

# Cost Function Design for Economically Optimal Grade Changes for a Polyethylene Gas Phase Reactor

Per-Ola Larsson, Johan Åkesson and Niklas Andersson

**Abstract**—This paper considers optimization of stationary production and dynamic grade changes for a gas phase polyethylene reactor. The designed cost function considers costs of inflows and revenues from produced polymer. At dynamic optimization, the cost function uses grade variable intervals for defining on-grade polymer and includes economical incentives to produce on-target polymer. Additionally, it also considers a preparatory time interval prior defined transition time, used for economical preparation of reactor state. A previously published model of a gas phase reactor is used and several grade changes are optimized, showing the effects of an economical cost function.

## I. INTRODUCTION

Polyethylene gas phase reactors (GPR) are today able to produce several different grades defined by industrial standard quality variables. Production is a continuous process and polyethylene properties are altered by manipulating the inflows of fresh raw material. This is valuable for producers since they can adapt to market conditions, both in terms of raw material pricing, product price and market demands. This has led to product campaigns varying in length between a few days up to weeks. During grade transition, i.e., the transferring of production from one product to another, there is in general production of polymer that is not acceptable as neither start nor end grade and must be sold at a lower price. This, together with inflow costs, must be taken into account when performing economic optimization of grade changes.

The grade change problem has been formulated and solved in several different ways. Quadratic criteria penalizing deviation from end grade multiplied by production rate, yielding less off-grade polymer, was used in [1] together with a sequential method. With a similar method, quality variable intervals defining polymer grades was used in [2] by having different quadratic functions inside and outside the intervals. Collocation based optimization of grade changes, using quadratic criteria has been considered in e.g., [3]. However, translating economics into weights in a quadratic criteria is a difficult task. Economics was considered to an extent in [4], comparing minimization of total transition time and minimization of off-grade polymer production. A more direct approach was considered in [5], where maximization of profit during the transition was performed using quality variable intervals and a sequential method. However, the optimization procedure did not enforce quality variables to be on-target, only inside acceptable intervals, and thus not considering

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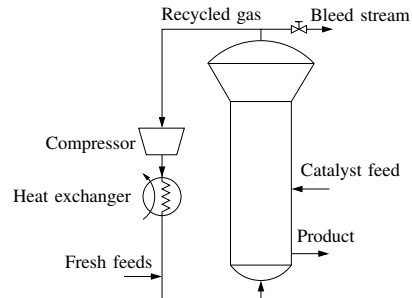


Fig. 1. Schematic diagram of a gas phase reactor with recycle system.

product consistency towards market and raw material and product price changes. The contributions of this paper are the development of a continuously differentiable cost function that considers plant economy and that uses quality variable intervals. The cost function also adds incentives to produce a polymer that is on-target. Additionally, the optimization includes a time interval prior defined transition time, used for economical preparation of reactor state. A model of a GPR previously published in [6] is used for demonstrating the cost function and its implications by maximizing profit during several different transitions.

## II. PROCESS DESCRIPTION

### A. Process Overview

The process consists of the reactor and a cooling system with a compressor and heat exchanger, see the schematic diagram in Figure 1 and also [6]. The gas phase, providing the fluidization in the reactor, consists of the monomer ethylene, co-monomer butene and hydrogen and also inert nitrogen, while the solid phase is polyethylene and a heterogeneous Ziegler-Natta catalyst. Ethylene is the main raw material, while butene and hydrogen are added for density and melt index control, respectively. Nitrogen is used as carrier for added catalyst and heat removal from the exothermic reaction [6]. The unreacted gas at the top of the reactor may either be bled off in the bleed stream used for pressure and impurity control of the reactor or it is recycled through the cooling system. The recycled part is added to the fresh gas feed and since the single pass conversion is as low as 2–5%, the recycle stream is much larger than the fresh feed [6]. The produced polyethylene is withdrawn at the bottom of the reactor.

### B. Modeling Assumptions

A first-principles model, capturing the main dynamics of the process, is presented in [6]. Several assumptions are made and motivated, keeping model complexity low, yielding it advantageous for grade transition optimization and evaluation

of cost function design. Gas and solid phases in the reactor are assumed well mixed, the temperature in the reactor is uniform and perfectly controlled, and a constant bed level is achieved by a perfect bed level controller. Variable bed level has been considered in e.g., [4] but this is often not used in practice due to the risk of polymer sticking to reactor walls, creating hot spots. Further, the time-delay associated with the recycle flow through compressor and heat exchanger is negligible compared to reactor dynamics and the gas exiting with the product outflow is captured directly and recycled.

