it only operates over a restricted (low) frequency range and does not reject higher frequency disturbances. Recovery from process upsets usually also takes much longer than required because of the limited bandwidth of the closed loop controlled process.

High performance control requires models with a bandwidth that cover all relevant process transfer dynamics over a frequency range given by the necessary disturbance rejection. The models have to enable accurate description of the process transfer dynamics in such a way that the model predicted outputs and the actual process outputs coincide both in amplitude and in phase over the relevant frequency range. Especially the requirement that the predicted and actual signal may not have a significant phase error makes that the bandwidth of the model has to exceed the closed loop bandwidth of the controlled process. Sensitivity for modeling errors over the full relevant frequency range is determined by the complexity of the process dynamics. Frequency ranges with large changes in phase shift between process inputs and outputs in general have to be treated with great care due to the sensitivity for poor performance or even instability in these frequency ranges. Processes often show large changes in phase shift between inputs and outputs especially around the cut-off frequencies, which makes that this frequency range almost always needs to be modeled accurately for high performance control.

First principles based modeling techniques in general are not very well suited to accurately model all process mechanisms that govern the higher frequency amplitude and especially phase characteristics. This is caused by the many interacting mechanisms that dominate the process behavior in this frequency range (e.g. inhomogenities in materials, temperatures, concentrations of components, turbulent flow patterns, non-homogeneous mixture of components, ...). Process identification techniques on the contrary are very well capable in capturing this behavior in models, if it is stationary. The following aspects are critical for process identification techniques to model process behavior accurately in the critical frequency ranges for high performance model based process control:

- The process needs to show stationary and reproducible behavior within the operating envelope
- The applied modelsets for system identification have to enable accurate modeling of the amplitude/phase characteristics of all process transfers in the critical ranges; i.e. complexity of the applied modelsets needs to be sufficiently high (Willems, 1986a,b, 1987)
- The process data used for estimation of the model parameters have to contain sufficient information on these process characteristics in ratio to encountered disturbances during testing; the process has to be persistently excited with adequate signal-to-noise ratio's at each of the process outputs (controlled variables) (Ljung, 1987)
- The test signals applied to the process have to excite the process in a balanced way to enable equally accurate modeling of low and high gain directions; this is of particular importance if the control system has to enable high performance in low gain directions of the process (e.g. dual quality control in distillation cf. Figure 3)
- The criterion function applied for estimation of the model parameters has to be consistent with the later use of the model in the model based control system, which usually implies prediction of future process outputs over some future time horizon on the basis of known past process inputs and known past process outputs.

High performance process control starts with the selection of appropriate process input (Manipulated Variables) and process output variables (Controlled Variables). The selected set of manipulated variables together with the information obtained from the measured disturbance variables have to enable compensation of the disturbances that affect the controlled variables. Furthermore the selected set of manipulated variables has to enable fast, predictable and reproducible transition between selected operating points of the process. Multivariate statistical analysis tools support selection of appropriate process inputs and process outputs for control (Yoon and MacGregor, 2000; Clarke-Pringle and MacGregor, 2000).

High performance model based process control in general requires process models that reflect process behavior

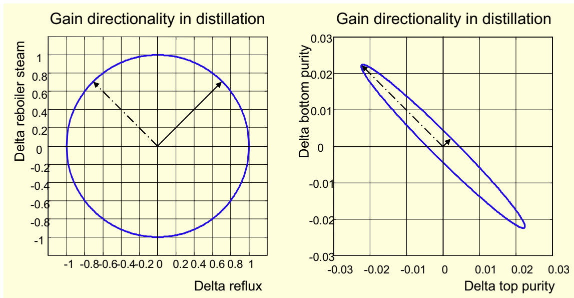

Figure 3: Directionality in process transfer characteristics of a local operating point in distillation.

