Hybrid Approach to Polymer Grade Transition Control

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A hybrid approach to model predictive control of a polymer grade transition problem is developed. The controller is posed as a mixed integer programming problem in which the discrete elements of the algorithm include both linear switching models used to approximate the nonlinear process and operating heuristics that are incorporated as propositional logic inequalities. The algorithm is tested in simulation on a polypropylene loop reactor system. Feed rates of monomer, hydrogen, and catalyst are manipulated to regulate slurry density, melt flow rate, and production rate, for various grades. Robust performance is demonstrated for grade transitional control. © 2004 American Institute of Chemical Engineers *AIChE J,* 50: 2502–2513, 2004
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Introduction

Modern polymer production encompasses a wide variety of products and techniques. Industrially produced polymers find use in many applications, such as beverage containers, bicycles, electronics, floor coverings, and specialty parts for automobiles and airplanes. In order to remain competitive and provide a wide array of products, polymer manufacturers must have the ability to produce many different types of polymers for use in these applications. Different types, or grades, of polymers are distinguished by various attributes such as density, average molecular weights, melt index, and other physical properties (McAuley and MacGregor, 1992). Each grade of polymer is characterized by a unique combination of these physical properties. Often these different grades of polymer are produced using dedicated plant equipment. Therefore, it becomes necessary to change the operating conditions of the reactor in order to shift production from one grade of polymer to another.

Grade transition is a process that requires the adjustment of the current steady state operating conditions of a polymer reactor in order to establish a new set of steady state operating conditions. This transition is accomplished through either manual adjustment of the process conditions or by automatic control systems through the adjustment of process set-points. Many of the variables controlling the transition are changing simultaneously. Some of these determine the rate of the transition while others determine the properties of the material being produced (Sinclair, 1987). The sequencing of these variables depends on the objectives of the transition. The minimization of the transition time is very important to maximize "prime" material production for the plant. Material that does

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not meet any specific grade requirement is denoted "off-specification" or "off-grade". During a transition, production of off-specification material results in a product that must either be blended with prime material or sold off at a (significantly) lower market price.

Grade transition control

The recent literature highlights several different methods used for the automatic control of grade transitions. These include the application of optimal control algorithms and industrial heuristics-based approaches. The work of McAuley and MacGregor (McAuley and MacGregor, 1992, 1993) is an example of the application of an optimal control algorithm to the control of polymer grade transition. In this study, three product grades were considered in a fluidized-bed polyethylene reactor. The optimal transition strategy was developed by defining an objective function combined with the use of a nonlinear programming solver. The decision variables used in the optimization were step changes in the manipulated variables. Another example of the use of an optimal control algorithm is the work of Takeda and Ray (Takeda and Ray, 1999). This study considers a bimodal loop polyethylene reactor. The manipulated variable profile was determined using the control-vector parameterization method. Wang et al. (Wang et al., 2000a,b) approached the problem of optimal control of an industrial slurry polyethylene reactor. The solution technique used for this study is similar to that of Takeda. The major difference in this study are the trial functions used in the control-vector parameterization. In this study the switching time of each trial function is allowed to vary and becomes a parameter in the optimization.

A heuristics-based approach to grade transition was taken by Debling, et al. (Debling et al., 1994). These heuristics, or experienced-based rules, were derived from industrial application or from the assumed advantages they offer. The heuristical strategies used consisted of changing process set-points, switching controllers on or off, and changing manipulated variables based on time. Two other studies that approached grade transition in a heuristical manner were those of Sirohi and Choi (Sirohi and Choi, 1997) and Lynch (Lynch, 2000). Sirohi and Choi applied a simple strategy manipulating the bed level and catalyst flow rate of a homogeneous stirred bed polyethylene reactor model according to two different heuristical strategies. Lynch applied industrially derived heuristics to Basell's *Spheripol* process.

Hybrid systems

A system that involves a grade transition can be cast as a hybrid system. A general class of hybrid systems consists of systems governed by continuous dynamics that are directed by discrete (logic) dynamics (Bemporad and Morari, 1999, 2001; Bemporad et al., 2000b; Branicky et al., 1998). Examples of continuous dynamic variables in the grade transition problem include temperatures, concentrations, and polymer properties, among others. Examples of discrete variables are valve positions, pump speeds, or various process status indicators. The hybrid aspects of the control problem also arise due to high-level decisions (recipe evolution or condition-based logic statements traditionally used in batch or PLC control) directing low-level continuous controllers (traditionally used in CSTR or DCS control).

To facilitate the application of hybrid systems theory to a control or optimization problem, an appropriate model structure is required. Both piecewise affine (PWA) (Sontag, 1981, 1996) and mixed logical dynamical (MLD) (Bemporad et al., 2000a, 1999; Bemporad and Morari, 2001; Bemporad et al., 2000b) systems have successfully been used for the description of such systems. The PWA and MLD system modeling approaches integrate continuous dynamics and discrete decisions in a framework that is readily adaptable to linear programming techniques, making them advantageous for use in on-line control. Hybrid system modeling and control has been applied in a variety of forms. The use of switched systems is probably the most prevalent use of hybrid systems theory in the literature. During the modeling of extremely nonlinear processes, linearization about multiple operating points is done in order to include the best linear approximation of the original system's dynamics. The operating regime dictates the relevant linearizations to be used. The switching of the various models can be accomplished by assigning integer variables to each linearization and activating the one that best describes the process at that time. Numerous control methods based on using multiple models are discussed in the book edited by Murray-Smith and Johansen (Murray-Smith and Johansen, 1997).

The approach that will be used in this study for the control of the grade transition problem relies on the description of the system as a hybrid system. The hybrid systems approach will allow the combination of various aspects of previous grade transition studies into a framework that models the automation of process logic/heuristics while at the same time allows optimization of the continuous grade transition problem. The logic/heuristics serve as high-level decisions or conditions that direct the low-level controller used in each study. The objective of this work is to utilize a hybrid systems modeling approach in order to combine heuristics with continuous grade transition so that an optimal grade transition may be found.

Piecewise affine (PWA) systems were introduced by Sontag (Sontag, 1981) over two decades ago as a method for modeling nonlinear control problems involving continuous and discrete dynamics. The PWA system is described by the following discrete state-space equations

$$x(k+1) = A_i x(k) + B_i u(k) + f_i \tag{1}$$

$$y(k) = C_i x(k) + g_i \tag{2}$$

for

$$\begin{bmatrix} x(k) \\ u(k) \end{bmatrix} \in \chi_i \tag{3}$$

where x, u, and y are the system states, inputs, and outputs respectively A_i, B_i, and C_i are constant matrices, f_i and g_i are constant vectors, and the ith matrix and vector is contained in the χ_ith partition of the state and input set. One way to accomplish the switching between partitions is through the use of logical if-then-else statements (Sontag, 1981). The switching from one partition of the state space to another may also be defined by linear equalities or inequalities.