### C. Mathematical Model

The process model, described in [6], is a macro scale model suited for grade transition optimization and control [7]. Based on the assumptions in II-B, the following mass balances are written for the gas phase components,

$$V_g \frac{dx_e}{dt} = u_e/M_e - b_e - r_e \quad (1)$$

$$V_g \frac{dx_b}{dt} = u_b/M_b - b_b - r_b \quad (2)$$

$$V_g \frac{dx_h}{dt} = u_h/M_h - b_h - r_h \quad (3)$$

$$V_g \frac{dx_n}{dt} = u_n/M_n - b_n, \quad (4)$$

where  $x_i$ ,  $i \in \{e, b, h, n\}$ , are molar concentrations of ethylene, butene, hydrogen and nitrogen, respectively. The concentrations are increased by fresh inflows of the gases, i.e.,  $u_i$ , and decreased by bleed flows  $b_i$  and reaction rates  $r_j$ ,  $j \in \{e, b, h\}$ , for the reactive components. The inflows together with the total bleed  $u_B$  are control variables and the component bleeds may be calculated from respective mole fraction and total bleed [6].  $M_i$  are the molar weights and  $V_g$  is the gas volume in the reactor and is assumed constant.

The Ziegler-Natta catalyst is assumed to have one active site, as in [4], and the number of moles of active catalyst sites in the bed,  $Y$ , may be modeled as [6]

$$\frac{dY}{dt} = u_Y a_Y - Y \frac{r}{B_w} - k_d Y - k_f Y x_h + k_h N x_e \quad (5)$$

$$N = \frac{Y k_f x_h}{k_h x_e + r/B_w}, \quad (6)$$

where  $N$  is the number of moles of sites deactivated by hydrogen, modeled using the stationary hypothesis. The bed weight  $B_w$  is assumed constant motivated by only minor variations in the gas mixture and polymer density. The first term on the right hand side of Eq. (5) is inflow of active sites where  $u_Y$  is a control flow and  $a_Y$  is a catalyst constant, while the second term is outflow of catalyst. Next, two terms of deactivation of catalyst are found, and the last term considers reactivation. The constants  $k_d$ ,  $k_f$ , and  $k_h$  are rate constants for deactivation, site deactivation by hydrogen, and reactivation reaction with ethylene, respectively. Parameter values for the model are found in Table I.

Reactor pressure  $P$ , with a reference value of  $P_v$ , is calculated using the gas components as,

$$P_i = x_i RT, \quad i \in \{e, b, h, n\} \quad (7)$$

$$P = P_e + P_b + P_h + P_n, \quad (8)$$

TABLE I  
PARAMETER AND CONSTANT VALUES IN PROCESS MODEL.

Param.	Value	Unit	Param.	Value	Unit
$P_v$	17.225	bar	$k_{ph}$	0.036	$\text{m}^3/(\text{molh})$
$T$	360	K	$k_h$	3.6	$\text{m}^3/(\text{molh})$
$M_e$	28.05	g/mol	$k_f$	0.3168	$\text{m}^3/(\text{molh})$
$M_h$	2.016	g/mol	$k_d$	0.36	1/h
$M_b$	56.11	g/mol	$k_1$	0.100	$(\text{g}/10\text{min})^{1/3.5}$
$M_n$	28.0	g/mol	$k_2$	0.400	$(\text{g}/10\text{min})^{1/3.5}$
$R$	$8.314 \cdot 10^{-5}$	$\text{m}^3 \text{bar}/(\text{molK})$	$k_3$	0.700	$(\text{g}/10 \text{ min})^{1/3.5}$
$V_g$	150	$\text{m}^3$	$p_1$	989	$\text{kg}/\text{m}^3$
$B_w$	35 000	kg	$p_2$	10.3	$\text{kg}/\text{m}^3/\ln(\text{g}/10\text{min})$
$a_Y$	0.548	mol/kg	$p_3$	-38.0	$\text{kg}/\text{m}^3$
$k_{pe}$	306	$\text{m}^3/(\text{molh})$	$p_4$	0.300	—
$k_{pb}$	10.8	$\text{m}^3/(\text{molh})$			

where  $R$  and  $T$  are the ideal gas constant and reactor temperature, respectively, and  $P_i$  is the partial pressure of component  $i$ . Due to the bed level assumption, the production rate  $r$  is equal to the total reaction rate, and found directly from the reaction rates and molar weights  $M_i$  as,

$$r = M_e r_e + M_b r_b + M_h r_h \quad (9)$$

$$r_i = Y k_{pi} x_i, \quad i \in \{e, b, h\}, \quad (10)$$

where  $k_{pi}$  are pseudo-propagation rate constants. Compared to [6], a small rate constant is added for hydrogen.