over a large frequency range. A distillation column may be used as a simple example to illustrate this. An industrial column with 15 trays will have a time to steady state of approximately 1.5 hours. A change in top product quality in response to a top pressure change will be noticed well within a minute however. This means that even for this simple column the range of dynamics to be covered already is ¿100. This number is the ratio of fastest relevant frequency (response to a pressure change in this example) over slowest relevant frequency (dynamics that govern settling towards steady state) for high performance model based control. A finite step response model needs at least 200 relevant samples to cover such a range of dynamics. The further the slowest and fastest relevant frequencies get apart the more parameters will be needed to describe this process behavior with finite step responses. The required sample rate for the model is governed by the highest relevant frequency. The time span that needs to be covered by the model is governed by the low frequencies that determine settling to steady state of the process. The time length of the model divided by the applied sampling time gives the complexity of the model for non-parametric type models like finite step responses or finite impulse responses. The complexity is a measure for the number of parameters of the model. This implies that these non-parametric types of models are requiring an increase in model complexity to cover all relevant dynamics, if the fastest and slowest relevant dynamic modes get further apart. In most of todays model predictive control applications the higher frequency characteristics of the process are not included in the models to prevent the models from becoming too complex.

The critical issue for high performance model based control is accuracy of the applied model in certain frequency ranges. Model sets that support coverage of wide frequency ranges without a necessarily large increase of model complexity are parametric models like e.g. state space models. State space models can handle the wide range of dynamics encountered in most industrial processes with a complexity dictated by the number of dynamic modes in the observed dynamic process behavior. The number of parameters required to accurately describe process behavior does not grow with the ratio of fastest and slowest relevant process dynamics, if parametric models are applied. It depends upon the complexity of the process dynamics i.e. the order of the difference equations that approximately describe the relevant process behavior with sufficient accuracy.

The data used for process identification has to contain information that enables reconstruction of the process transfer characteristics at the critical frequency ranges with the required accuracy. This implies that test signals applied to the process have to span the input space later used by the control system in such a way that all relevant frequencies are well excited and that the variables that will be controlled are showing balanced responses. This also has to hold for the directions that show the largest and the smallest gains over the relevant frequency range. Model accuracy obtained from process identification is governed by the signal-to-noise ratios encountered over the full frequency range over all output directions (Zhu and Backx, 1993; Zhu et al., 1994).

Subspace and orthonormal basis function based techniques are latest developments in multivariable process identification techniques that enable modeling of a wide range of process dynamics, without requiring detailed a-priori knowledge on the order and structure of the multivariable system (Van Overschee and De Moor, 1993, 1994; Verhaegen and Dewilde, 1993a; Viberg, 1995; Heuberger et al., 1995; Van den Hof and Bokor, 1995; Van Donkelaar et al., 1998). Essential in both approaches is that observed input-output behavior of the process as represented by the process data collected and pre-treated for identification are projected to a subspace spanned by a set of (orthonormal) basis functions that can represent all relevant process dynamics. The difference between both methods stems from the type of basis functions applied and by the way the selection of these basis functions is established.

Subspace identification techniques determine the basis functions directly from Hankel U and Y matrices constructed from the process input and process output data applied for process identification. The basis functions are obtained by data compression via an RQ factorization (Verhaegen and Dewilde, 1993a,b).

$$\begin{aligned}
\begin{bmatrix} U \\ Y \end{bmatrix} &= \begin{bmatrix} R_{11} & 0 \\ R_{21} & R_{22} \end{bmatrix} \cdot \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} \\
&= \begin{matrix} (n-1)p \rightarrow \\ p \rightarrow \\ (n-1)q \rightarrow \\ q \rightarrow \end{matrix} \begin{bmatrix} \overbrace{R_{11}^1}^{np} & \overbrace{0}^{nq} \\ * & 0 \\ R_{21}^1 & R_{22}^1 \\ * & * \end{bmatrix} \cdot \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} \\
&= \begin{matrix} p \rightarrow \\ (n-1)p \rightarrow \\ q \rightarrow \\ (n-1)q \rightarrow \end{matrix} \begin{bmatrix} \overbrace{r_u}^{np} & \overbrace{0}^{nq} \\ R_{11}^2 & 0 \\ r_{y1} & r_{y2} \\ R_{21}^2 & R_{22}^2 \end{bmatrix} \cdot \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}
\end{aligned} \tag{5}$$