A relatively new approach to the modeling of hybrid systems is the mixed logical dynamical (MLD) system framework (Bemporad et al., 2000a, 1999; Bemporad and Morari, 2001; Bemporad et al., 2000b). This modeling method allows for the inclusion of discrete dynamics through the use of constraints in the form of mixed-integer linear inequalities. Discrete (logic) decisions in the process are represented as Boolean expressions. Next, in order to incorporate the logic decisions into the dynamics of the system, the variables are transformed into 0-1 integers, and included in the state equations. Once this is done, the constraints on the continuous and integer values may then be expressed as mixed-integer linear inequalities. An MLD system is represented in discrete time form as

$$x(k+1) = Ax(k) + B_1u(k) + B_2\delta(k) + B_3z(k) \quad (4)$$

$$y(k) = Cx(k) + D_1u(k) + D_2\delta(k) + D_3z(k) \quad (5)$$

$$E_2\delta(k) + E_3z(k) \leq E_1u(k) + E_4x(k) + E_5 \quad (6)$$

where x, u, and y are the states, inputs, and outputs respectively, δ and z are vectors of auxiliary (Williams, 1985) binary and continuous variables, and A, C, B_i, D_i, and E_i are suitable constant matrices. The states, inputs, and outputs may be made up of both continuous or logic values (that is, $x \in \{x_c, x_l\}$, $u \in \{u_c, u_l\}$, $y \in \{y_c, y_l\}$). The auxiliary variables (δ, z) appear as a consequence of the development of mixed-integer linear inequalities (Bemporad et al., 2000a, 1999; Bemporad and Morari, 2001; Bemporad et al., 2000b).

A benefit of using the MLD system method for the modeling of hybrid systems is that the HYSDEL (HYbrid Systems DEscription Language) (Torrisi et al., 2000) compiler has been developed to efficiently generate the MLD realization from a description of the system. This tool is very effective in reducing the model and constraints to a minimal form by eliminating redundant constraints that are introduced through the conversion from logic statements to mixed-integer inequalities. Another benefit of MLD systems is that they have been shown to be equivalent to other hybrid system modeling techniques, such as the PWA system (Heemels et al., 2001).

Model Predictive Control

The use of feedback control allows for the compensation of process disturbances and modeling errors. Model Predictive Control (MPC) has been identified as a successful feedback control strategy for model-based control applications. The model predictive controller solves an on-line optimization problem at time step, with the goal of minimizing a specific objective. A primary objective is the minimization of the future deviations of a controlled variable from a set-point (Morari et al., 2002). MPC makes use of a process model to predict the response to specific process inputs. Two of the major benefit of MPC are: (1) the explicit incorporation of process constraints into the optimization problem, and (2) the handling of multivariable problems of arbitrary (and possibly nonsquare) dimension (García et al., 1989). A potential disadvantage of MPC is that it must solve an on-line optimization problem at each sample time. For very large problems, the solution time could increase to the point that real-time implementation is compromised.

MPC has been shown to be adaptable for application to hybrid systems in several instances (Bemporad et al., 1999; Bemporad and Morari, 2001; Gatzke and Doyle III, 2001; Morari, 2001). Specifically, references (Bemporad et al., 1999; Bemporad and Morari, 2001; Morari, 2001) detail the use of the MLD realization to formulate a hybrid model predictive controller. A similar strategy is adopted in this work, resulting in a mixed integer programming problem. The term "mixed-integer" arises from the fact that some of the variables in the optimization are restricted to take on integer values, usually 0 or 1. The solution of mixed-integer problems can be achieved through several methods including branch-and-bound, outer-approximation, generalized Benders decomposition, cutting plane, and other methods (Bemporad and Morari, 2001; Grossman and Kravanja, 1995; Winston, 1995). The optimization software used for this research is ILOG CPLEX 6.5 which utilizes the branch-and-bound technique.

Modifications of the branch and bound technique have been applied in order to increase the computational efficiency of the algorithm (Gatzke and Doyle III, 2002). This becomes necessary due to the fact that the addition of integer variables to an optimization problem increases the difficulty of the problem. It is known that, as a worst case, the solution time for a mixed-integer problem grows exponentially with the size of the problem (Raman and Grossman, 1991). Because of this, large mixed-integer optimizations may be too computationally intensive to solve for an on-line control problem. Recent advances in processor speed, and the efficiency of the available solvers, coupled with the inherently slow time constants in process systems, indicate promise for the feasibility of real-time solution of these problems.

Loop Reactor Model

The polymer reactor used for the control study discussed in this article is an extension of a model developed by Zotti (Zotti, 1999). The reactor model under consideration is the first loop in a multistage industrial olefin loop reactor. Specifically, propylene, and propylene/ethylene (co)polymerization grade transitions are studied in this reactor. Figure 1 shows the multistage loop reactor train. Each reactor is shaped like a loop, as the name implies, with the first and second loops connected in series. Studies of polymerization in loop reactors in the past have focused on detailed kinetic, residence time distribution, heat and mass transfer, species population balances, and sedimentation effects (Takeda and Ray, 1999; Zacca et al., 1996, 1997; Zacca and Ray, 1993) of the reactor. The process model used in this study includes the previously mentioned effects (excluding sedimentation) but relies on a lumped-parameter model instead of population balances to detail the dynamics of the system.

In the previous studies, liquid slurry loop reactors have either been modeled as a distributed (loop) system, or have been approximated as a continuous stirred-tank reactor (CSTR). Zacca and Ray (Zacca and Ray, 1993) have shown that when the recycle rate in the loop reactor is very high, the CSTR approximation is justified. The reactor considered in this study has a high recycle rate, and the time per pass in the loop is much lower than the approximate one h. residence time in

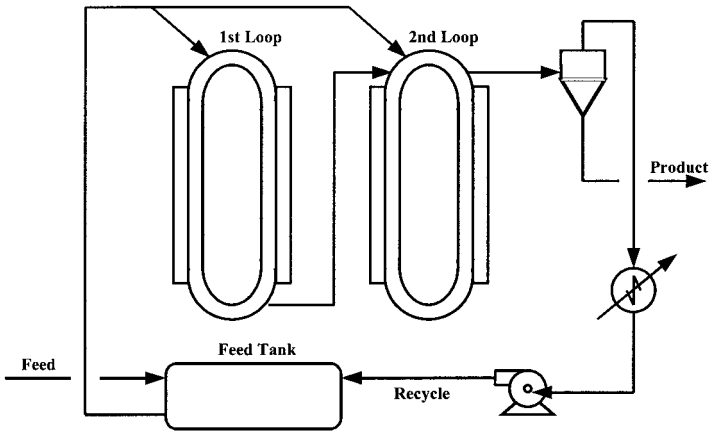

Figure 1. Loop reactor train.