The two most frequently used quality variables for polyethylene are melt index  $MI$ , an indirect measure of the molecular weight, and density  $\rho$ , see e.g., [7]. Polymer produced at a certain time instant has in general different quality variables values than the mixture of polymer in the reactor, i.e., the cumulative values of the bed. This is because the polymerization reaction is much faster than the dynamics of the gas and solids phase in the reactor [8]. Instantaneous values for  $MI$  and  $\rho$  in this study are calculated as

$$MI = (k_1 + k_2 x_h/x_e + k_3 x_b/x_e)^{3.5} \quad (11)$$

$$\rho = p_1 + p_2 \ln MI + p_3 (x_b/x_e)^{p_4}, \quad (12)$$

while the cumulative values are found as

$$\frac{d}{dt} MI_c^{-\frac{1}{3.5}} = \frac{1}{B_w/r} \left( MI^{-\frac{1}{3.5}} - MI_c^{-\frac{1}{3.5}} \right) \quad (13)$$

$$\frac{d}{dt} \left( \frac{1}{\rho_c} \right) = \frac{1}{B_w/r} \left( \frac{1}{\rho} - \frac{1}{\rho_c} \right). \quad (14)$$

The four equations above have the same structure as derived in [8]. The parameter values used in this paper can be found in Table I.

The reactor states, algebraic variables and control flows in the model are collected in  $\mathbf{x}$ ,  $\mathbf{w}$  and  $\mathbf{u}$ , respectively.

### III. GRADE DEFINITION AND PRICES

The two cumulative quality variables  $MI_c$  and  $\rho_c$  in the previous section define a polyethylene grade and are also center values for the intervals that define acceptable values for premium priced product. Added to the list of quality variables is the reactor pressure with a target value of  $P_v$ , see Table I. The pressure has not a direct effect on product properties in the model, but can instead be seen as a reactor operations quality variable affecting long term production.

TABLE II  
GRADE DEFINITIONS WITH INTERVALS, POLYMER SELL PRICES AND  
INSTANTANEOUS PROFITS.

Grade $j$	$MI_j$	$\rho_j$	$P_j$	$x_h/x_e$	$x_b/x_e$	$S_j$	$R_j$
A	0.35	944.0	$P_v$	0.40	0.70	10.35	21544
B	0.35	948.5	$P_v$	0.84	0.44	10.35	21847
C	0.90	952.0	$P_v$	0.75	0.83	10.64	25063
D	0.50	952.0	$P_v$	1.03	0.45	9.45	9575
E	0.25	942.0	$P_v$	0.38	0.61	11.25	33882
Interval	$\pm 0.025$	$\pm 1$	$\pm 0.15$	-	-	-	-

TABLE III  
COSTS OF INFLOWS AND OFF-GRADE POLYMER SELL PRICE.

$C_e$	$C_b$	$C_h$	$C_n$	$C_Y$	$S_{\text{off}}$
8	10	60	0.03	750	6.75

The quality variable values and intervals for all grades A–E considered in this paper can be found in Table II.

The polymer sell price (\$/kg) depends on the polymer properties. Premium sell price for grade  $j$ , denoted  $S_j$ ,  $j \in \{A, \dots, E\}$ , is assumed to be given only if all quality variables are inside their defined intervals, otherwise the off-grade price  $S_{\text{off}}$  (\$/kg) is given. However, for e.g., consistency reasons to the market, the quality variables should be as close to target values as possible. Table II gives the premium prices  $S_j$ , and Table III gives the inflow costs  $C_i$  (\$/kg),  $i \in \{e, b, h, n, Y\}$ , and off-grade polymer sell price  $S_{\text{off}}$ .

