MARKET-ORIENTED SCHEDULING, ECONOMIC OPTIMIZATION AND STOCHASTIC CONSTRAINED CONTROL OF CONTINUOUS MULTI-GRADE CHEMICAL PROCESSES

O.H. Bosgra * **R.L. Tousain** *,1 **D.H. van Hessem** *,2

* *Delft Centre for Systems and Control, Delft University of Technology, Mekelweg 2, 2628CD Delft, The Netherlands*

Abstract: In this paper an approach for flexible production scheduling for continuous multi-grade chemical processes is proposed. The approach integrates the economics of production and of company-market interaction for single-machine multi-grade continuous processes. The resulting grade transitions are realized using a newly developed closed-loop stochastic MPC framework, that decomposes this task into a deterministic feedforward constrained trajectory optimization task and a stochastic feedback disturbance suppression task. The back-off used in the former is provided by the latter. The approach is demonstrated on a gas phase HDPE manufacturing plant.

Keywords: process optimal operation, continuous scheduling, grade transitions, closed-loop model predictive control, stochastic MPC, process control

1. INTRODUCTION

During the past decades the chemical industry has been faced with a major change into a *globally competing* and *demand driven* mode of operation. Companies are required to respond quickly to changing market situations and must meet customer-specified product specifications. A main challenge and a key to demand-driven operation, is the allocation of production resources to comply with orders and physical constraints such as plant capacity and storage facilities. Such problems are generally referred to as *scheduling* problems, and their role in the internal supply chain is broadly acknowledged. An overview can be found in (Reklaitis, 1992). Although most of the scheduling literature focuses on *batch* operations, there is recent work on continuous process scheduling see (Mendez and Cerda, 2002), (Giannelos and Georgiadis, 2002). The approach here will consider continuous, single-machine, multi-grade chemical plants, and differs from the work cited in several aspects. Our way of including the effect of process transitions on the material flows appears new. Further, most scheduling studies assume the order base to be fixed in advance and strive for 'minimum makespan' or 'minimum lateness'. In our approach, the negotiation of sales orders and purchases is an integral part of the decision making that is supported by the scheduler, and to this end the scheduler selects a set of appealing purchase and sales transactions from a larger set of possible transactions (denoted *opportunities*).
The optimal scheduling approach considered here includes a formulation of the grade change problem that includes a truly economic objective. To

[1] Present affiliation: Philips Centre for Industrial Technology, P.O. Box 218, 5600 MD Eindhoven, The Netherlands
[2] Present affiliation: Shell International Chemicals B.V. P.O. Box 38000, 1030 BN Amsterdam, The Netherlands

implement grade changes under practical process conditions, the off-line computed process trajectories will be transferred into reality by a real-time MPC algorithm. We will extend current MPC capabilities (Rawlings, 2000) for this purpose to deal with back-off under stochastic disturbances, and to obtain guaranteed control performance with respect to disturbance suppression. Lee and Ricker (Lee and Ricker, 1994) have proposed to decompose the stochastic MPC problem into an optimal Gaussian estimation and a deterministic prediction problem, to be solved as separate optimization problems in a receding horizon implementation. This view has become a major paradigm for MPC research, in which stochastics are considered in the past but not in the future. Three limitations of this paradigm are (1) there is no back-off to the constraints, (2) there is no possibility to tune the implied feedback properties and (3) the underlying assumption of the validity of the certainty equivalence property may be questionable in the case of active inequality constraints. The approach taken here suggests to decompose the predictive control formulation into a feedforward trajectory and a feedback controller. By creating a back-off to the constraints, the feedback controller retains its linear behaviour, enabling feedback properties to be assigned using an appropriate disturbance suppression objective. This in turn provides an estimate for the back-off to be used in the feedforward trajectory optimization, as in a bootstrap technique. Consequently, optimal plant transitions can be realized using feedforward whereas the inequality constraints are guaranteed not to be violated under the closed-loop control. The paper presents a survey of work available in detail in (Tousain, 2002) and (van Hessem, 2004).

2. DEMAND DRIVEN OPERATION

The scheduling task concerns the timing of feedstock and grade changes. Most of today's multi-grade plants are still operated according to a predetermined sequence of product grades, called a *product slate* or a *product wheel*, see figure 1 (Sinclair, 1987). The sequence is constructed such that the necessary grade changes are relatively easy, safe and well-known by the operating staff. In order to operate market-responsive, short-term production scheduling should consider the internal supply chain in interaction with the markets involved. The simple model is represented schematically in figure 2. It provides a new, broader scope for *process control* from a perspective of *intentional dynamics*, (Marquardt *et al.*, 1998). It captures some of the main mechanisms in practical chemical supply chains: company-market interactions, inventory control, process

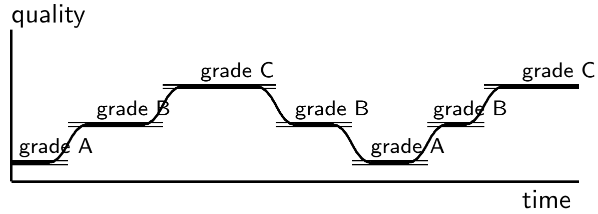


Fig. 1. A product grade slate A-B-C-B-A with on-spec-ranges

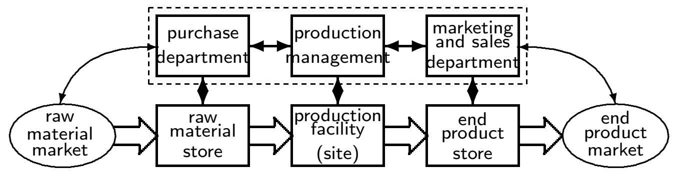


Fig. 2. A simple supply chain model for a continuous chemical manufacturing site

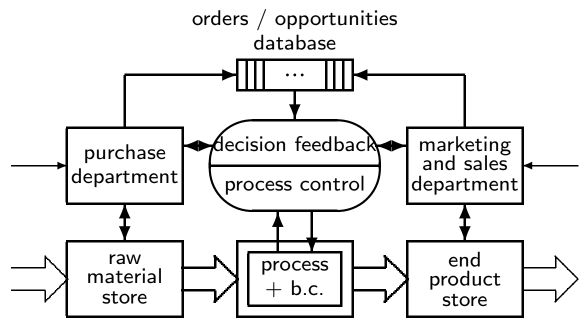


Fig. 3. A single level approach to supply-chain-conscious production management and process control

dynamics such as transitions, load changes, and internal supply chain organization. Although dynamic supply chain phenomena such as demand amplification (Towill, 1996) are important, here we focus on production management decisions for multi-grade processes. These involve scheduling, plant optimal operation and control tasks. The integration of these tasks needs care to avoid inconsistencies. In (Bassett *et al.*, 1996), three types of model-based integration are distinguished: *single-level control*, *multi-level control* and *conceptual decomposition*. A *single-level control strategy* to the problem of supply-chain-conscious process operations implies to control the process while supporting the purchasing and sales decision making tasks, as represented schematically in Figure 3. This necessitates to include all relevant time scales of the operations problem (i.e. weeks/months to capture market changes, and seconds/minutes to describe plant dynamics which should be controlled) into one control problem. This will generally lead to combinatorial control problems which are of enormous dimension and hence computationally infeasible. The main decomposition that we propose is hence to deal separately with the