In these equations n denotes the order of the state space system representation, p denotes the number of inputs and q denotes the number of outputs. Calculation of the singular value decomposition of the matrix $[(R_{21} - H_n \cdot R_{11})\ R_{22}]$ that links future process output behavior to past and current input manipulations:

$$\begin{aligned}
\Lambda_n \cdot X_l &= Y - H_n \cdot U \\
&= [(R_{21} - H_n \cdot R_{11})\ R_{22}] \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} \\
&= U_s \cdot S_s \cdot V_s^T \cdot \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}
\end{aligned} \tag{6}$$

provides the matrix U_s^1 by selection of the first $(n-1) \cdot q$ rows of U_s. H_n is the Hankel matrix constructed from n Markov parameters estimated from the available process input output data.

The state space system matrices are subsequently calculated by least squares solution of the following set of equations:

$$\begin{aligned}
&\begin{bmatrix} U_s^{1^*} \cdot (R_{21}^2 - H_{n-1} \cdot R_{11}^2) & U_s^{1^*} \cdot R_{22}^2 \\ r_{y1} & r_{y2} \end{bmatrix} = \\
&\begin{bmatrix} A & B \\ C & D \end{bmatrix} \cdot \begin{bmatrix} U_s^{1^*} \cdot (R_{21}^2 - H_{n-1} \cdot R_{11}^1) & U_s^{1^*} \cdot R_{22}^1 \\ r_u & 0 \end{bmatrix}
\end{aligned} \tag{7}$$

Orthonormal basis function based algorithms use an initial basis function generation step in which a rough low order approximation of the process dynamics is used in combination with an inner transfer function to generate the applied set of basis functions (Van Donkelaar et al., 1998; Heuberger et al., 1995; Van den Hof and Bokor, 1995).

$$G(z, \vartheta) = \sum_{i=1}^{N} W_i(\vartheta) \cdot F_i(z) \tag{8}$$

represents the process transfer as a function of time shifts z and of the model parameters . Wi() indicates the weights on each of the basis functions and Fi(z) refers to the basis functions applied.

A well known set of basis functions commonly applied in industrial applications is the pulse basis:

$$f_i(z) = z^{-i} \tag{9}$$

Substitution of this basis in (8) gives the Finite Impulse Response representation of the process. This basis requires many parameters Wi to describe all relevant process dynamics, if the process dynamics cover a wide range as discussed above. A significant reduction in the number of parameters required for describing all relevant process dynamics may be obtained by using Laguerre or Kautz sets of basis functions:

Laguerre:

$$f_i(x) = \sqrt{1 - a^2} \cdot \frac{(1 - az)^i}{(z - a)^{i+1}} \tag{10}$$

Kautz:

$$\begin{aligned}
&f_{2i}(z) = \\
&\quad z\frac{\sqrt{1-c^2} \cdot (z-b)}{z^2 + b(c-1)z - c} \cdot \left[\frac{-cz^2 + b(c-1)z + 1}{z^2 + b(c-1)z - c}\right]^i \\
&f_{2i+1}(z) = \\
&\quad z\frac{\sqrt{(1-c^2) \cdot (1-b^2)}}{z^2 + b(c-1)z - c} \cdot \left[\frac{-cz^2 + b(c-1)z + 1}{z^2 + b(c-1)z - c}\right]^i
\end{aligned} \tag{11}$$

A significant reduction in the number of parameters N is achieved by selecting the coefficients of these basis functions—parameter a in the Laguerre basis functions and parameters b, c in the Kautz basis functions—in such a way that the first elements of the set of basis functions closely represents the relevant process dynamics. The Laguerre basis works well for systems that show smoothly damped behavior. The Kautz basis works fine for system with badly damped transfer characteristics. To achieve a close approximation with a few basis functions of actual processes that show more complicated transfer dynamics, a better performance is obtained by making use of a generalized orthonormal basis as described in (Heuberger et al., 1995). This allows the selection of a set of orthonormal basis functions of which the first functions closest approximate the actual observed process dynamics.

