Control-Relevant Scheduling of Polymer Grade Transitions

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Grade transition is a critical step in the operation of a polymerization reactor. The nonlinear input-output behavior of the reactor can lead to severe differences in the dynamic response of different grade transitions. These differences are analyzed under the assumption that the polymerization reactor is regulated by a linear controller. The cost of each transition is calculated based on a linear first-order model of the transition. Robust control theory is employed to propose screening tools and heuristics for the identification of the transitions that are "difficult" from an operational perspective in the presence of uncertainty. The dependence of the transition cost on the gain and the time constant of various transitions is analyzed to determine the effect of process nonlinearities on the scheduling problem. This approach is demonstrated on the problem of scheduling grade transitions in an isothermal methyl methacrylate polymerization reactor.

Introduction

Increased competition in the chemical process industries has forced chemical plants to operate in highly nonlinear regimes, and recycle material and energy streams for cost effectiveness. In the polymer industry, this translates into the production of different products with the same manufacturing equipment to reduce capital costs. This requires efficient transitions between products to avoid the cost intensive phases of startup and shutdown of the process.

In a typical polymer production, various grades are made in a sequence which may be cyclic, where each grade is made in an amount proportionate to the total demand for that grade. The sequence of the grades is repeated over time to effectively manage storage costs. Since the end use properties of the different grades of the polymer demand specific characteristics of the polymer in terms of properties such as melt index, molecular weight, and density, excursions outside a restricted range result in the production of large amounts of off-specification (off-spec) product. An extended discussion of the practical issues associated with grade transitions is presented in Sinclair (1987) and Debling et al. (1994). Depending on the severity of the excursions, blending of the products might be a required additional processing step (Ohshima and Tanigaki, 2000). Due to nonlinearities inherent in these processes, the dynamic characteristics of a transition from one grade to another can be significantly different from the reverse transition.

The area of grade transition control has been an active subject of academic research. McAuley and MacGregor (1992) have proposed solution methodologies based on dynamic optimization using control vector parameterization to determine the optimal grade transition policy in a gas-phase polyethylene reactor. Approaches based on nonlinear geometric control (Alvarez et al., 1994) and nonlinear optimization (Farber and Laurence, 1986; Sirohi and Choi, 1997) for controlling the dynamics of startup and grade transitions have been presented earlier. Wang et al. (2000) and Hillestad and Andersen (1994) have proposed nonlinear model predictive control strategies for tracking the predetermined optimal policy obtained using an off-line optimizer in the presence of disturbances and model mismatch.

Determining the optimal sequence of the transitions for a process with a large number of grades can pose a challenging problem as the number of possible sequences grows combina-

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torially with the number of grades. The production schedule should also consider the demand for the grades, the inventory costs, and also the costs associated with the off-spec product formed during transition (Debling et al., 1994). In this article, the emphasis is on the dynamic transition cost. Scheduling problems dealing with plant-wide operations that are batch, semicontinuous, and continuous have been addressed in the past by various researchers. See, for example, Applequist et al. (1997), Pinto and Grossmann (1995), Harjunkoski et al. (2000), Djavdan (1993), and Ierapetritou and Floudas (1998). Recently Mèndez and Cerdá (2000) and Orcun et al. (2001) have presented optimal scheduling approaches based on mixed integer linear programming (MILP) and mixed integer nonlinear programming (MINLP). A discussion of the computational issues relating to the MILP formulations is presented in Shah et al. (1993) and Orcun (1999). However, there have been very few publications which take into account the issues relating to control with the exception of Shobrys and White (2000) and Perea-Lopez et al. (2000).

The objective of this article is to analyze the schedule of grade transitions for a polymerization reactor, which is controlled by a simple linear controller [PI or internal model control (IMC)]. The dominant factor determining the schedule of grade transitions is the transition cost relating to the off-specification product. Techniques from robust control theory are used to investigate the effect of input constraints in the presence of uncertainty and to propose screening tools and heuristics that aid in the understanding of the scheduling problem. A simple representation of the plant as a first-order model is used to generate physical insight on the effect of the differences in the time constant and the gain of the model on the transition cost and the schedule. A scheme based on identification of first-order models using closed-loop data is employed to characterize the system. A screening tool has been proposed to determine the sequence of the grades for a nonlinear MMA free radical polymerization reactor, so that transitions involving the production of a significant amount of off-spec product can be minimized. A cost based on the economics of each transition is calculated and the analysis of all the transition costs yields the optimal product wheel. Such an approach would also be useful to provide a warm-start solution and other heuristics for a mixed integer nonlinear programming (MINLP) problem in the situation where a fundamental model is available. This could potentially result in increased computational efficiency of the solution method. The effect of uncertainty in the model parameters has also been considered in the analysis presented in this article.