#### IV. MODELING AND OPTIMIZATION FRAMEWORK

The process is modeled using the Modelica language, which is a high level language for complex physical models, where the user may mix differential and algebraic equations. For optimization, the open source platform JModelica.org is used [9]. This platform has been successfully used on significantly larger reactor models, see [10].

JModelica.org contains an implementation of a simultaneous optimization method based on collocation on finite elements [11]. State and algebraic variables are parametrized by Lagrange polynomials of order three and two, respectively, based on Radau points, while the inputs are constant during each finite element. This yields a non-linear program (NLP) with structure, which is exploited by the solver IPOPT [12].

#### V. OPTIMIZATION FORMULATION

##### A. General Process Constraints

Specifications of  $MI_c$  and  $\rho_c$  sets the ratios of the reactants, but not the production level. If the product sell price is greater than the inflow costs, the production level will in general be as high as possible, limited by, for instance, safety, post-processing capacity, lump formation due to too high ethylene partial pressure or catalyst amount and insufficient heat removal. This sets limits on e.g., ethylene concentration, and subsequently, limits on the other reactant concentrations may be set. For the reactor pressure to be on its target value, nitrogen is added, which also should be able to remove enough heat. In addition, to handle impurities, a non-zero

bleed is preferred in industry, see [1] and [4], which sets a lower limit on the bleed. The behavior of the inflows, both in terms of range and rate of change, is limited due to e.g., pump capacities and safety.

##### B. Stationary Optimization

During stationary production, the quality variables should be on targets, while the reactor is operated in an economically beneficial way, respecting process safety and constraints. The instantaneous production profit for grade  $j$ , denoted  $R_j$ , is the difference between revenue from sold polymer and inflow costs as

$$R_j = S_j r - \sum_{i \in \{e, b, h, n, Y\}} C_i u_i.$$

The profit may be maximized during stationary production by solving the following optimization problem,

$$\begin{aligned} \min_{\mathbf{x}, \mathbf{x}, \mathbf{w}, \mathbf{u}} \quad & -R_j \\ \text{s.t. Eqs. (1)–(14)} \\ & \mathbf{x}_{\min} \leq \mathbf{x} \leq \mathbf{x}_{\max} \\ & \mathbf{w}_{\min} \leq \mathbf{w} \leq \mathbf{w}_{\max} \\ & \mathbf{u}_{\min} \leq \mathbf{u} \leq \mathbf{u}_{\max} \\ & \dot{\mathbf{x}} = \mathbf{0} \\ & MI_c = MI_j, \rho_c = \rho_j, P = P_j, \end{aligned} \quad (15)$$

The inequality constraints are related to the limitations in the previous section and the three last equality constraints yield production corresponding to grade  $j$  in Table II.

##### C. Dynamic Optimization

Upon performing a transition it is important not to only focus on the end grade. Before the actual transition, preparations may be performed in the reactor state such that the transition becomes easier. If a transition time  $t_T$  is defined, then the grade transition cost function may be divided into two parts that concentrate on start and end grade, respectively. In each part, the revenue is a function of the quality variables and production rate. In the ideal case, if all quality variables are inside their interval, the sell price is  $S_j$ , while if at least one is outside, the product sell price is  $S_{\text{off}}$ . Considering the first part, i.e., time before  $t_T$ , the instantaneous profit for start grade  $j$  is,

$$R_j = ((S_j - S_{\text{off}})\theta_j(Q) + S_{\text{off}})r - \sum_{i \in \{e, b, h, n, Y\}} C_i u_i,$$

where the effective sell price is  $(S_j - S_{\text{off}})\theta_j(Q) + S_{\text{off}}$ .  $Q$  contains the quality variables, i.e.,  $Q = [MI_c, \rho_c, P]$ , and  $\theta_j(Q) = 1$  if all quality variables are inside their intervals defined by grade  $j$ , else  $\theta_j(Q) = 0$ .  $R_j$  is non-linear and discrete due to  $\theta_j(Q)$  and must be made continuously differentiable for efficient optimization. One approximation is

$$\tilde{\theta}_j(Q) = \left( \sum_{i=1}^{n_Q} \left( 2 \frac{q_i - q_{ji}}{w_{ji}} \right)^{n_i} + 1 \right)^{-1},$$