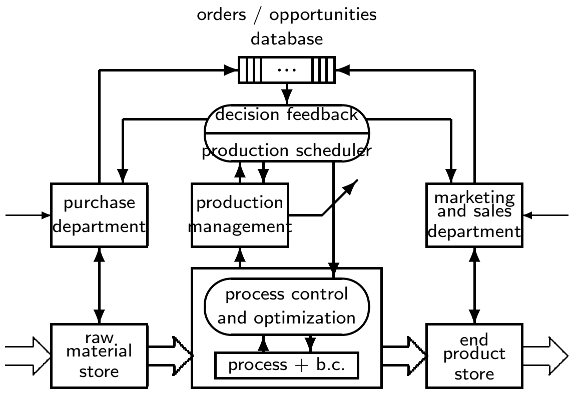


Fig. 4. Decomposition of supply-chain-conscious production management and process control

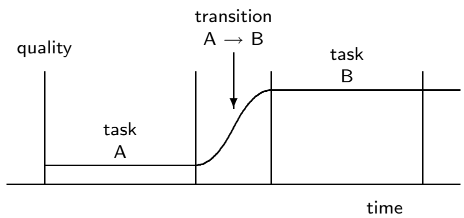


Fig. 5. Operation of a multi-grade process considering static production tasks and transition tasks

two questions 1: what products/feedstocks will be produced/processed when? and 2: how will the production be realized? We split up the production management problem into a *production scheduling problem* (section 3), and a *production control problem*, (section 5), see figure 4. Both solutions utilize the same dynamic model, which is an important prerequisite for the consistency of the decomposition approach.

3. SHORT TERM SCHEDULING DESIGN

To solve the production scheduling problem, we concentrate on a description of the plant in terms of operating tasks with accompanying precedence rules. The use of quasi-static and dynamic tasks in modeling the behavior of a continuous multi-grade plant is illustrated in figure 5. Let a model of the plant, *including the basic control system*, be given by the following set of DAE's

$$\begin{aligned} \dot{x} &= f(x,u,y) \\ 0 &= g(x,u,y) \\ z &= C_x x + C_u u, \end{aligned} \tag{1}$$

where $x(t) \in \mathbb{R}^{n_x}$, $u(t) \in \mathbb{R}^{n_u}$, and $y(t) \in \mathbb{R}^{n_y}$ are respectively the state, input and algebraic variables of the model. For ease of notation, the dependency of these variables on time will be omitted in the remainder. $z \in \mathbb{R}^{n_z}$ contains the so-called performance channels, i.e. all variables that are required for the performance evaluation of the plant. The performance computation involves a so-called objective function as well as the violation of constraints. These operating constraints are expressed as

$$h(z) < 0. \tag{2}$$

All feasible steady state operating conditions are given by the set

$$\begin{aligned} \mathcal{F} = \{x, u \mid \exists\, y, z \ \text{ such that } f(x,u,y) = 0, \\ g(x,u,y) = 0,\ z = C_x x + C_u u,\ h(z) < 0\} \end{aligned} \tag{3}$$

In general we are only interested in a limited number of interesting scenarios, e.g. a finite number of product grades or feedstock conditions. The production grade conditions $\mathcal{G}_g$ are by definition given by specific sets of conditions (z) that obey the corresponding constraints:

$$\begin{aligned} \mathcal{G}_g = \{(x,u) \in \mathcal{F} \mid \exists z = C_x x + C_u u, \text{ such that} \\ g_g(z) < 0\} \end{aligned} \tag{4}$$

where g_g defines the quality bounds of grade g. For example, in a distillation plant, these would be lower and upper limits on the purity. The different production grades are connected via process transitions. We define a transition T_g^h from an element $(x^g, u^g) \in \mathcal{G}_g$ to an element $(x^h, u^h) \in \mathcal{G}_h$ as a quadruple (x, u, y, z) satisfying

$$\begin{array}{llll} \text{plant} & \text{init. cond.} & \text{end cond.} & \text{constraints} \\ \dot{x} = f(x,u,y) & x(0) = x^g, & x(T) = x^h, & h(z) < 0 \\ 0 = g(x,u,y) & u(0) = u^g & u(T) = u^h & \\ z = C_x x + C_u u & & & \end{array} \tag{5}$$

for some $T > 0$. Let $\mathcal{T}_g^h$ be the set of all these transitions. The sets $\mathcal{G}_g$ and $\mathcal{G}_h$ are said to be compatible if there exists a transition T_g^h from any $(x^g, u^g) \in \mathcal{G}_g$ to any $(x^h, u^h) \in \mathcal{G}_h$. Finally, all sequences of transitions are feasible if all pairs $[g, h]$ are compatible. The verification of such conditions is not straightforward, only for specific cases there may exist a computationally feasible approach. We assume that during the static production tasks, the operating conditions are determined according to the *maximization* of an economic criterion. As the basic economic criterion we will use the *added value*. Let C_r and Y_e denote the consumption of raw materials and utilities r, and the production of end product e, respectively. We assume these are given as functions of the performance variables: $C_r = C_r(z)$, $Y_e = Y_e(z)$. Then, in case of a static production task, the added value rate is given by

$$L(z) := -\sum_r p^{C,r} C_r(z) + \sum_e p^{Y,e} Y_e(z) \tag{6}$$

where $p^{C,r}$ and $p^{Y,e}$ are the instantaneous prices of respectively raw material r and the product e. Using this expression for the added value and disregarding the effect of noise and disturbances, the optimal operating conditions for grade g are found by solving the following, static optimization problem

$$(\bar{x}^g, \bar{u}^g) = \text{argmin}\, \{-L(z) \mid \exists z = C_x x + C_u u \text{ such that } (x,u) \in \mathcal{G}_g\} \quad (7)$$

and the corresponding raw material and product flows are given by $C_r^g = C_r(\bar{z}^g)$ and $Y_e^g = Y_e(\bar{z}^g)$, where $\bar{z}^g = C_x \bar{x}^g + C_u \bar{u}^g$. The dynamic transition tasks are designed to be the solution of a dynamic optimization with an economic criterion as performance index. We also require that the process control system governing the implementation of process transitions is based on dynamic optimization involving the same criterion. A general formulation of the corresponding trajectory optimization problem is given as follows

$$\min_{T, u \in \mathcal{U}} \left\{ \int_0^T L^d(z)dt \,\middle|\, \exists x, y, z, \text{ s.t. } (x,u,y,z) \in \mathcal{T}_{\bar{g}}^{\bar{h}}, \; x(0) = \bar{x}^g, \; x(T) = \bar{x}^h \right\} \quad (8)$$

where L^d is chosen so as to represent the economics of the transition. In case of a **demanding market**, the main incentive is to maximize production. Then transition times should be limited to the minimum. Transition costs are of secondary importance. In case of **low demand** and moderately filled order books, there is no incentive to minimize the transition times. Instead, the difference between the transition revenues and the transition costs should be maximized. This leads to a truly economic transition optimization, where $L^d(z)$ is selected to represent the negative added value rate during the transition. The grade change optimization problem is hard to solve using standard gradient-based numerical optimization techniques due to the fact that the production rate of a certain grade depends discontinuously on the quality variables. One possible approach uses a smooth approximation of the definition of the grade region and exploits the structure of the problem in the definition of a Nonlinear Programming (NLP) based inner loop optimization to compute accurate search directions. A second approach uses integer variables to describe the grade regions and solves a sequence of MILP's to converge to a solution. The grade change problem is non convex and both approaches can be expected to converge to local minima only. However they are believed to do so much faster than the conventional control parametrization method.