Feed to the loops consists of liquid propylene monomer, catalyst, hydrogen (as a chain transfer agent), and ethylene as a comonomer. The polymer is extracted from the effluent of the second reactor as product and a recycle stream is cooled and returned as feed to the first reactor.

the loop, motivating a CSTR model. Polymerization schemes carried out in loop reactors are usually designed to be multistage, with two loops being placed in series in the plant. The reaction conditions from one reactor to another are varied in order to control the properties of the polymer product. A single loop of this process is considered in this work, since this model can be easily extended to the second.

Liquid monomer, Zeigler-Natta catalyst, and hydrogen is charged to the loop as feed. The monomer here consists of propylene containing a variable amount of propane which depends on the purity of the feed. Liquid ethylene may also be charged for random copolymerization with the propylene. The catalyst considered in this study is modeled with one active site and includes temperature effects governed by an Arrhenius dependence. Hydrogen acts as a chain transfer agent in polymerization reactions to control molecular weight. Increases in the hydrogen concentration in the reactor will reduce the average molecular weight of the polymer being produced. In low to moderate concentrations hydrogen is known to activate the catalyst, however, in large concentrations it can deactivate the catalyst in the reactor. In this model, the activity of the catalyst is dynamically effected by the hydrogen concentration. Although both reactor temperature and hydrogen concentration can effect the deactivation of the catalyst, the value of the deactivation coefficient is considered constant in this model. The rate of polypropylene production is given by

$$R_1 = \frac{L_1 M_{\mathrm{Cat1}}}{K\tau_1 + 1} \tag{7}$$

where L_1 is the activity of the catalyst, M_{Cat1} is the mass of the catalyst, K is the catalyst deactivation constant, and τ_1 is the loop residence time. For copolymerization, the polypropylene production rate is adjusted according to the copolymerization equation (Ravve, 2000). It is assumed for the purposes of this study that there are no side reactions. The model allows the ability to use the temperature set point of the reactor either as a manipulated input in the optimization problem or the reactor temperature as a disturbance to the process. Figure 2 shows the typical process output response around one steady state to a series of step changes in the inputs. One important response to note is that of the melt flow rate to a step decrease in the monomer flow rate. As can be seen, the final melt flow rate for the five percent monomer flow rate decrease is greater than the final melt flow rate for the 10% monomer flow rate decrease. This gain change is due to competing effects of the hydrogen concentration, density, and production rate in the reactor. Figure 3 shows that the final hydrogen concentration in the reactor for the five percent monomer flow rate decrease is greater than the ten percent case.

The mass balances for the species present in the reactor are the following

$$V_R x_1 \frac{dC_{H2}}{dt} = q_0 C_{H2_0} - q_1 x_{1,\mathrm{eff}} C_{H2} - Fac_{H2} \frac{MW_{H2}}{MW_{PP}} R_P \tag{8}$$

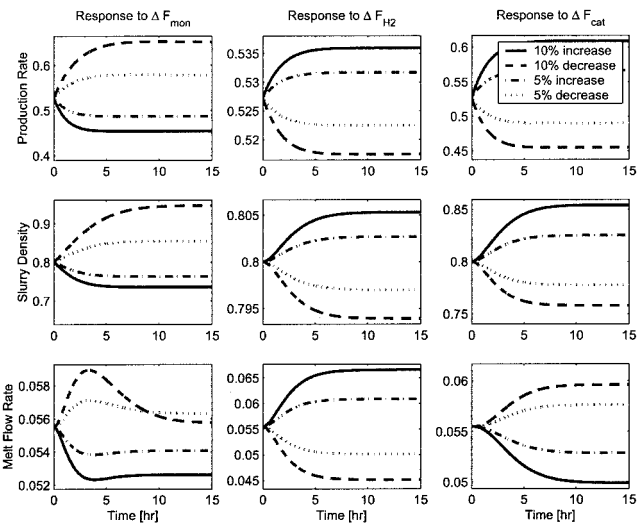

Figure 2. Process output responses to positive and negative step changes in the inputs.

The columns show the separate controlled variable responses to step changes in the manipulated monomer flow, hydrogen flow, and catalyst flow, respectively. The values given in the graph for the production rate, slurry density, and the melt flow rate are scaled by their maximum expected values.

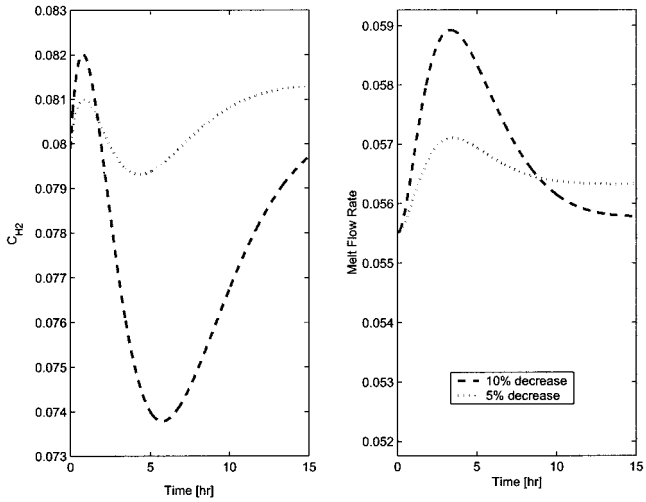

Figure 3. Process responses to negative step changes in the monomer flow rate.

The values given in the graph for the hydrogen concentration and the melt flow rate are scaled by their maximum expected values.

$$V_R \frac{dC_{\text{Cat1}}}{dt} = q_0 C_{\text{Cat1}_0} - q_1 F_{\text{Dis}} C_{\text{Cat1}} \tag{9}$$

$$V_R \frac{dC_{PP}}{dt} = -q_1 F_{\text{Dis}} C_{PP} + R_P \tag{10}$$

$$V_R x_1 \frac{dC_{C3e}}{dt} = q_0 C_{C3e_0} - q_1 x_{1,\text{eff}} C_{C3e} - Fac_{C3e} R_1 \tag{11}$$

$$V_R x_1 \frac{dC_{C3a}}{dt} = q_0 C_{C3a_0} - q_1 x_{1,\text{eff}} C_{C3a} \tag{12}$$

$$V_R x_1 \frac{dC_{C2e}}{dt} = q_0 C_{C2e_0} - q_1 x_{1,\text{eff}} C_{C3e} - Fac_{C2e} R_2 \tag{13}$$

where the subscripted species $H2$, $Cat1$, PP, $C3e$, $C3a$, $C2e$ designate hydrogen, catalyst 1, polymer, propylene, propane, and ethylene, respectively. C_i, Fac_i, and MW_i are concentrations, consumption factors, and molecular weights of species i, F_{Dis} is the discharge factor of polymer from the reactor that takes into account a greater slurry density being withdrawn than the average in the reactor, V_R is the slurry volume in the reactor, which is assumed to be constant, q_0 and q_1 are the flow rates of the feed and effluent streams, R_P, R_1, R_2 are the overall reaction rate, and the rate of consumption of propylene and ethylene, respectively. Finally, x_1 and $x_{1,\text{eff}}$ are the volume fractions of liquid monomer in the reactor and effluent stream. The catalyst average residence time distribution balance is given by

$$V_R \frac{dC_{\text{Cat1}}\tau_1}{dt} = -q_1 F_{\text{Dis}} C_{\text{Cat1}}\tau_1 + M_{\text{Cat1}} \tag{14}$$

where $C_{\text{Cat1}}\tau_1$ is the product of the concentration of catalyst and the average residence time distribution, and M_{Cat1} is the mass of catalyst in the reactor. The relative reaction rates of propylene and ethylene during copolymerization are determined by the combination of reactivity ratios and the corresponding kinetic expressions (Ravve, 2000).