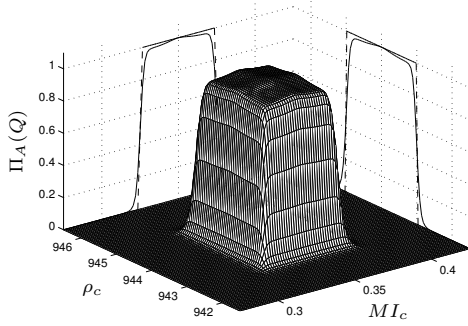


Fig. 2. Example of  $\Pi_A(Q)$  with only  $MI_c$  and  $\rho_c$ , i.e.,  $n_Q = 2$ , with parameters  $n_i = 20$ ,  $p = 0.95$ ,  $h_{Ai} = w_{Ai}/6$ . Projections of  $\Pi_A(Q)$  (–) and  $\theta_A(Q)$  (--) are also shown for comparison.

where  $n_Q$  is the length of  $Q$ ,  $q_i$  is the  $i$ th quality variable in  $Q$ ,  $q_{ji}$  and  $w_{ji}$  are  $q_i$ 's target value and interval width, respectively, specified by grade  $j$ , and  $n_i$  is a sufficiently large even integer giving satisfying approximation error. An alternative would be to use e.g., trigonometric functions [5].

An incentive to be on-target is that premium sell price  $S_j$  is only given when all quality variables are on-target, i.e., a reward for product consistency towards the market. This can be formulated by giving a large percentage of  $S_j$  when on-grade but off-target, and then add the small remainder depending on how close the quality variables are their target values. This is an approximation of the relation between price and quality variables in Section III. However, the small remainder should only be greater than the cost of change of inflows required to move the quality variables from the interval boundary to the target. This cost is in general very small in comparison to the cost of the fresh feeds. Thus,  $\tilde{\theta}_j$  may be given an extension fulfilling these properties as,

$$\Pi_j(Q) = \tilde{\theta}_j(Q) \left( p + \frac{1-p}{n_Q} \sum_{i=1}^{n_Q} \left( \left( 2 \frac{q_i - q_{ji}}{h_{ji}} \right)^2 + 1 \right)^{-1} \right),$$

where  $p \in [0, 1]$  determines the percentage of the difference  $S_j - S_{\text{off}}$  that at least is given additionally when on-grade compared to off-grade,  $q_i$  is the  $i$ th quality variable in  $Q$ ,  $q_{ji}$  is  $q_i$ 's target value for grade  $j$  and  $h_{ji}$  defines the width of the effective sell price peak at target value for quality variable  $q_i$  and grade  $j$ . Thus, for every quality variable being on-target, a  $(1-p)/n_Q$ -part of  $S_j - S_{\text{off}}$  is added to the effective sell price. An example of  $\Pi_A(Q)$  with only  $MI_c$  and  $\rho_c$  can be found in Figure 2.

The start grade  $j$  and the end grade  $k$  at a transition have different on-grade functions, i.e.,  $\Pi_j$  and  $\Pi_k$ . To calculate the approximated total profit during a transition, a switch between  $\Pi_j$  and  $\Pi_k$ , defined by  $t_T$ , is included in the instantaneous profit  $R$  during a grade change as

$$\begin{aligned} R = & (S_j - S_{\text{off}})\Pi_j(Q)T(t_T)r \\ & + (S_k - S_{\text{off}})\Pi_k(Q)(1 - T(t_T))r \\ & + S_{\text{off}}r - \sum_{i \in \{e, b, h, n, Y\}} C_i u_i, \end{aligned}$$

The switch may be well approximated by

$$T(t_T) = 1/2 - \arctan(\gamma(t - t_T)) / \pi,$$

with a large  $\gamma$ . In this study,  $\gamma = 500$  has been used, which gave a sufficiently small approximation error compared to an ideal step function.

The dynamic optimization problem on the time interval  $t_{\text{start}} \leq t \leq t_{\text{end}}$  of transferring production from grade  $j$  to grade  $k$  may be stated using the above  $R$ , as