The **company-market interaction** is represented here by a transactions-based framework. The sales actions are **(1) orders** originating from long term sales contracts or short term commitments to customers; the main order attributes are the quantity, the price and the time span during which the order can be delivered; **(2) opportunities** arising from predictions of the market-

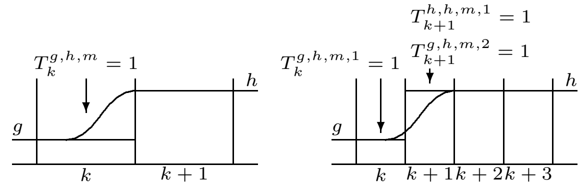


Fig. 6. Representation of transition tasks in UDM framework in case (left) transition time is smaller than τ, and (right) transition time is smaller than 2τ

company interaction made by the sales decision makers. In opportunities they express their estimate of future sales deals. The attributes of the opportunities are the same as those of the orders. The representation of the time axis is discussed by (Zentner *et al.*, 1998). Here we adopt the *Uniform Discretization of time Modeling* (UDM) framework, in which the horizon is divided into a finite number of time slots of uniform length. Only at the beginning of each interval changes may occur. The choice of the interval length, denoted τ in the sequel, is a trade-off between solution resolution and computational tractability. Transition tasks can occur within a single time interval or within more than one, as shown in figure 6. Here we will only consider the first case. We introduce decision variables G_k^g, $g = 1, \ldots, n_g$ as the *production decision* variables, where $G_k^g = 1$ means that production task g is started at the beginning of the k-th time span and executed during this time span. Only one task can be performed at the same time:

$$\sum_g G_k^g = 1. \quad (9)$$

To model the transitions we introduce variables $T_k^{g,h,m}$ which, if equal to 1, indicate that a transition from grade g to h and of mode[3] m is executed at the end of time span k. $T_k^{g,h,m}$ relates to G_k^g and G_{k+1}^h in the following manner.

$$\sum_g \sum_h \sum_m T_k^{g,h,m} = 1, \; \sum_m T_k^{g,h,m} \leq G_k^g, \; \sum_m T_k^{g,h,m} \leq G_{k+1}^h. \quad (10)$$

Further, let TM_k^m be one if transition mode m is executed in time span k and zero otherwise. Then the following holds:

$$T_k^{g,h,m} < TM_k^m. \quad (11)$$

Because all transition times are shorter than τ we need to take the quasi-static production preceding the transition into account to arrive at the appropriate production attributes (raw material consumption and end product yield). Let the transition time for a mode m transition from grade g to grade h be denoted $\tau^{g,h,m}$. Then, the

[3] The transition mode m refers to the market scenario for which the transition characteristics are computed.

consumption of raw material r and the production of end product e for the corresponding transition are computed as

$$TC_r^{g,h,m} = (\tau - \tau^{g,h,m})C_r^g + C_r^{g,h,m}, \quad (12)$$
$$TY_e^{g,h,m} = (\tau - \tau^{g,h,m})Y_e^g + Y_e^{g,h,m}. \quad (13)$$

For 'transitions' $T_k^{g,g,m}$ the transition time is zero which yields the corresponding steady state production figures: $TC_r^{g,g,m} = \tau C_r^g$ and $TY_e^{g,g,m} = \tau Y_e^g$. C_r^g, Y_e^g, $C_r^{g,h,m}$, and $Y_e^{g,h,m}$ are the consumption and yield variables as defined in the previous section. To formulate the *transaction-based market description*, a binary decision variable $S_k^{e,s} \in \{0,1\}$ is used to indicate whether sales order/opportunity s for end product e is executed in time span k (in which case $S_k^{e,s} = 1$) or not ($S_k^{e,s} = 0$). Further, for each order/opportunity we introduce a set of time spans $\Omega^{e,s}$ outside which it may not be executed. Attached to each sales order/opportunity the market database stores the amount of product, $SA^{e,s}$ and the unit price offered, $S\$^{e,s}$. By definition of $\Omega^{e,s}$ we have:

$$S_k^{e,s} = 0, \quad \forall k \notin \Omega^{e,s}. \quad (14)$$

Further, each order must be executed exactly once and each opportunity at most once. This gives rise to the following constraints

$$SO^{e,s} \le \sum_{k\in\Omega^{e,s}} S_k^{e,s} \le 1, \quad (15)$$

where $SO^{e,s}$ is zero if s is an opportunity and one if s is an order. Similar reasoning for purchasing orders and opportunities leads to the introduction of binary decision variables $P_k^{r,p}$ and the constraints

$$P_k^{r,p} = 0, \qquad \forall k \notin \Omega^{r,p}, \quad (16)$$
$$PO^{r,p} \le \sum_{k\in\Omega^{r,p}} P_k^{r,p} \le 1, \quad (17)$$

where $\Omega^{r,p}$ is defined as the set of time spans k outside which purchase ord./opp. p may not be executed and $PO^{r,p}$ is zero if transaction p for raw material r is a purchase opportunity and 1 if it is an order. The purchase attributes are $PA_k^{r,p}$ and $\$P_k^{r,p}$: the amount of feedstock r and its unit price for purchase ord./opp. p. Let us introduce ES_k^e as the storage level of end-product e at the beginning of time span k and RS_k^r as the storage level of raw material r at the beginning of time span k. The *material balances* for the raw material storage and the end-product storage are defined as follows

$$ES_{k+1}^e = ES_k^e + \sum_g\sum_h\sum_m T_k^{g,h,m} TY_e^{g,h,m} - \sum_s S_{k+1}^{e,s} SA^{e,s}, \quad (18)$$

$$RS_{k+1}^r = RS_k^r - \sum_g\sum_h\sum_m T_k^{g,h,m} TC_r^{g,h,m} + \sum_p P_k^{r,p} PA^{p,r} \quad (19)$$

with initial conditions $ES_1^e = ES_{initial}^e$ and $RS_1^r = RS_{initial}^r$. Note that the recursive formulation is conservative. Minimum and maximum constraints on the *storage capacity* can be imposed as follows

$$ES_l^e \le ES_k^e \le ES_u^e, \quad (20)$$
$$RS_l^r \le RS_k^r \le RS_u^r. \quad (21)$$

In a simple form, the cumulative added value (CAV) is the difference between all revenues through sales of end products and all expenses on raw materials over a certain period of time. Here, the objective is defined as the CAV extended by interest on the capital balance, and can be formulated as follows

$$V_{k+1} = (1+\gamma)V_k + \sum_e\sum_s S_{k+1}^{e,s} SA_S^{e,s} \$^{e,s} - \sum_r\sum_p P_{k+1}^{r,p} PA^{r,p} P\$^{r,p} \quad (22)$$

$$J = V_H + \sum_r RS_{r,H} RV_r + \sum_e ES_{e,H} EV_e \quad (23)$$

where γ is the fractional interest rate and H is the horizon length. The last two terms in (23) account for end-storage appreciation which is necessary because we solve a finite horizon approximation of an infinite (or much longer)-horizon problem. The number of binary variables changes with the choice of the transition modeling. A formulation with multiple, distinct transition modes leads to the introduction of $H(n+m)$ binary variables *only* for the production modeling. Additional binary variables arise from the modeling of the purchase and sales actions. Their number can be limited through an appropriate choice of the validity sets $\Omega^{e,s}$ and $\Omega^{r,p}$.