A balance on the mass fraction of ethylene in the copolymer is also included in the model, as this value is important for determining the properties of the product

$$V_R \frac{dC_{C2e,PP}}{dt} = -q_1 F_{\text{Dis}} C_{C2e,PP} + R_2 \tag{15}$$

Here, $C_{C2e,PP}$ is the mass fraction of ethylene in the polymer product. Another important property for determining the product grade is the melt index (MI) or melt flow rate (MFR) of the polymer. The cumulative MI (MFR) of the polymer is calculated using a correlation relating it to the cumulative intrinsic viscosity (IVc) of the polymer in the reactor

$$\ln(MFR) = a_1 + a_2 IVc + a_3 IVc^2 + a_4 IVc^4 \tag{16}$$

where a_i are appropriate constants derived from experiments. The cumulative intrinsic viscosity is found through the following balance equation

$$V_R \frac{dIVcM_{PP}}{dt} = IViR_P - IVcM_{PP} F_{\text{Dis}} q_1 \tag{17}$$

where $IVcM_{PP}$ is the product of the IVc and the polymer mass in the reactor, IVi is the instantaneous intrinsic viscosity of the polymer. The IVi of the polymer can be found through a correlation relating it to the concentration of hydrogen in the reactor.

Table 1 lists the continuous states of the model and their corresponding initial state values.

The polymerization reactions studied here are exothermic and it is necessary to remove heat from the reactor in order to control its temperature. The reactor is unstable at the desired operating point, and the optimization framework described here requires that the process must be open-loop stable. However, the reactor can be stabilized by a PI controller on the reactor temperature. It is assumed that the cooling water tem-

Table 1. Initial State Values for the Loop Reactor Grade Transition

State	Value	Units
C_{H2}	7.9892×10^{-6}	kg H_2/L liquid
C_{Cat1}	1.4107×10^{-5}	kg Cat1/L slurry
C_{PP}	0.28270	kg polymer/L slurry
C_{C3e}	0.21450	kg propylene/L liquid
C_{C3a}	0.18980	kg propane/L liquid
C_{C2e} †	0	kg ethylene/L liquid
$C_{\text{Cat1}}\tau_1$	1.9373×10^{-5}	(kg cat—hr)/L slurry
$C_{C2e,PP}$ †	0	kg ethylene in polymer/L slurry
$IVcM_{PP}$ †	2.8930×10^4	(dL—kg polymer)/g
Tr	343.15	K
Twi †	323.15	K

(Values obtained from Zotti (Zotti, 1999), except † which are derived for this work.)

Table 2. Parameter Values for The Loop Reactor Grade Transition

Parameter	Value	Units
Vr	4.8675×10^4\	L slurry
Tcr	364.6	C
$MWH2$	2.016	kg/kmol
$MWC3e$	42.081	kg/kmol
$MWC3a$	44.097	kg/kmol
$MWC2e$	28.054	kg/kmol
DPP	0.900	kg polymer/L polymer
$FacH2$	1.0	kmol H_2/kmol polymer
$FacC3e$	1.0	kg propylene/kg polymer
$Fdis$	1.2	(L polymer/L slurry) in effluent/ (L polymer/L slurry) in reactor
K	0.25	1/hr
R	8.314	J/(mole—K)
Ea	5.024×10^4	J/mole
$Tref$	298.15	K
$CpC3e$	2.6563	kJ/(kg—K) @ 25 C
$CpC3a$	2.7460	kJ/(kg—K) @ 25 C
$CpC2e$	6.6828	kJ/(kg—K) @ 25 C
$CpPP$‡	2.0	kJ/(kg—K) @ 25 C
$CpH2$	14.275	kJ/(kg—K) @ 25 C
Cpw	4.1802	kJ/(kg—K) @ 25 C
dHr‡	2219.0	kJ/(kg—K) @ 25 C
$r1$†	0.1	
$r2$†	25.0	
Fw*	6.7909×10^5	kg water/hr
AU*	1.0663×10^6	kJ/(K—hr)
kp*	2.075	
ki*	124.62	

(Values obtained from Zotti (Zotti, 1999), except † from Moore (Moore Jr., 1996), ‡ from Shouche (Shouche, 2002), and * which are derived for this work.)

perature can be controlled instantaneously through use of a cooling unit integrated into the recycle jacket stream. The gain and time constant for the controller are listed in Table 2. The energy balance for the reactor takes the following form

$$Cp_R V_R \frac{dTr}{dt} = Hfd - Heff - Q + Hr \tag{18}$$

where Hfd, $Heff$, and Hr are the enthalpies of the feed, effluent, and the reaction, respectively. Q is the heat removed by the cooling water, Tr is the temperature of the reactor, and Cp_R is the total heat capacity of the reactor contents.

Model Predictive Control of the loop reactor

As discussed previously, MPC requires the solution of an optimization problem at each sample time based on a specified performance objective. On the basis of a model of the process, the optimization routine makes use of a series of predictions of future process outputs over a specified horizon to minimize the performance objective.

MLD system formulation of the loop reactor

The MLD system model developed for the loop reactor grade transition problem consists of 13 continuous and four logic states. 11 continuous states are described by the 10 differential equations given in the previous section plus a state that is required to define the integral term of the PI controller used to stabilize the temperature of the process. The remaining two continuous states are used to define current measured density and melt flow rate of the process. The logic states included are introduced in order to describe the evolution of the model. Three of the logic states are introduced in order to describe the allowed phases of the model. The allowed phases and their associated discrete state representations are shown in Figure 4. The phases associated with these states are used to incorporate a set of grade transition heuristics. The remaining logic state is introduced in order to specify whether a specific process set point has been reached. Table 3 lists the logic variables used and their interpretation.

The heuristics used here are in the form of scheduled set point changes. Ordinarily, this polymer production system is composed of two reactors in series, where the product from the first is introduced as feed to the second. An example of the set-point heuristics used in the two reactor scheme is as follows:

(1) The production rate and density in the first reactor are decreased to a predetermined value, while in the second reactor the density is maintained relatively constant.