$$\begin{aligned} \min_{\dot{\mathbf{u}}} & \int_{t_{\text{start}}}^{t_{\text{end}}} (-R + \dot{\mathbf{u}}^T \mathcal{U}_d \dot{\mathbf{u}}) dt \\ \text{s.t.} & \text{Eqs. (1)–(14), } \mathbf{u} = \int_{t_{\text{start}}}^t \dot{\mathbf{u}} d\tau \\ & \mathbf{x}_{\min} \leq \mathbf{x} \leq \mathbf{x}_{\max} \\ & \mathbf{w}_{\min} \leq \mathbf{w} \leq \mathbf{w}_{\max} \\ & \mathbf{u}_{\min} \leq \mathbf{u} \leq \mathbf{u}_{\max} \\ & \dot{\mathbf{u}}_{\min} \leq \dot{\mathbf{u}} \leq \dot{\mathbf{u}}_{\max} \\ & \mathbf{x}(t_{\text{start}}) = \mathbf{x}_j, \mathbf{u}(t_{\text{start}}) = \mathbf{u}_j \\ & \mathbf{u} = \mathbf{u}_k, t \geq t_{\text{end}} - T_c \end{aligned} \quad (16)$$

where  $\mathbf{x}_j$  and  $\mathbf{u}_j$  are state and control flows from stationary optimization of grade  $j$  and  $\mathbf{u}_k$  is from stationary optimization of grade  $k$ .

In order to penalize highly varying inflows, the control flow derivatives  $\dot{\mathbf{u}}$  are used as optimization variables and a quadratic term with the diagonal matrix  $\mathcal{U}_d$  is introduced.

The control signal constraint of holding  $\mathbf{u}$  constant to end grade specified values during a time interval of  $T_c$  at the end of the optimization interval is due to the finite optimization horizon. If the constraint is not included, it would be economically beneficial to close all inflows just prior  $t_{\text{end}}$  since this will not effect production until after  $t_{\text{end}}$  due to reactor dynamics. Thus, in this case, the instantaneous profit would be greater at  $t_{\text{end}}$  than found at stationary optimization, but the end point is not stationary and impossible to retain.  $T_c$  should be chosen large enough such that the system essentially is in stationarity at  $t_{\text{end}}$ , independently of the control flow movement prior  $t_{\text{end}} - T_c$ .

Inequality constraints on  $MI$  and  $\rho$  are set for preventing excessive under- and overshoots since this may give a product with a mixture of polymers that have significantly different  $MI$  and  $\rho$ . Even though the cumulative values are on-target, the transition polymer may in these cases differ considerably from on-target polymer produced at stationarity, see [1] for a further discussion.

## VI. OPTIMIZATION RESULTS

As all grades cost less than sell price to produce, the stationary optimization aims to maximize production, which has limits as pointed out in Section V-A. Assuming the limit of raw material is high, it is the ethylene partial pressure, catalyst, and down-stream capacity that sets the limits. To minimize the amount of expensive catalyst used, the ethylene partial pressure should be as high as possible. Table IV shows the most important limits used at all optimizations, both static and dynamic. At all economically optimal stationary solutions, both ethylene partial pressure and production rate

TABLE IV  
VARIABLE LIMITS AT OPTIMIZATION.

Variable	Lower limit	Upper limit
$r$	5000	13500
$P_e$	1	6
$u_B$	5000	10000
$MI$	$\min(MI_j, MI_k) - 2w_{j1}$	$\max(MI_j, MI_k) + 2w_{j1}$
$\rho$	$\min(\rho_j, \rho_k) - 2w_{j2}$	$\max(\rho_j, \rho_k) + 2w_{j2}$
$P$	$P_v - 0.3$	$P_v + 0.3$

are on their upper bounds, and amount of catalyst is well inside limits. Additionally, the bleed flow is at its minimum, yielding minimum waste of raw materials and diluent. In Table II, the resulting instantaneous profits  $R_j$  are reported together with the ratios  $x_h/x_e$  and  $x_b/x_e$ . It is mainly the sell price  $S_j$  that contribute to the differences in profits as the inflow costs are similar for all grades, dominated by ethylene.

From the stationary optimization, initial and end values are given to the dynamic optimization which is specified to be 36 h long and divided into three parts,

- 12 h before transition time  $t_T$ .
- 12 h after transition time  $t_T$ .
- 12 h with control flows equal to stationary optimization result of end grade, i.e.,  $T_c = 12$  h.

This does not specify the transition time, only upper limits on preparation and completion times are defined.

The on-grade functions  $\Pi_j$  in the optimizations utilizes  $MI_c$ ,  $\rho_c$  and  $P$  as quality variables with the intervals in Table II. For simplicity, all quality variables are treated equally by setting the function parameters as in the example in Figure 2. The under- and overshoot limits on  $MI$  and  $\rho$  are given by using start and end grade values and intervals, see Table IV. These limits are process and user specific and are trade-offs between fast change of cumulative values and the range of instantaneous polymer properties in the end product. Hard limits are also set on the reactor pressure due to e.g., safety reasons. The cost of highly varying inflows is set by  $U_d$ , yielding smooth control flows.