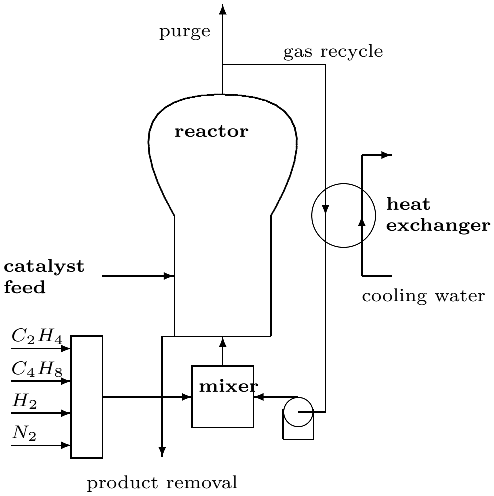
Because the objective as well as all constraints are linear and the total set of variables contains binary as well as continuous variables, the scheduling problem is a MILP:

maximize the objective J (23) subject to the objective recursion (22), the storage constraints (20, 21), the inventory recursion (18, 19), the purchase constraints (16, 17), the sales constraints (14, 15), the transition constraints (10, 11), and the grade constraints (9).

This MILP is, like most scheduling problems, NP-hard. This means that no polynomial time algorithm has been found for solving the problem. For NP-hard problems one can in general only hope that an acceptable solution be found in a reasonable time.

4. CASE STUDY: GAS PHASE HDPE PLANT

We consider a nonlinear model of an industrial high density poly-ethylene (HDPE) fluidized bed



performance channels (z)		inputs (u)	
1	polymer density	1	butylene feed flow
2	polymer melt index	2	hydrogen feed flow
3	production flow	3	catalyst feed flow
4	cooling water flow	4	setpoint pressure control
5	ethylene feed flow		
6	butylene feed flow		
7	hydrogen feed flow		
8	catalyst feed flow		
9	setpoint pressure control		

Fig. 7. Schematic process flow sheet of the gas phase HDPE polymerization process

Table 1. The five production grades for the HDPE reactor.

g	constraints	constraints
1	$932.8 < z^1 < 933.2$	$0.8 < z^2 < 1.2$
2	$937.8 < z^1 < 938.2$	$0.8 < z^2 < 1.2$
3	$937.8 < z^1 < 938.2$	$2.8 < z^2 < 3.2$
4	$932.8 < z^1 < 933.2$	$2.8 < z^2 < 3.2$
5	$942.8 < z^1 < 943.2$	$0.8 < z^2 < 1.2$

reactor, schematically described in figure 4. Here we consider 5 different product grades. The product grades are defined by bounds on the density (z^1) and the natural logarithm of the melt index (z^2) of the polymer as given in Table 1. The model is based on (Choi and Ray, 1985) and (McAuley, 1991) and further refined by Tousain and Van Brempt [4]. It contains about 1000 variables amongst which 40 differential variables. The model has the following properties:

- The fluidized bed consists of a bubble phase, an emulsion gas phase and an emulsion polymer phase. Both emulsion phases are assumed perfectly mixed. Mass transfer between the bubble phase and the emulsion gas phase is modeled using Fick's law.
- Co-polymerization reactions (butylene comonomer) occur on the surface of Ziegler-Natta catalyst particles in the emulsion polymer phase. The following reactions are modeled according to Ziegler-Natta kinetics (Dotson *et al.*, 1996): 1. catalyst activation, 2. chain initiation, 3. chain propagation, 4. chain transfer, 5. catalyst deactivation.
- On top of the reactor a wide gas cap is modeled as being ideally mixed.
- The counter current heat exchanger is modeled using a multi-compartment model.
- A purge outlet flow makes it possible to remove nitrogen (and other gases) from the reactor.
- Four low-level PI controllers stabilize the process
- A flow driven representation is used.

[4] IMPACT (Eureka project number E! 2063), IPCOS Technology, Leuven, Belgium

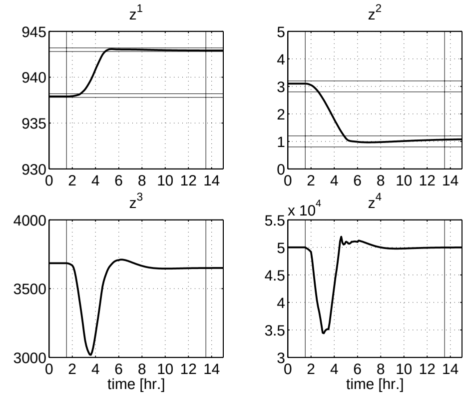


Fig. 8. (SSQP) Optimal trajectories of the density (z^1), melt index (z^2), production (z^3) and cooling water flow (z^4) for a transition from grade 3 to grade 5

The general mathematical formulation of the grade change problem is given by (8). For the HDPE process, the economic objective is defined as

$$V_{ec} = \int_0^T \left(\sum_{r=1}^{3} p_F^r C_r(z) - \sum_{e \in \{g,h,6\}} p_P^e Y_e(z) \right) dt, \tag{24}$$

where the feed flows are given by $C_1(z) = z^5$, $C_2(z) = z^6$, and $C_3(z) = z^7$. Y_g and Y_h refer to the production flows of the departure grade and the target grade, respectively. Y_6 refers to the production of off-spec material. It is assumed that during a transition, all material that is not within the specifications of either one of the grades connected by the transition is *off-spec* material. With the product prices, chosen according to a representative market scenario, 20 grade transitions have been optimized. These are used to construct the production database for the scheduler. A typical optimized transition result is shown in Figure 8.

A uniform discretization of time is chosen with production intervals of 12 hours. All transition times being smaller than 12 hours, we can use the single-interval transition model using production data which is computed on the basis of the static optimization of the grades and the dynamic optimization of grade transitions using (12,13). In

Table 2. Sales order and opportunity database for the HDPE production facility.

Sales of grade 1

s	$SA^{1,s}$	$S\$^{1,s}$	$\Omega_{1,s}$	$SO^{1,s}$
1	300,000	0.7	{8}	1
2	150,000	1.55	{15,22}	0
3	200,000	0.71	{15,22}	1
4	250,000	0.72	{43,50}	1
5	180,000	1.20	{71,78}	0

Sales of grade 2

s	$SA^{2,s}$	$S\$^{2,s}$	$\Omega_{2,s}$	$SO^{2,s}$
1	250,000	0.70	{8,15}	1
2	200,000	1.31	{22,29}	0
3	250,000	1.60	{28,35}	0
4	150,000	1.20	{43,50,57}	0
5	200,000	0.65	{64,71}	1

Sales of grade 3

s	$SA^{3,s}$	$S\$^{3,s}$	$\Omega_{3,s}$	$SO^{3,s}$
1	250,000	1.60	{8,15}	0
2	300,000	0.70	{22,29}	1
3	200,000	1.65	{50,57}	0
4	150,000	1.30	{64,65}	0

Sales of grade 4

s	$SA^{4,s}$	$S\$^{4,s}$	$\Omega_{4,s}$	$SO^{4,s}$
1	250,000	0.70	{8}	1
2	200,000	1.15	{22,29,36}	0
3	300,000	0.71	{36,43,50}	1
4	150,000	1.20	{57,64,71}	0