(2) Once the density of the first reactor reaches the specified set point, the melt flow rate of the first reactor is increased, and

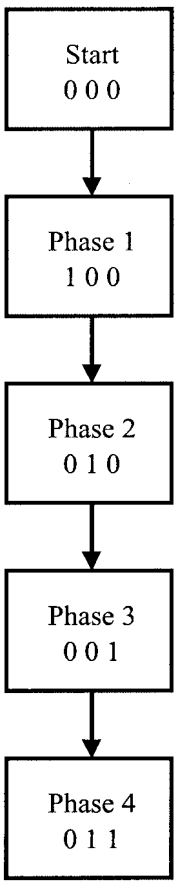

Figure 4. Allowed phases, transitions, and discrete states of the grade transition problem.

For the logic states, the first digit is the first state, the second digit the second state, and so on. In Phase 1, the production rate and density set-points of the first reactor are lowered. Phase 2 increases the melt flow rate and density set-points of the first reactor. Phase 3 increases the production rate of the first reactor. Phase 4 holds all values constant.

Table 3. Logic Variables Used in the Loop Reactor Grade Transition Hybrid Description

Logic Variable	Interpretation
$p1$	first of three states used to define phase of model
$p2$	second of three states used to define phase of model
$p3$	third of three states used to define phase of model
$sp2$	state, indicates density set-point of the second loop is reached
$sp1$	variable, indicates density set-point of the first loop is reached
$sp3$	variable, indicates mfr set-point of the first loop is reached
$spn1$	state value for sp1 at current sample time
$spn2$	state value for sp2 at current sample time
$spn3$	state value for sp3 at current sample time
$md1$	model switching parameter relying on density
$md2$	model switching parameter relying on production rate
$ca1$	no catalyst in reactor
$pn1$	state value for p1 at current sample time
$pn2$	state value for p2 at current sample time
$pn3$	state value for p2 at current sample time
$tr1$	reference trajectory 1 indicator
$tr2$	reference trajectory 2 indicator
$tr3$	reference trajectory 3 indicator
$da1$	linear model 1
$da2$	linear model 2
$da3$	linear model 3
$da4$	catalyst linear model 1
$da5$	catalyst linear model 2
$da6$	catalyst linear model 3
$da7$	no catalyst in reactor
$da8$	use current measured variable value

the density of the second reactor is decreased. The density of the first reactor is also slowly increased during this time.

(3) When the density of the second reactor reaches its specified set point, the production rates of the first and second reactors are increased and the density and melt flow rate of the second reactor is also increased.

(4) When the densities of the two reactors reach their respective set points and the melt flow rate of the second reaches its set point, the transition is finished.

This type of grade transition is practiced in order to keep the product of the second reactor constant for as long as possible during the procedure before the reactor conditions are changed to those of the desired new product. It has been found that this can reduce the amount of off-specification material and transition time. The amount of comonomer in the final product can also be manipulated through this method (Lynch, 2000).

As only one loop reactor is considered in this model, the interaction with a second loop is accomplished by specifying a new (Boolean) variable that indicates the status of the density of the reactor (that is, at set point or not). approximate per The successful evolution of the density set point for the second reactor will become a logic value that is introduced at a random time in an appropriate interval after the first reactor density set point is reached. In this study, the logic value for the second reactor density set point is introduced one to two h. after the first reactor reaches its density set point.

The heuristics incorporated in this problem are similar to those described for the full two reactor system. In order to show the flexibility of the hybrid modeling approach, the grade transition procedure is modified slightly and the phases of evolution allowed are conducted in the following way:

(1) The phase "Start" initiates the grade transition problem from an initial set of conditions. Specification of these initial conditions invokes the switch to the next phase.

(2) When "Phase 1" is initiated, the system decreases the production rate and density set points of the first reactor.

(3) "Phase 2" is engaged once the density reaches five percent of the new set point. (The production rate responds more quickly than the density, and will have reached its set point before the density set point is reached.) In this phase, the melt flow rate and the density in the first reactor are increased, while the production rate is held constant.

(4) "Phase 3" is activated when the logic variable representing the density set point of the second reactor takes the appropriate value. In this phase, the set point for the production rate of the first reactor is returned to its initial value.

(5) "Phase 4" is invoked when the melt flow rate reaches five percent of its final set point and is held constant. (The values for the density and production rate respond much more quickly and will have already reached their set points by this time.)

As the polymerization process studied here is highly nonlinear, and given the fact that grade transition usually involves large set point changes, multiple linear models are used to characterize the nonlinear dynamics of the system. An illustration of the nonlinear process character is shown in Figure 5, where individual step responses are compared at different operating points.

Linearization points of the model are chosen based on the expected evolution of the system according to the allowed phases. Each linearization point is chosen to be the operating point where the model moves from one phase to the next. For example, when Phase 1 is started, the density, production rate,

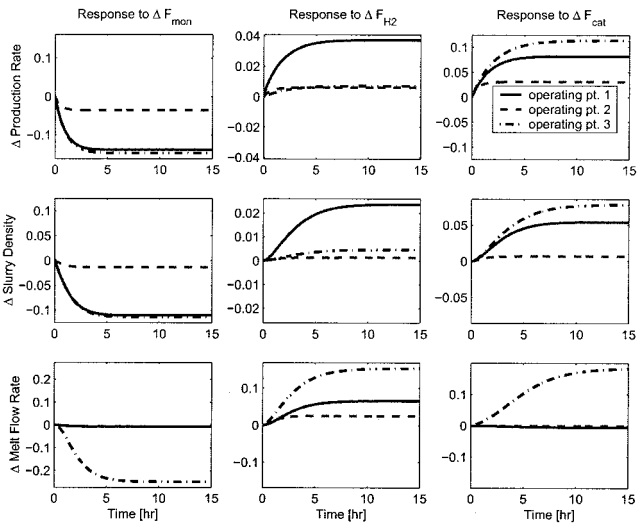

Figure 5. Process output magnitude responses to positive step changes in the inputs.

The columns show the separate magnitude changes of the controlled variables to step changes in the manipulated monomer flow, hydrogen flow, and catalyst flow, respectively. The values given in the graph for the production rate, slurry density, and the melt flow rate are scaled by their maximum expected values and show deviation from each steady state operating point. Monomer, hydrogen, and catalyst flows (all scaled) were increased by 0.1, 0.1, and 0.05, respectively, at time zero.

and the melt flow rate of the first reactor are at their initial points. This is considered to be one of the operating points of the process. At the start of Phase 2, the density, production rate, and the melt flow rate are at their low set points. This is considered to be another operating point of the process. The model then switches from one linearization to the next at a convenient point during the set point change, when one linear model may be more accurate than the other. In this research, the convenient points chosen were the mid-transition points of the controlled variables that were used as a trigger in a specific phase. The only discontinuity due to this type of model switching that caused any significant deviation from the nonlinear model was the prediction of the melt flow rate. It was predicted to change more quickly than the full nonlinear model response during the switch between Phase 3 and 4. Other discontinuities (state, output) were not large enough to be noticeable graphically or computationally. A logic statement that can accomplish this takes the following form

$$\text{IF } (y_i \leq \text{condition 1}) \wedge (y_i \geq \text{condition 2}),$$

$$\text{THEN model } M_i \text{ is active}$$

where y_i is the variable in question, and M_i is the matrix of model parameters that is active when the logic statement is true. For example, switching linear models during the first set point change, is accomplished through a logic statement that checks to see if the predicted density of the reactor is less than or equal to the midpoint specified for the model switch. If the predicted density meets this requirement the parameters used to define the evolution of the states switch from one set to the next. This method of switching is convenient as the controller can switch between appropriate models along the prediction horizon during each optimization step.