Both methods—the subspace method and the orthonormal basis function method—don't directly give an optimum model with minimum output error. In general the models are very good starting points for a final nonlinear output error optimization as described in (Falkus, 1994). This output error optimization allows fine tuning of the state space model to accurately describe process dynamics in the critical frequency ranges. Application of the identification techniques in closed loop process operation allows the identification techniques to automatically concentrate on realizing the highest model accuracy in the critical frequency ranges for closed loop control (Hjalmarsson et al., 1996).

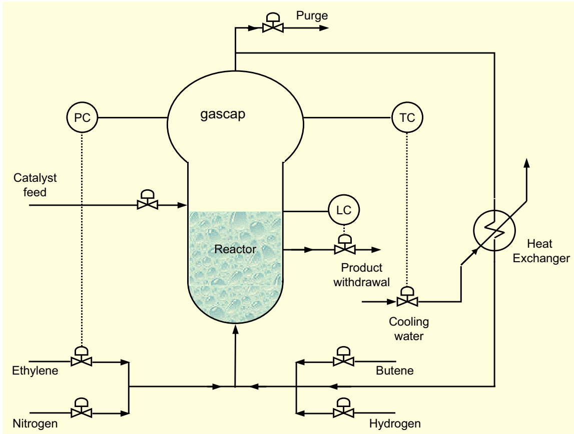

Figure 4: Fluidized bed gas phase HDPE reactor.

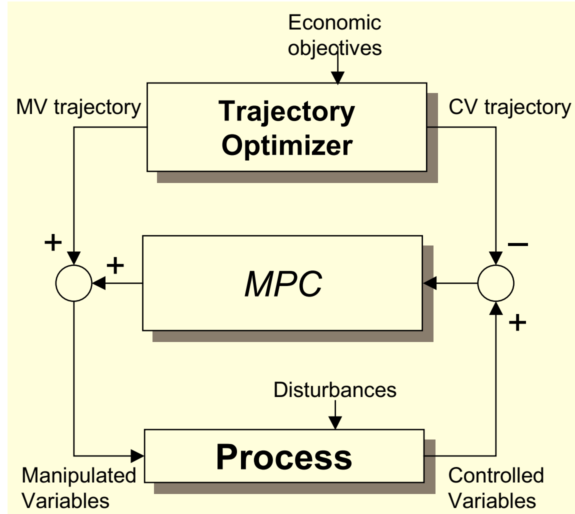

Figure 5: Integration of the delta mode MPC system and the rigorous model based dynamic trajectory optimizer.

Some Results

Control of a gas phase fluidized bed HDPE polymer reactor is used as an example to show some initial results of performance improvement that can be achieved by integrated high performance model based control and dynamic optimization (Figure 4). As discussed in the previous sections performance of the model predictive control system and the dynamic optimizer is governed by accuracy of the applied models.

In this example a set of approximate linear models is applied to realize a high performance model predictive transition control system that optimizes polymer production performance both during normal operation as well as during grade transitions. The dynamic grade transition optimization is done on the basis of a first principles based dynamic model of the process as discussed in section 2 and implemented in gPROMS.

The model predictive control system developed for control of the polymerization reactor has been designed to cover a broad operating range of the process. The control system simultaneously manipulates Monomer/Co-monomer ratio, Hydrogen/Monomer ratio, Catalyst flow, Gascap Pressure and bed Temperature. The model predictive control system controls Density, Melt Index and Production Rate. Direct or inferential measurements of the controlled variables needs to be available for this purpose. The control system operates in delta mode and includes linearizing functions to cover the large, non-linear operating range of the process with sufficient accuracy (Figure 5).