Sales of grade 5

s	$SA^{5,s}$	$S\$^{5,s}$	$\Omega_{5,s}$	$SO^{5,s}$
1	200,000	0.60	{8,15}	1
2	250,000	1.35	{15,22,29}	0
3	200,000	1.50	{29,36,43}	0
4	220,000	0.73	{50,57,64}	1
5	150,000	1.25	{71,78}	0

Sales of off-spec material

s	$SA^{6,s}$	$S\$^{6,s}$	$\Omega_{6,s}$	$SO^{6,s}$
1	100,000	0.32	{8,..,36}	0
2	100,000	0.33	{43,..,78}	0

Table 3. Raw material storage attributes for the HDPE plant.

r	RS^r_l	RS^r_u	RS^r_1	$RS^r_{H,l}$	$R\$^r$
1	0	10,000,000	1,100,000	600,000	0.45
2	0	450,000	60,000	35,000	0.60
3	0	2,000	250	100	3.30

addition, a fictional order/opportunity database has been constructed such that about 80% of the production capacity is used for production orders, the remaining is to be used for attractive sales opportunities. The sales order/opportunity database is given in Table 2. The sets of time instances at which transactions can take place are chosen sparse in order to limit the number of binary decision variables. The order/opportunity database should be seen as being the result of previous interactions of sales managers with the market. Initial inventory levels, the storage constraints and the end-storage appreciation of respectively the raw materials and the end products are finally given in tables 3 and 4. In traditional slate scheduling, the slate is going back and forth through a sequence of grades. The sequence is determined in such a way that the overall grade change effort, which can be characterized for example by grade change time or off-spec production, is minimized. Here, we exploit that further improvements can be achieved if, by means of advanced process control technology, all transitions are enabled, leading to a flexible scheduling approach. In this approach the production is allowed to switch to any other grade at each production interval, providing much improved flexibility to deal with changes in the market situation and to react to attractive sales opportunities. A solution to the flexible scheduling problem was found in several hours and to a guaranteed optimality of slightly more than 2.3 %. The objective value was equal to 3,339,845 which is over 16.8 % better than

Table 4. End product storage attributes for the HDPE plant.

e	ES^e_l	ES^e_u	ES^e_1	$ES^e_{H,l}$	$E\$^e$
1	0	5,000,000	325,000	300,000	1.02
2	0	5,000,000	315,000	300,000	0.98
3	0	5,000,000	270,000	300,000	1.06
4	0	5,000,000	270,000	300,000	1.05
5	0	5,000,000	306,000	300,000	1.03
6	0	5,000,000	22,000	0	0.33

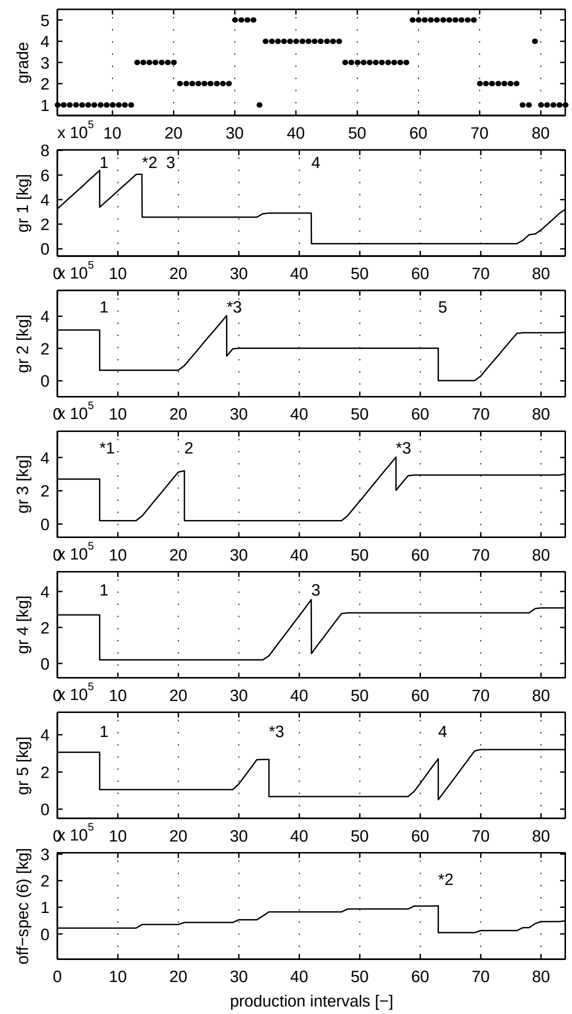


Fig. 9. Flexible schedule for HDPE production. Grades (top) and storage levels of the end-products (bottom)

the performance achieved with a fixed-duration slate. The result is displayed in figure 9.

5. CLOSED-LOOP STOCHASTIC MPC

In this section a closed-loop stochastic model-predictive control formulation will be discussed. The formulation is model-based and predictive, with constraints on the process variables. The approach is developed using the following observations:

- The smooth dynamic model (1) is assumed to be available, enabling to determine numerically a trajectory along which a time-varying linearized model can be computed. The trajectory is initially given by the scheduler and is subsequently improved in an iterative implementation of the closed-loop MPC formulation (CLMPC)
- CLMPC exploits the availability of future measurements, i.e. future feedback, and derives desirable feedback properties from this structure
- CLMPC considers stochastic disturbances, here assumed as Gaussian
- The constraints are taken into consideration with a backoff resulting from the effect of the stochastic disturbances
- In (van Hessem and Bosgra, 2003) we have shown that for any controller of the CLMPC there exists an equivalent finite horizon LQG controller (FHLQG) having the same performance and which can be implemented in a receding horizon mode
- The receding horizon CLMPC controller implementation inherits the stability properties of the optimal CLMPC solution
- In (van Hessem and Bosgra, 2002*a*),(van Hessem and Bosgra, 2002*b*) it has been shown how a Youla parametrization that renders CLMPC convex can be replaced by an innovations feedback controller structure which allows the solution to be put in a receding horizon formulation. It has an observer-based structure as shown in figure 11.
- For its actual solution, the CLMPC problem is decomposed into a deterministic constrained optimization problem and a minimum variance problem
- The solution of the latter provides the back-off used in the former
- The idea is shown in figure 10 based on a strong concept of classical LQG control (Athans, 1971). The deterministic optimization using the back-off is implemented as feedforward, the minimum variance controller provides the feedback. In fact any (robust) feedback controller with desirable disturbance-suppressing properties can be used here.