As explained previously, heuristics are included in the model through the specification of process set points. The selection of which set points are active at any one time during the evolution of the model is dependent on the process conditions at that point. Previous MPC techniques have scheduled multiple set point changes based on time. In these approaches, the times that the set points are changed are chosen *a priori* and the set points that are supplied to the controller depend on where the process is time-wise in its evolution based on a specified starting point. Specifying set point changes in this manner does not take into consideration the speed at which a process can reach new set points or a controller can reject disturbances. For example, suppose a time-based scheme is employed that will make a set point change corresponding to the switch between Phase 1 and Phase 2 of the hybrid scheme. In order to correspond precisely to the hybrid scheme, it is necessary to know *a priori* exactly when the new density set point of the first reactor is reached. In reality, disturbances to the plant can affect the amount of time it takes to reach this set point, and the exact time cannot be determined in advance for each transition. Conversely, the approach taken here is that the controller responds to a logic value that represents a set point being reached and internally switches to a new set point. This control scheme bases the switching routine on three process measured variables, the density, and melt flow rate of reactor 1, and the density of reactor 2. The switch from Phase 1 to Phase 2 is accomplished by comparing the current measured value of the density of reactor 1 to a suitable logic statement. When this statement is true, the controller is allowed to transition to the next phase. Similarly, the transition from Phase 3 to Phase 4 relies on the current measured value of the melt flow rate in reactor 1. However, the transition from Phase 2 to Phase 3 is accomplished by the introduction of a logic value as described previously.

The set points that are active are specified by which phase the model is in at any point in the evolution. A logic statement that can accomplish this takes the form

$$\text{IF phase } i,$$

$$\text{THEN vector } S_i \text{ is active}$$

where S_i is the vector of set points that is active when the logic statement is true. By specifying logic statements that define when a specific vector of set points is active and including these statements along with the corresponding set point vectors in the hybrid model, the set points can be dynamically switched in the model. Table 3 lists the remaining required logic variables and their interpretation. Table 4 lists the z variables used in the hybrid model.

Included in the model are constraints on the controlled variables and manipulated variables. The logic necessary to describe the system was combined with the continuous equations, and a textual description of the model and system logic was written according to the method described by Torrisi et al. (Torrisi et al., 2000).

MPC formulation

The MPC problem for this grade transition problem is formulated as a MILP problem. The objective function that is solved for this problem is

$$\min_{v} \sum_{i=n}^{n+p} \|\Gamma_y \mathbf{e}(i)\|_1 + \|\Gamma_v \mathbf{v}(i)\|_1 \tag{19}$$

where $\| \quad \|_1$ denotes the 1-1 norm of the vector, $\mathbf{e}(i)$ is a vector of the process error at time (i), and $\mathbf{v}(i)$ is a vector of the process inputs, auxiliary binary, and auxiliary continuous variables. The term p is the model prediction horizon. After a time m, all process inputs in the model are assumed held constant, where $m \leq p$. Γ_y is used to weight the importance of the elements of the error vector, while Γ_v is a diagonal matrix that is used to weight the penalties incurred on the process inputs and auxiliary variables. The error vector is defined as

$$e = y_r - y_m \tag{20}$$

where e is the error, y_r is the reference value for the controlled variable, and y_m is the measured value for the controlled variable. The prediction algorithm used in this research is based on the state-space prediction model developed by Ricker (Ricker, 1990). The predicted values are related to the measured values at time i through the equation

Table 4. The Following z Variables are Combined or Used Individually to Calculate MLD Model Values Depending on which Phase is Active in the Model

z Variable	Interpretation
$zH21$, $zH22$, $zH23$	The three linearizations for hydrogen concentration
$zCt11$, $zCt12$, $zCt13$, $zCt14$	The four linearizations for catalyst concentration
$zPP1$, $zPP2$, $zPP3$	The three linearizations for polymer concentration
$zCT1$, $zCT2$, $zCT3$	The three linearizations for average residence time distribution
$zC3e1$, $zC3e2$, $zC3e3$	The three linearizations for propylene concentration
$zC3a1$, $zC3a2$, $zC3a3$	The three linearizations for propane concentration
$zC2e1$, $zC2e2$, $zC2e3$	The three linearizations for ethylene concentration
$zTr1$, $zTr2$, $zTr3$	The three linearizations for reactor temperature
$zC2P1$, $zC2p2$, $zC3P3$	The three linearizations for copolymer fraction
$zTw1$, $zTw2$, $zTw3$	The three linearizations for coolant temperature integral
$zVP11$, $zVP12$, $zVP13$	The three linearizations for the cummulative viscosity
$zmDSL$	Current measured value of the slurry density
$zmMFR$	Current measured value of the melt flow rate
$zrT1$, $zrT2$, $zrT3$	The three linearizations for reactor temperature prediction
$zRp1$, $zRp2$, $zRp3$	The three linearizations for production rate prediction
$zDSL1$, $zDSL2$, $zDSL3$	The three linearizations for the slurry density
$zFr1$, $zFr2$, $zFr3$	The three linearizations for copolymer fraction prediction
$zMFR1$, $zMFR2$, $zMFR3$	The three linearizations for melt flow rate prediction
$zTsp1$, $zTsp2$, $zTsp3$	The three values for the temperature set-point
$zRsp1$, $zRsp2$, $zRsp3$	The three values for the production rate set-point
$zDsp1$, $zDsp2$, $zDsp3$	The three values for the slurry density set-point
$zFsp1$, $zFsp2$, $zFsp3$	The three values for the copolymer fraction set point
$zMsp1$, $zMsp2$, $zMsp3$	The three values for the melt flow rate set point

The reader is referred to the references on MLD systems for a more detailed explanation of the formulation of z variables.

$$y_m = y_p + d \tag{21}$$

where y_p is the model prediction and d is a disturbance variable that is a consequence of system noise, plant-model mismatch, or other factors. As is standard in many MPC applications, a DMC disturbance model is assumed in which the current value of d is assumed to be a bias that is held constant for future points in the prediction horizon.