In case no on-line measurement of the controlled variables are available, the controller will calculate the required control actions on the basis of model predictions of these variables between the updates of the real measured process values. This functionality enables robust operation of the control system at various sample rates of the product quality (Melt Index and Density) measurement. It will make the control rather insensitive for changes in the sample rate as long as the model predictions don't show severe errors.

The control system is designed for high performance, robust control of the polymer properties over a broad operating range of the process. Table 1 gives an overview of the total set of grades covered by the integrated control and dynamic optimization system. Performance of the control system is stable over this operating range. Figure 6 shows the results of the transitions from O7 to P3 (left two columns) and R0 to P3 (right two columns) as an example of two grade changes subject to a variety of external disturbances acting on the process. The picture clearly shows the improvements obtained over traditional grade transition control. The transitions are fast and the polymer properties remain well within specifications at both grades.

The transitions shown are shortcuts in the normal grade slate. The transitions involve a large change in the density of the polymer, which implies a large change in the co-monomer/monomer ratio. In order to enable a fast transition the production rate is heavily decreased to get a minimum amount of wide spec product during the transition. The large change in production rate implies that a severe change is process behavior is encountered due to the wide operating range spanned. The models applied for prediction in the control system have to accurately describe these changing process characteristics to enable close tracking of the optimum transition trajectory calculated by the optimizer. The performance improvement achieved by the integrated MPC and dynamic trajectory optimization in this example represents an economic benefit of €117330 for the transition of O7 to P3. The benefit related to the improvement of R0

Grade Names			DENS 964 966	DENS 954 956	DENS 944 946	DENS 934 936	DENS 924 926	DENS 914 916	DENS 904 906	DENS 894 896
LNMI	-2.4	-2.6	GO	G1	G2	G3	G4	G5	G6	G7
LNMI	-1.4	-1.6	H0	H1	H2	H3	H4	H5	H6	H7
LNMI	-0.4	-0.6	I0	I1	I2	I3	I4	I5	I6	I7
LNMI	0.6	0.4	J0	J1	J2	J3	J4	J5	J6	J7
LNMI	1.6	1.4	K0	K1	K2	K3	K4	K5	K6	K7
LNMI	2.6	2.4	L0	L1	L2	L3	L4	L5	L6	L7
LNMI	3.6	3.4	M0	M1	M2	M3	M4	M5	M6	M7
LNMI	4.6	4.4	N0	N1	N2	N3	N4	N5	N6	N7
LNMI	5.6	5.4	O0	O1	O2	O3	O4	O5	O6	O7
LNMI	6.6	6.4	P0	P1	P2	P3	P4	P5	P6	P7
LNMI	7.6	7.4	Q0	Q1	Q2	Q3	Q4	Q5	Q6	Q7
LNMI	8.6	8.4	R0	R1	R2	R3	R4	R5	R6	R7
LNMI	9.6	9.4	S0	S1	S2	S3	S4	S5	S6	S7

Table 1: Grade definition table.

to P3 represents a value of € 49081 at the given market values. The actual benefit and the corresponding optimum transition strategy strongly depend upon market conditions for first grade and wide spec products.

Conclusions

Changing market conditions enforce chemical processing industries to better utilize process capabilities. Process operation needs to be closer tied with market demand to improve capital productivity. Currently applied state-of-the-art model predictive control and model based optimization techniques don't support close tracking of optimum operating conditions. A main reason for this is the limitation in accuracy of the models applied for control and optimization. High performance control requires models that accurately describe all relevant process dynamics over a wide operating range. Especially the frequency ranges where the process is showing huge changes in its transfer phase characteristics are critical and need to be modeled accurately. High performance in general requires models that cover the full process transfer frequency range accurately. The frequency range covered accurately by the model dictates the ultimate bandwidth of the closed loop model predictive control system. This bandwidth in its turn governs the disturbance rejection capabilities of the control system and therefore the resulting capability to achieve product and process quality requirements. The bandwidth of the control system furthermore governs the capabilities to closely track transition trajectories that enable cost effective changeovers between various operating points.