Consider a linear discrete time-varying stochastic system derived from the model (1):

$$\begin{pmatrix} x_{k+1}(\xi) \\ z_k(\xi) \\ y_k(\xi) \end{pmatrix} = \begin{pmatrix} A_k & G_k & B_k \\ C_k^z & O & D_k^z \\ C_k & F_k & O \end{pmatrix} \begin{pmatrix} x_k(\xi) \\ w_k(\xi) \\ u_k(\xi) \end{pmatrix} \quad (25)$$

where ξ is a Gaussian random process, $w_k(\xi)$ is a white noise sequence with variance matrix W_k and with the property $G_k W_k F_k^T = 0$ (process and measurement noise are independent). In 'lifted' form (see (Furuta and Wongsaisuwan, 1993)) over a time horizon of n samples, the vector-stochastic processes are

$$\mathbf{y}_k(\xi) = \begin{pmatrix} y_k(\xi) \\ \vdots \\ y_{k+n}(\xi) \end{pmatrix}, \mathbf{z}_k(\xi) = \begin{pmatrix} z_k(\xi) \\ \vdots \\ z_{k+n}(\xi) \end{pmatrix} \quad (26)$$

and so on, representing each signal $\mathbf{y}, \mathbf{z}$ from sample k to sample $k+n$. The two stochastic processes $\mathbf{y}, \mathbf{z}$ are the measured and performance output process, respectively; $\mathbf{z}$ contains variables appearing in the objective function or in the constraints, or in the inputs.

$$\begin{aligned} \mathbf{y}_k(\xi) &= G_{yx} x_k(\xi) + G_{yu} \mathbf{u}_k(\xi) + G_{yw} \mathbf{w}_k(\xi) \\ \mathbf{z}_k(\xi) &= G_{zx} x_k(\xi) + G_{zu} \mathbf{u}_k(\xi) + G_{zw} \mathbf{w}_k(\xi) \end{aligned}$$

Define a finite horizon observer, having time varying-feedback gains

$$\begin{pmatrix} \hat{x}_0(\xi) \\ \hat{x}_1(\xi) \\ \vdots \\ \hat{x}_n(\xi) \end{pmatrix} = \begin{pmatrix} I \\ \Phi_{1,0}^e \\ \vdots \\ \Phi_{n,0}^e \end{pmatrix} \hat{x}_0(\xi) + \begin{pmatrix} O & O & \cdots & O \\ B_0 & O & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ \Phi_{n,1}^e B_0 & \Phi_{n,2}^e B_1 & \cdots & O \end{pmatrix} \begin{pmatrix} u_0(\xi) \\ u_1(\xi) \\ \vdots \\ u_n(\xi) \end{pmatrix} + \begin{pmatrix} O & O & \cdots & O \\ N_0 & O & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ \Phi_{n,1}^e N_0 & \Phi_{n,2}^e N_1 & \cdots & O \end{pmatrix} \begin{pmatrix} y_0(\xi) \\ y_1(\xi) \\ \vdots \\ y_n(\xi) \end{pmatrix} \quad (27)$$

where the transition matrix $\Phi_{k,j}^e$ for the observer system mapping $\hat{x}_j$ to $\hat{x}_k$ is given for $k > j$ by

$$\Phi_{k,j}^e = A_{k-1}^e A_{k-2}^e \cdots A_j^e, \quad \Phi_{j,j}^e = I, \quad A_k^e = A_k - N_k C_k$$

and N_k is the Kalman predictor gain. Define

$$e_k(\xi) := x_k(\xi) - \hat{x}_k(\xi) \quad (28)$$

which recursively satisfies

$$e_{k+1}(\xi) = \underbrace{(A_k - N_k C_k)}_{A_k^e} e_k(\xi) + \underbrace{(G_k - N_k F_k)}_{G_k^e} w_k(\xi) \quad (29)$$

In lifted form: $\mathbf{e}_0(\xi) = G_{ee} e_0(\xi) + G_{ew} \mathbf{w}_0(\xi)$ and in terms of $(\Phi_{k,l}^e, G_k^e)$:

$$\begin{pmatrix} e_0(\xi) \\ e_1(\xi) \\ \vdots \\ e_n(\xi) \end{pmatrix} = \begin{pmatrix} I \\ \Phi^e_{1,0} \\ \vdots \\ \Phi^e_{n,0} \end{pmatrix} e_0(\xi) + \begin{pmatrix} O & O & \cdots & O \\ G^e_0 & O & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ \Phi^e_{n,1}G^e_0 & \Phi^e_{n,2}G^e_1 & \cdots & O \end{pmatrix} \begin{pmatrix} w_0(\xi) \\ w_1(\xi) \\ \vdots \\ w_n(\xi) \end{pmatrix} \tag{30}$$

The corresponding innovation sequence (Kailath, 1968), is given by

$$v_k(\xi) := y_k(\xi) - \hat{y}_k(\xi) = C_k e_k(\xi) + F_k w_k(\xi)$$

In lifted form

$$\mathbf{v}(\xi) = G_{ve} e_0(\xi) + G_{vw}\mathbf{w}(\xi) \tag{31}$$

and in terms of the matrices $(\Phi^e_{k,l}, G^e_k, C, F)$

$$\begin{pmatrix} v_0(\xi) \\ v_1(\xi) \\ \vdots \\ v_n(\xi) \end{pmatrix} = \begin{pmatrix} C_0 \\ C_1\Phi^e_{1,0} \\ \vdots \\ C_n\Phi^e_{n,0} \end{pmatrix} e_0(\xi) + \begin{pmatrix} F_0 & O & \cdots & O \\ C_1 G^e_0 & O & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ C_n\Phi^e_{n,1}G^e_0 & C_n\Phi^e_{n,2}G^e_1 & \cdots & F_n \end{pmatrix} \begin{pmatrix} w_0(\xi) \\ w_1(\xi) \\ \vdots \\ w_n(\xi) \end{pmatrix} \tag{32}$$

In (van Hessem and Bosgra, 2003) it has been shown that for the optimal CLMPC problem, an optimal output feedback controller can be equivalently replaced by an optimal innovations feedback controller. Let this be the law (assuming zero reference trajectories w.l.o.g.)

$$\mathbf{u}_0(\xi) = K_0 \mathbf{v}_0(\xi) \tag{33}$$

where $K_0 \in$ is a non-anticipative controller, i.e.

$$K_0 = \begin{pmatrix} K^{11} & O & \cdots & O \\ K^{21} & K^{22} & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ K^{n1} & K^{n2} & \cdots & K^{nn} \end{pmatrix}.$$

Then, at any time instant in the future, there exist matrices L_k and K_k of appropriate dimension, such that the control law

$$\mathbf{u}_k(\xi) = L_k \hat{x}_k(\xi) + K_k \mathbf{v}_k(\xi) \tag{34}$$

generates the optimal control sequence for the remainder of the horizon, provided the matrices are appropriately parametrized. This is a solution to a receding horizon implementation, using a recursive expression for the variance matrices and the feedback law. Observe that the actual controls applied at each instant are given by L^1_k and K^{11}_k which are the first n_u rows of the control law L_k and K_k respectively:

$$u_k = L^1_k \hat{x}_k + K^{11}_k v_k$$

From the preceding analysis it follows that $\mathbf{z}_k(\xi)$ in closed-loop is some function of $\hat{x}_k(\xi), e_k(\xi), \mathbf{w}_k(\xi)$. Since $\hat{x}_k(\xi), e_k(\xi)$ are independent of $\mathbf{w}_k(\xi)$ it follows that we only need to keep track of the joint