Also included in the MPC formulation is the use of an asymmetric objective to ensure that the output responses do not overshoot upper reference trajectories excessively. Gatzke and Doyle (Gatzke and Doyle III, 2001) reported the use of such objectives to penalize either positive or negative tracking error more strongly than the other. This type of objective formulation is useful when a reference trajectory is near an undesired output value. In this research, the upper density set point of the reactor is near an undesired larger density value. Any slurry density above this undesired value could cause the reactor to plug. To prevent this, the output error measurement is weighted more heavily when the density is above the set point. The error and input move weights are shown in Table 5.

Table 5. Values for the Error and Input Move Weights

	$e = y_r - y_m$ Positive	$e = y_r - y_m$ Negative	Δu
R_P	1.2×10^5	1.2×10^5	—
DSL	1.5×10^5	3.9×10^5	—
MFR	9.0×10^4	2.8×10^5	—
F_{mon}	—	—	5.0×10^3
F_{H2}	—	—	1.0×10^4
F_{cat}	—	—	7.0×10^3

R_P, DSL, and MFR are the overall production rate, the slurry density and the melt flow rate, respectively. F_{mon}, F_{H2}, and F_{cat} are the monomer, hydrogen, and catalyst flowrates, respectively.

General constraints on the input, output, and states can be formulated. The MLD system constraints that describe the evolution of the system dynamics and logic are also included as follows

$$E_2\delta(k) + E_3z(k) \le E_1u(k) + E_4x(k) + E_5 \tag{22}$$

$$x_{c,\min} \le x_c \le x_{c,\max} \tag{23}$$

$$u_{c,\min} \le u_c \le u_{c,\max} \tag{24}$$

$$y_{c,\min} \le y_c \le y_{c,\max} \tag{25}$$

$$z_{c,\min} \le z_c \le z_{c,\max} \tag{26}$$

$$x_1,\ u_1,\ y_1,\ \delta \in \{0,\ 1\} \tag{27}$$

where the subscript c refers to continuous variables, and the subscript l refers to Boolean logic variables. Additional constraints are on the maximum allowed input move to prevent large instantaneous changes in the individual inputs to the process, and a lower constraint on the minimum allowed monomer flow rate to the reactor. The numerical values of these constraints are given in Table 6.

This constrained optimization problem is solved at each sample time, and the first control move is implemented on the system. This problem is resolved at each sample time, and this optimization process is repeated at each sample time until the end of the simulation. For the formulations described here, and tuning values described in the next section, a typical solution

Table 6. Values for the Lower Constraints and Maximum Allowed Input Moves for the Process

	Minimum u	Maximum Δu
F_{mon}	0.2195	0.4
F_{H2}	0.0	0.4
F_{cat}	0.0	0.4

The values for each input are scaled by their maximum expected values.

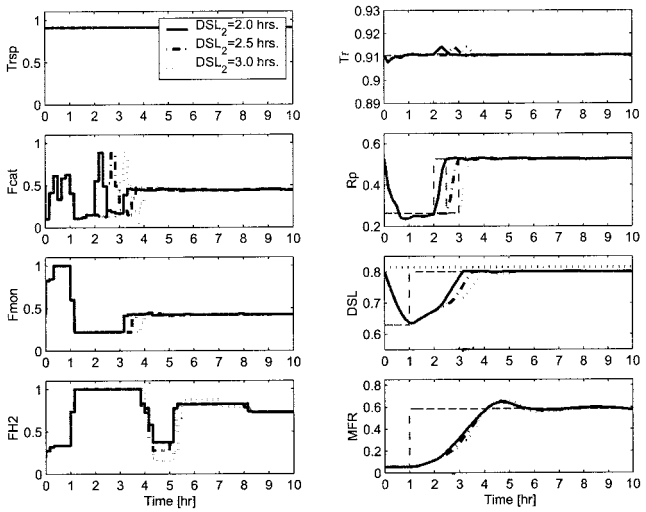

Figure 6. Evolution of the first reactor during the hybrid grade transition problem.

The solid line shows the density of the second reactor reaching its low set-point at 2 h, the dashed-dot line at 2.5 h, and the dotted line at 3 h. Also, the dashed line shows the set point and the horizontal dotted line shows the density soft constraint.

time per iteration was 60 sec (Sun Sparc Enterprise 333MHz/512MB).

Results and discussion of the applied control technique

All of the results shown for the grade transition problem are reported in scaled variables. The inputs and outputs of the process were scaled by the maximum expected values during the grade transition study. Ten minute sample times were used in this study, and the move (m) and prediction (p) horizons used are three and eight, respectively.

A ten minute sampling time was chosen to achieve a compromise between the time needed for appropriate corrective action to the process (including the availability of measurements, such as melt flow rate), and the system's time constants. An additional consideration was the feasibility of solving the ensuing mixed integer programming problem in real-time. The prediction horizon was chosen to allow a horizon large enough to see the upcoming set point changes associated with the transition, and the move horizon was chosen to allow a qualitatively quick response time with minimal overshoot.

The temperature, production rate, and the density of the polymer are all measurements that can be taken online with the instrumentation currently available to industry. The melt flow rate can be estimated using other measurements available, and the parameters used for this estimation can be adjusted periodically or biased based on lab measurements.

The quality of the solution to hybrid grade transition MPC problem for the first reactor was affected mainly by the response of the evolution of the second reactor. As can be seen in Figure 6, when the second reactor reaches its low density set point at 2 h all of the reactor outputs reach, and track their reference trajectories by about 5 h. into the simulation. The approaches of each of the outputs are fast and experience little to no overshoot. When the low density set point of the second reactor is reached at 2.5 h., as seen in the figure, the density of the first reactor takes about a half hour longer to reach its set point, and the melt flow rate reaches its set point at about the same time. Figure 6 also shows the process responses when the low density set point of the second reactor is reached at 3 h. Again, the density of the first reactor responds more slowly and reaches its set point at about an hour longer than the 2 h. case. The melt flow rate reaches its set point at about the same time, but experiences a slightly larger overshoot than the previous examples.

In addition to smooth control of the process during the grade transition, the controller must be able to correct for process sensor bias. Figure 7 shows the case where there are positive and negative biases (± 0.05 scaled) in the measured density at 5 h. The controller is able to successfully bring all outputs except the melt flow rate to the desired set-points. This is caused by the fact that the hydrogen flow rate meets its upper constraint, which causes a slight offset in the melt flow rate set-point. Smaller positive bias in the measured density will be rejected completely by the controller if the input constraint on the hydrogen flow rate is not met. Also evident in Figure 7 is the fact that the asymmetric objective rejects positive bias in the density more quickly than negative, which helps to maintain the density below the upper soft constraint.

Noise rejection is another important feature of an effective control design. Figure 8 indicates that the designed controller can successfully reject such output disturbances. In this case, 1 percent noise was added to the temperature measurement, and 10 percent noise was added to the remaining measurements. As can be seen from the figure, when noise is added to the process measurements the first set point switch takes place two sample times later than the case where no noise is added. These results do not include noise added to the density measurement of the second reactor, otherwise the set point change in the production rate may occur at a different sample point in the procedure.