Accurate modeling of all relevant process dynamics for the entire process operating envelope envisaged requires integration of rigorous modeling techniques with process identification techniques to be economically feasible. Process testing needs to be minimized due to the high cost involved with plant tests. Extensive (re-)use of a-priori knowledge on process dynamics is enabling a significant reduction in test time required. Plant tests have to focus primarily on critical frequency ranges for control. These dedicated tests can be relatively short and less expensive in general.

Optimum transition control is not supported by steady state optimization techniques. New concepts based on the use of dynamic plant models have been discussed that enable exploitation of plant dynamics for optimization of economic performance of plants. Consistency between model-based optimization and model-based control is crucial for high performance in dynamic plant operation. Intential dynamic operation of a plant opens opportunities for very significant improvement of plant economics and capital productivity. Market driven operation of plants becomes feasible, if plant and process designs support it.

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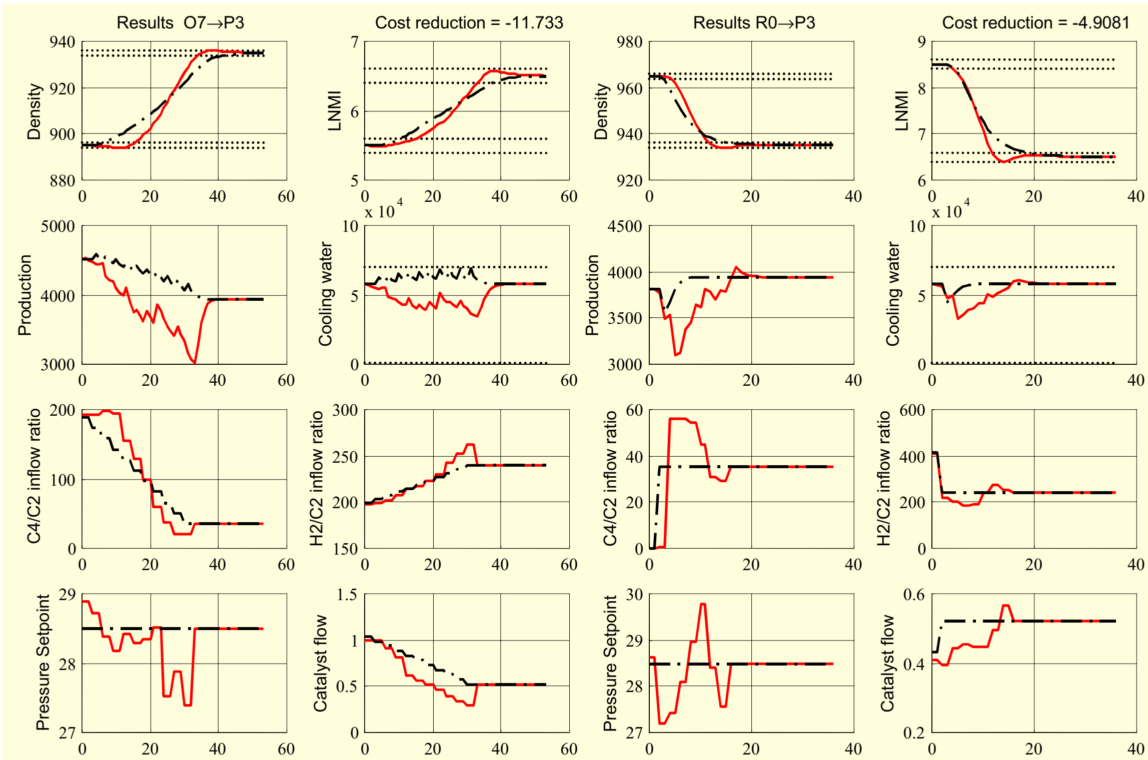

Figure 6: Process values and manipulated variables for two optimized grade changes. The dashed lines represent the initial trajectory, while the solid lines correspond to the optimized controlled trajectory.

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