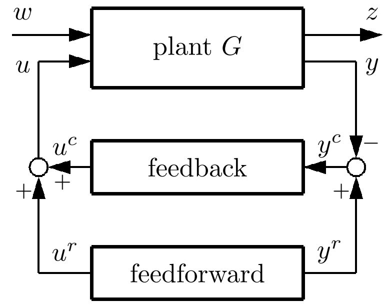


Fig. 10. Generalized plant for MPC

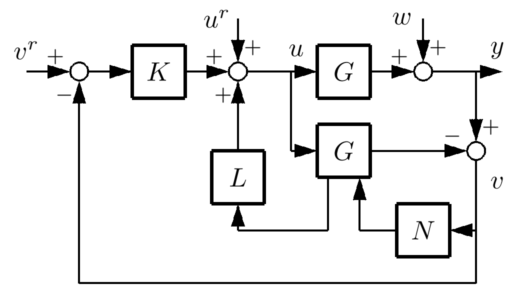


Fig. 11. Feedback part of CLMPC using innovations and state feedback

variance matrix V_k of $\hat{x}_k(\xi)$ and $e_k(\xi)$, generated by

$$\begin{pmatrix} \hat{x}_{k+1}(\xi) \\ e_{k+1}(\xi) \end{pmatrix} = \begin{pmatrix} A_k + B_k L^1_k & (N_k + B_k K^{11}_k)C_k \\ O & A_k - N_k C_k \end{pmatrix} \begin{pmatrix} \hat{x}_k(\xi) \\ e_k(\xi) \end{pmatrix} + \begin{pmatrix} (N_k + B_k K^{11}_k)F_k \\ G_k - N_k F_k \end{pmatrix} w_k(\xi)$$

and recursively given by

$$V_{k+1} = \begin{pmatrix} A_k + B_k L^1_k & (N_k + B_k K^{11}_k)C_k \\ O & A_k - N_k C_k \end{pmatrix} V_k \begin{pmatrix} \star & \star \\ \star & \star \end{pmatrix}^T + \begin{pmatrix} (N_k + B_k K^{11}_k)F_k \\ G_k - N_k F_k \end{pmatrix} W_k \begin{pmatrix} \star \\ \star \end{pmatrix}^T, \quad V_0 = \begin{pmatrix} O & O \\ O & P_0 \end{pmatrix}$$

As $e_k(\xi) \perp \hat{x}_k(\xi)$ for any k, the joint variance matrix V_k is block-diagonal for each k by construction. Thus the variance matrices follow from the Riccati recursions for the estimation error

$$P^e_{k+1} = A_k P^e_k A^T_k - N_k (C_k P^e_k C^T_k + F_k W_k F^T_k) N^T_k + G_k W_k G^T_k$$

having boundary condition $P^0_e = P_0$. The recursion for the state-estimate

$$P^{\hat{x}}_{k+1} = (A_k + B_k L^1_k) P^{\hat{x}}_k (A_k + B_k L^1_k)^T + (N_k + B_k K^{11}_k)(C_k P^e_k C^T_k + F_k W_k F^T_k)(N_k + B_k K^{11}_k)^T$$

having boundary condition $P^{\hat{x}}_0 = O$. L^1_k and K^{11}_k are given externally in every cycle by the solution of the control problem. The Kalman gain is

$$N_k = A_k P^e_k C^T_k (C_k P^e_k C^T_k + F_k W_k F^T_k)^{-1}$$

The factored variance matrix of the initial condition and disturbances are

$$P^x_k = E x_k(\xi) x_k(\xi)^T = P^{\hat{x}}_k + P^e_k = F_x F^T_x, \quad W_k = F_w F^T_w.$$

On the basis of the previous development, the closed-loop MPC problem is defined as

$$\textbf{(CLMPC)} \quad \min_{\mathbf{z}^r_k \in \mathbb{R}^{n_u}, K \in \mathbf{K}_0} f(\mathbf{z}^r_k) \quad r\sqrt{h^T_j Z_k h_j} + h^T_j \mathbf{z}^r \leq g_j \tag{35}$$

where $Z = E(\mathbf{z}_k(\xi) - \mathbf{z}_k^r)(\mathbf{z}_k(\xi) - \mathbf{z}_k^r)^T$. and f is a convex function. The constraints above follow from the nominal inequality constraints which trajectories must obey:

$$h_j^T \mathbf{z}^r \leq g_j, \quad j = 1 \ldots n_z$$

The extra term $r\sqrt{h_j^T Z_k h_j}$ in CLMPC is added as back-off to the constraints using an ellipsoidal relaxation, with the intention to prevent violation of constraints under stochastic disturbances. This problem is a convex optimization problem that can be solved for the global optimum using a solver for second-order cone problems, (Lobo *et al.*, 1998) . However, it is a computationally expensive problem in its present format for medium- and large-sized problems with many constraints and long prediction horizons, due to the present state of development of state-of-the-art cone programming solvers. These solvers utilize a vectorization of the problem data and given the large number of parameters in the controller K, the size of the problem tends to grow. This especially holds for the number of Lagrange multipliers in primal-dual interior-point methods. One solution to this situation is to derive new algorithms exploiting the ellipsoidal structure of the **(CLMPC)**, see for example (Dabbene *et al.*, 2003). However, there exists a different approach. Given the quadratic objective function

$$E \sum_{k=1}^{n} (z_k(\xi) - z_k^r)^T Q_k (z_k(\xi) - z_k^r) + \Delta u_k(\xi)^T R_k \Delta u_k(\xi) \tag{36}$$

where $\Delta u_k = u_k - u_{k-1}$, and given the fact that the optimal solution to **(CLMPC)** is a finite horizon LQG controller. Then in the absence of any inequality constraints, (36) can be separated into a deterministic optimal control problem and a stochastic optimal feedback problem by the separation property of LQG optimal control. The fact that the inequality constraints are treated with a back-off implies that the unconstrained case is effective for the stochastic problem. This motivates to separate (36) in a stochastic feedback problem and a deterministic feedforward problem. This implies a considerable simplification in the computational load of the problem, and makes real-time implementation a realistic opportunity. Assume that the weighting matrix $R = R^T > 0$ has a full rank Cholesky factorization $F_R F_R^T$. R and S are weighting parameters in the quadratic performance index in an LQG problem. The first step is to solve for given F_R, S, s the minimal variance problem (subproblem $\mathbf{CFHLQG}^A$):

$$\min_{K \in \mathbf{K}} \ \text{tr}\ S F_R F_Z F_Z^T F_R^T S^T \tag{37}$$

for

$$F_Z = \left(G_{zx} F_x \ \ G_{zw} F_v\right) + G_{zu} K \left(G_{vx} F_x \ \ G_{vw} F_v\right)$$

Suppose one has solved this problem for the optimal $Q^\star$, then the optimal variance matrix $Z^\star$ is also known, and the back-off terms using the ellipsoidal relaxation are readily computed:

$$\nu_j^\star = r\sqrt{h_j^T Z^\star h_j} \tag{38}$$

In the second step (subproblem $\mathbf{CFHLQG}^B$) one solves the optimal transition, in which the terms 38 are used to keep back-off to the constraints:

$$\begin{aligned} &\min_{\mathbf{u}^r} \qquad (S\hat{\mathbf{z}} - s)^T R (S\hat{\mathbf{z}} - s) \\ &\nu_j^\star + h_j^T \mathbf{z}^r \leq g_j, j = 1, \ldots, m \\ &\mathbf{z}^r = G_{zx} x_0^r + G_{zu} \mathbf{u}^r + G_{zw} \mathbf{w}^r \end{aligned} \tag{39}$$

where the performance weighting matrix S and vector s have to be chosen. Note that the separation into two subproblems also implies that separate tuning of the feedback part and of the feedforward transition part has been realized. This enables especially to modify the criterion in the second step to include a strong component representing the economic performance of a transition.