Four consecutive grade changes, A to E, have been optimized, and quality variables, control flows, on-grade functions, production and economics are found in figures 3–5. The element length in the discretization is chosen to 10 min. and the figures show only the first 24 hours of optimization, since stationarity is reached at this time for all optimizations.

Considering the first grade change, A–B, only an increase of density requires changes in both hydrogen and butene concentrations. To prepare a fast transition, inflows of hydrogen and butene do small changes that first decrease the instantaneous value  $\rho$ . Then, by making fast changes in the inflows, the rate of change of  $\rho_c$  during the off-grade time is greater than if the preparation not had been performed. This is since  $\rho$  was given time to accelerate to a greater rate of change before leaving start grade specification. Preparative operations like this are found in all considered grade changes. They are the preparation equivalents of making under- and overshoots in the instantaneous values after the start grade has been left, which is also performed at the transitions.

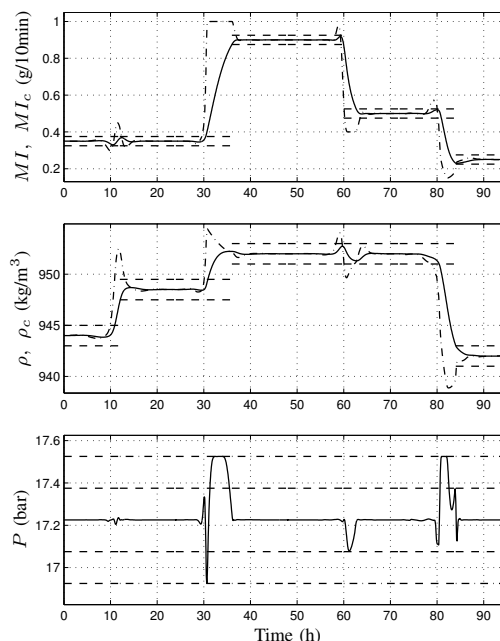


Fig. 3. Upper and middle: Instantaneous  $MI$  and  $\rho$  (· · ·), cumulative  $MI_c$  and  $\rho_c$  (—) and quality variable intervals (---). Bottom:  $P$  (—) with quality interval (---) and limits (· · ·).

Additionally, the inflows are synchronized such that the polymer is on-grade during only a short time interval, even though the inflows change over a significantly longer time period. In this first grade change, the overshoot of  $\rho$  reaches the constraint set in Table IV. During the transition, inflow of nitrogen is closed, making room for the hydrogen overshoot and an increase of catalyst holds production high even with the undershoot of butene inflow, yielding time constants for  $MI_c$  and  $\rho_c$  as small as possible. Only a small increase of bleed is used, minimizing waste, and the transition is performed in approximately 1 h as can be seen from the on-grade functions in Figure 5.

At the second grade change, B–C, starting at  $t = 24$  h, both  $MI$  and  $\rho$  are to be increased. Rapid increase of  $u_b$  and decrease of  $u_e$  and a small increase in  $u_h$  causes  $MI$  to be on overshoot limit, thus giving as fast rise of the cumulative value as possible. However,  $u_e$  may not be decreased too much since this will decrease the production and hence increase the time constant for  $MI_c$  and  $\rho_c$ . The overshoot constraint of  $MI$  is kept active while decreasing  $u_h$  and increasing  $u_e$  and  $u_b$  such that  $\rho$  is as large as possible. To make room for more butene in the reactor without too much bleed,  $u_n$  is completely closed and reactor pressure is at its upper limit. The transition is performed in approximately 6 h.

A decrease of only  $MI_c$ , as in the change C–D, is performed by decreasing  $u_b$  and increasing  $u_h$ . More nitrogen is added to the reactor to keep pressure at target due to the loss of butene. Production rate is kept high with increased  $u_e$  and  $u_Y$ , making time constants for  $MI_c$  and  $\rho_c$  small. As quality variables come close to grade D specifications, the nitrogen is turned off and the reactor is filled with correct concentrations of hydrogen and butene. The transition takes 2.5 h and hold both  $\rho_c$  and  $P$  inside quality variable intervals.