To establish a basis for comparison, an open-loop manual control approach is designed in which predefined manipulated variable set points are used in the control sequence. In this manner, a series of manipulated variable moves that will

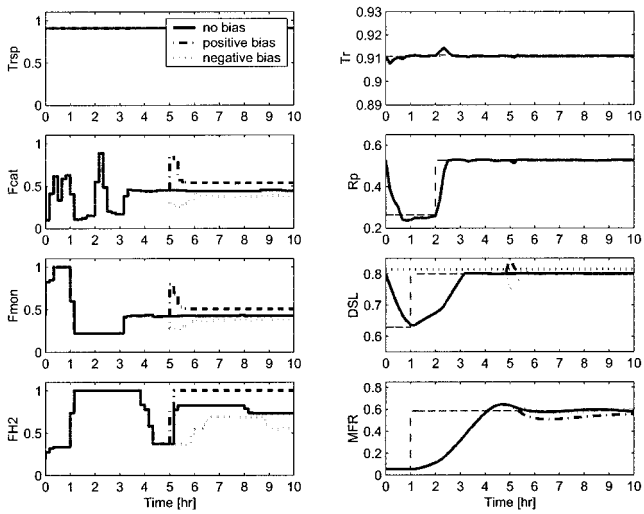

Figure 7. Positive and negative sensor bias (± 0.05 scaled) in the measured density at 5 h.

The sensor bias is present for all time after 5 h.

achieve the desired reference trajectory tracking results are given to the process at appropriate times during the procedure. The goal in this grade transition study is to apply manipulated variable set points that provide an appropriate controlled variable response that corresponds to the grade transition logic. Figure 9 shows the results of such a procedure and compares them to the closed-loop feedback control profiles. As can be seen, the hybrid MPC controller results in earlier set point changes and quicker reference tracking. Feedback control can significantly decrease the amount of time that the transition takes, and in this case, significantly decrease the amount of off-specification material that is produced during the transition. Also, it can be seen that the manipulated variable profiles F_{cat} and F_{mon} at the end of the procedure are the same for the open-loop and closed-loop procedure. However, the two profiles for F_{H2} are not the same at the end of the procedure.

Conclusions

The problem of polymerization grade transition control has been formulated as a hybrid system, and the corresponding mixed integer version of MPC has been developed and solved. The discrete components of the algorithm include both linear switching models used to approximate the nonlinear process, and operating heuristics that are incorporated as propositional logic inequalities. This is a novel algorithm for industrial control of polymer grade transitions. While there are methods to include heuristics (in an ad hoc manner) in control design via, for example, PROGRAMMABLE logic CONTROLLER (PLC), and there are methods for optimized the continuous variables in a grade transition using nonlinear optimization, there are no tools available for combining the heuristics, and the continuous (process) variables in a common framework. Consequently, this leads to optimal incorporation of the constraints in a model predictive control framework. The solution

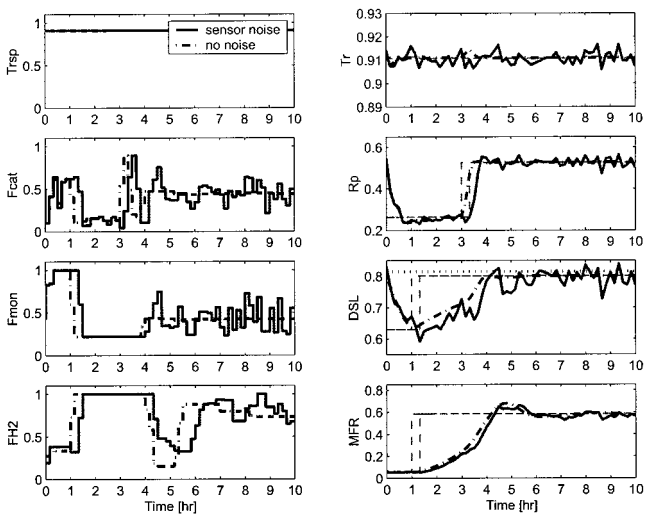

Figure 8. Effect of output measurement noise on controller performance. In the noise-free profile, the second reactor reaches its density set point at 3 h.

The temperature measurement is subjected to 1 percent noise, all other measurements are subjected to 10 percent noise.

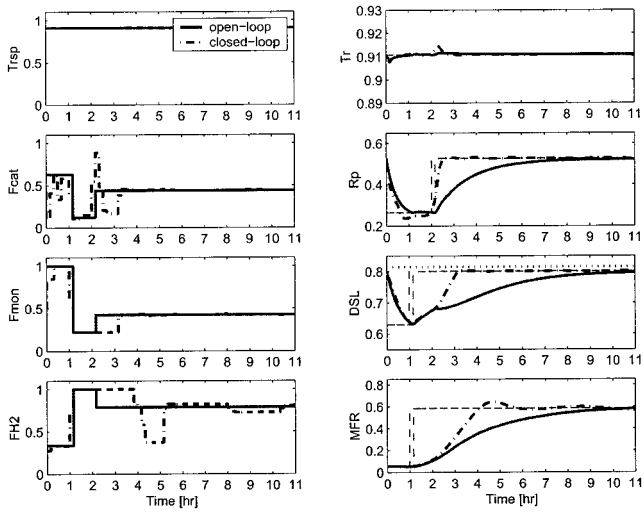

Figure 9. Comparison of open-loop manual control to feedback control of the grade transition problem.

Here the density of the second reactor reaches its set point one hour after the density set-point of the first reactor is reached.

times per iteration were approximately 60 s. (Sun Sparc Enterprise 333MHz/512MB), demonstrating real-time feasibility.

This article considers the problem of transitions in a production scheme having two polymer grades. Larger grade slates would add the complexity of more linear models (if necessary) to represent the operating regimes encountered during the transitions. Also, integer variables would be added to the problem in the form of constraints that activate set points, and the order of execution of the grade transition. The number of the added integers greatly depends on the formulation of the MLD model. Computationally, the difficulty of solving the problem increases exponentially with the number of integers in the problem. In order to solve the problem in a satisfactory time, algorithm engineering of the solution may be required.

The resulting model predictive controller was able to successfully complete the grade transition problem in minimal time for the case where there were no output disturbances as compared to the open-loop example. The timing of the second reactor in reaching its density set point had a large effect on the profile of the production rate, and the density and a negligible effect on the profile for the melt flow rate in the first reactor. Large sensor bias in the production rate and density were completely rejected, although bias in the melt flow rate was not successfully rejected. This was found to be the case when the bias entered at different times during the transition problem. Realistic output measurement noise was added to the process model, and the controller was able to reject it successfully and track reference trajectories during the grade transition. The asymmetric objective was able to successfully reject the appropriate sensor bias errors more quickly. Also, it was shown that closed-loop feedback control results in a significant improvement over the heuristic open-loop control policy.

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