6. CASE STUDY (CONTINUED)

Application of a grade change from grade 5 to grade 3 has been investigated for the CLMPC approach. We require the grade change to be done under two bias disturbances: +0.0025 kg/h on the catalyst flow, and −0.05 kg/h on the hydrogen flow, results of imprecise valve positions and errors in flow measurements. The hydrogen bias influences the melt-index and a negative value of this disturbance is chosen to counteract the transition from grade 5 to grade 3. The controller must increase the hydrogen feed to compensate for this bias possibly violating the feed limitation. A positive bias in the catalyst feed leads to a significant increase in energy hold-up. The PI loop in the basic control loop increases the cool water flow threatening to saturate the flow constraint. Additionally, measurement noise is active on all output measurements, such that controller parameters cannot grow unbounded (high gain feedback) to compensate the persistent disturbances, which adds robustness to the control design. The performance index has appropriately chosen quadratic weights on performance variables 1, 2 and 4 and on inputs 1, 2 and 3. The constraints are given in table 5. The computed open-loop performance

Table 5. Constraints on process variables

Variable		lo	up
z_4	[10^4kg/h]	2.5	5.2
z_5	[10^2kg/h]	0.0	1.5
z_6	[kg/h]	0.1	1.0
z_7	[kg/h]	0.2	2.0
z_9	[bar]	0.0	1.0

trajectories of density, melt index, coolwater flow and production rate are shown in figure 12. Without feedback a serious offset results from the computed optimal reference trajectories, due to the active disturbances which are not taken into consideration in the optimization. In figure 13, the

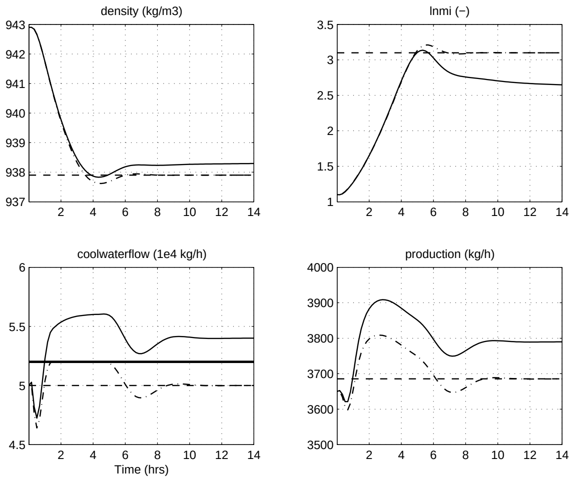


Fig. 12. Open loop: real (solid), reference (dash-dot), target (dash)

performance trajectories of the same performance variables are shown under closed-loop CLMPC feedback. We see no violation of the feedwater flow constraint as a consequence of the appropriate back-off in the computation of the reference trajectories. Figures 14 and 15 shows a close-up

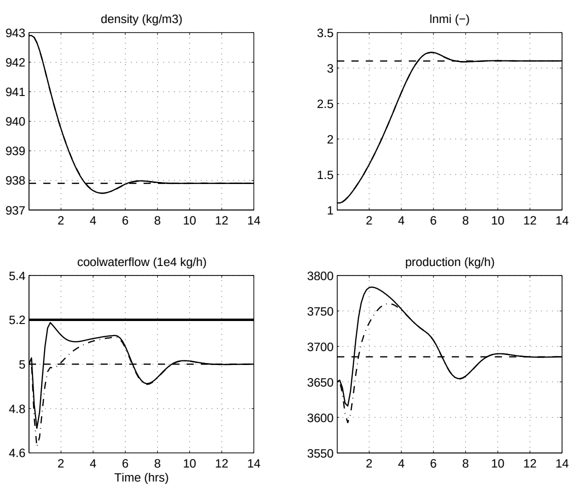


Fig. 13. Closed-loop: real (solid), reference (dash-dot), target (dash)

of the reference trajectories of the cool water and hydrogen feed flows, respectively, where the back-off is visualized via the 1-dimensional confidence intervals (projected ellipsoids). Due to the back-off, inequality constraints play no role in the part of the control moves related to disturbance rejection. Consequently, the control updates needed to remove the biases on the feeds are very smooth. Apart from the real actual trajectories, the error bars in the figures show the evolution of the variance disturbances which are expected (and can be accomodated) by the CLMPC controller.

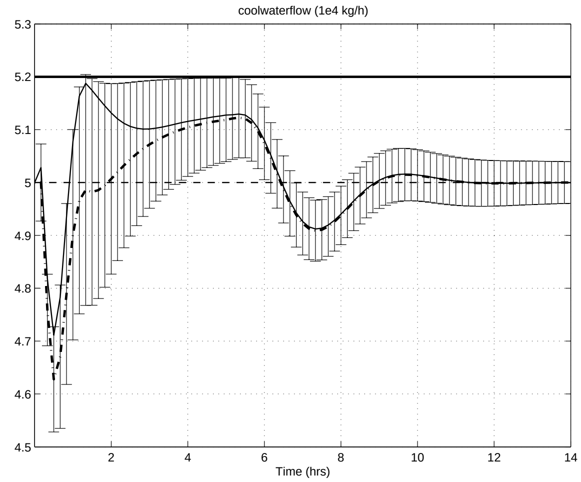


Fig. 14. Closed-loop cool water flow: real (solid), reference (dash-dot), target (dash)

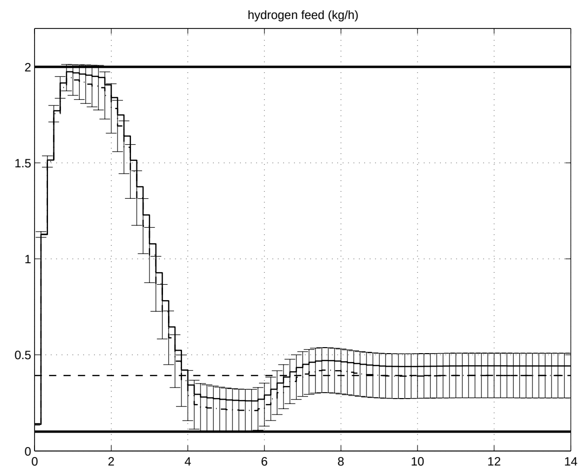


Fig. 15. Closed-loop hydrogen feed flow: real (solid), reference (dash-dot), target (dash)

7. CONCLUSIONS

In this paper a scheduling approach has been presented that enables the production management of a multi-grade chemical plant to operate the plant according to a market-responsive and economics-based objective. For single-machine multi-grade processes, such a scheduler can be designed by capturing the purchasing, production and sales decisions and their effect on the company's objective into a MILP which can be solved using standard software. Process transitions and their effect on material flows are included in the formulation without the need to introduce additional binary variables. Reasonable solution times were encountered for the HDPE production test problem that was considered in this paper. The application of the flexible short term scheduling approach to a gas phase HDPE manufacturing plant for a fictional market situation demonstrates a significant increase in added value compared to the traditional fixed and variable duration slate scheduling.

For the actual realization of grade transitions the paper has presented a new closed-loop MPC formulation that separates a stochastic MPC problem into a deterministic constrained feedforward trajectory optimization solution and a stochastic minimum-variance feedback solution. The stochastic solution provides the back-off needed in the feedforward part. Conversely, the implementation of the back-off allows the feedback control to realise a proper disturbance suppression task. The combined scheduling and closed-loop MPC solution provides a coherent integration of process control tasks covering the days-to-minutes range of time scales.

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