Grade changes with large decreases in hydrogen concen-

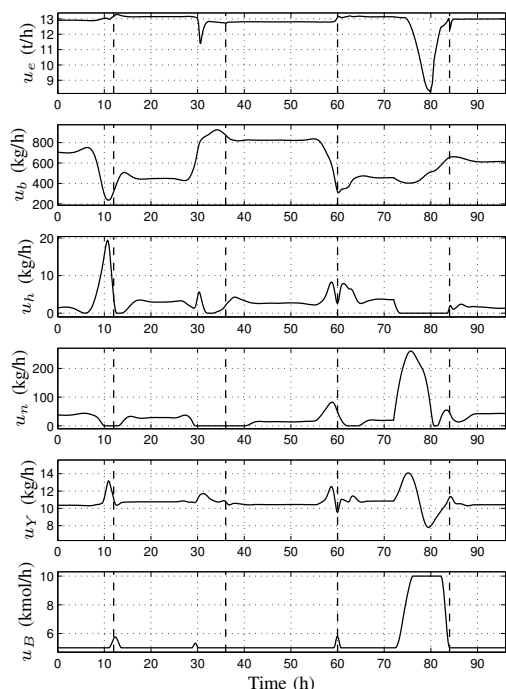


Fig. 4. Control flows at transitions. Vertical lines (--) indicate transition times defined by  $t_T$ .

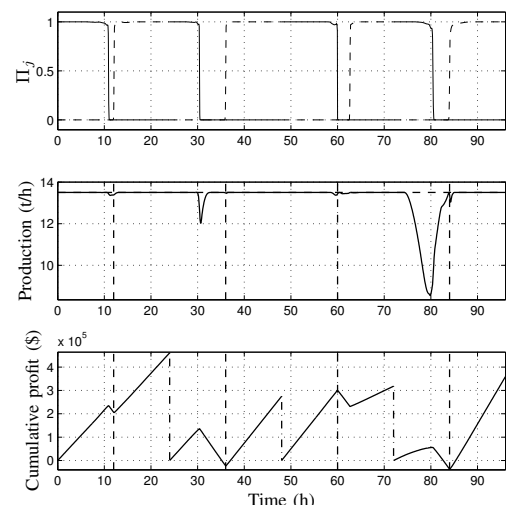


Fig. 5. Upper: On-grade functions  $\Pi_j$  (— and --). Middle: Production rate. Bottom: Cumulative profit, set to 0 at optimization start. Vertical lines (--) indicate transition times defined by  $t_T$ .

tration are considered hard, see e.g. [1], due to the slow hydrogen dynamics in the reactor. This is seen in the last transition, D–E. To lower the hydrogen concentration as fast as possible,  $u_h$  is completely closed and the bleed is at maximum. To minimize raw material waste,  $u_e$  is decreased substantially, and the amount of catalyst in the reactor is increased such that the production rate is not decreased too much. A large amount of inexpensive nitrogen is instead inserted into the reactor to keep pressure and to bleed off until enough hydrogen is removed. Close to transition time,  $u_e$  and  $u_n$  are again increased and decreased, respectively, making time constants for  $MI_c$  and  $\rho_c$  small again, yielding fast transfer. A small overshoot of  $u_b$  and small corrective actions in  $u_h$  give fast settling of  $MI_c$  and  $\rho_c$  and the transition takes approximately 4 h. This transfer shows that

a bleed stream is effective for hydrogen decreases.

For all transitions, the grade change is made such that the grade with highest instantaneous profit is produced as for a long time as possible, as seen in Figure 5. This is due to the maximization of cumulative profit.

## VII. SUMMARY

An economic cost function, with a preparatory time interval prior grade change, utilizing quality variable intervals and giving incentives to produce on-target polymer, has been presented and used for several transitions. The main effects of the cost function are

- the grade with highest profit of the two transition grades is produced for as long time as possible.
- control flows are synchronized to yield short off-grade periods and are actively changed over larger time intervals than the off-grade periods.
- hydrogen and butene inflows make preparations of instantaneous variables before defined transition time, and the transitions are performed with significant under- or overshoots. This yields the cumulative values, defining the grade, to move fast through the off-grade interval.
- production rate is often as high as possible, set mainly by ethylene and catalyst inflows, yielding a small time constant for cumulative quality variables.

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