Model Identification

The process under consideration is the isothermal free radical polymerization of methyl methacrylate (MMA) with azobis-isobutyronitrile as initiator and toluene as the solvent (Congalidis et al., 1989; Daoutidis et al., 1990). The model equations are summarized below and the corresponding parameter values are given in Table 1

$$\frac{dC_m}{dt} = -\left(k_p + k_{f_m}\right)C_m\left[\frac{2f^*k_IC_I}{k_{T_d}+k_{T_c}}\right]^{0.5} + \frac{F\left(C_{m_{in}} - C_m\right)}{V}$$

$$\frac{dC_I}{dt} = -k_IC_I + \frac{F_IC_{I_{in}} - FC_I}{V}$$

$$\frac{dD_0}{dt} = \left(0.5k_{T_c} + k_{T_d}\right)\left[\frac{2f^*k_IC_I}{k_{T_d}+k_{T_c}}\right] + k_{f_m}C_m\left[\frac{2f^*k_IC_I}{k_{T_d}+k_{T_c}}\right]^{0.5} - \frac{FD_0}{V}$$

$$\frac{dD_1}{dt} = M_m\left(k_p + k_{f_m}\right)C_m\left[\frac{2f^*k_IC_I}{k_{T_d}+k_{T_c}}\right]^{0.5} - \frac{FD_1}{V}$$

$$y = \frac{D_1}{D_0} \tag{1}$$

Four different operating points based on the molecular weight are defined as the different polymer grades. The designated grades are A, B, C, and D with molecular weights of 15,000, 25,000, 35,000, and 45,000, respectively. Thus, the number of possible transitions is 12 ($n(n-1)$, where n is the number of the grades) and the number of distinct schedules/product wheels is 6 [$(n-1)!$]. First-order models of each transition

Table 1. States and Parameters

Symbol	State/Parameters	Value
C_m	Monomer concentration	kmol/m^3
C_I	Initiator concentration	kmol/m^3
D_0	Molar concentration of dead chains	kmol/m^3
D_1	Mass concentration of dead chains	kg/m^3
T	Temperature of the reactor	335 K
F	Monomer flow rate in	1.00 m^3/h
F_I	Initiator flow rate out	m^3/h
P_0	Molar concentration of live chains	kmol/m^3
f_s	Initiator efficiency	0.58
k_p	Propagation rate constant	2.50×10^6 m^3/kmol·h
k_{Td}	Termination by disproportionation rate constant	1.09×10^{11} m^3/kmol·h
k_{Tc}	Termination by coupling rate constant	1.33×10^{10} m^3/kmol·h
CI_{in}	Inlet initiator concentration	8.0 kmol/m^3
$C_{m_{in}}$	Inlet monomer concentration	6.0 kmol/m^3
k_{fm}	Chain transfer to monomer rate constant	2.45×10^3 m^3/kmol·h
k_I	Initiation rate constant	1.02×10^{-1} h^{-1}
M_m	Molecular weight of monomer	100.12 kg/kmol

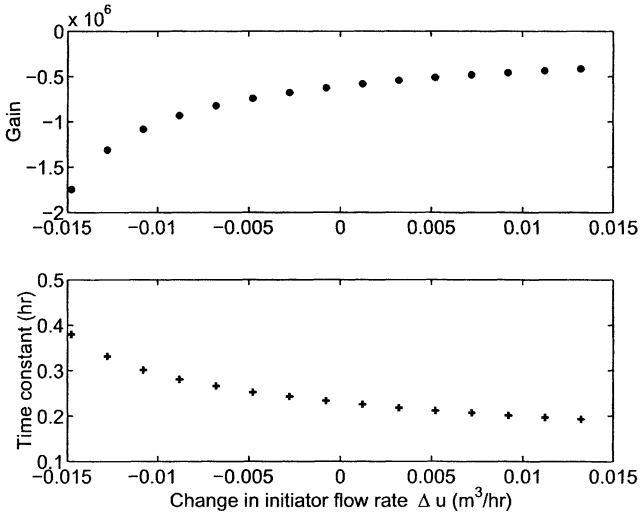

Figure 1. Gain and time constant of identified linear models for various changes in initiator flow rate from nominal value corresponding to grade B.

were obtained by fitting the response of the nonlinear model to a step change in the input. The time constants for the transitions vary from 0.16 to 0.41 h, highlighting the differences in the speed of response of the various transitions. The gain and the time constant of the various linear models identified from steps of different magnitude in the initiator flow rate from the nominal value for grade B are given in Figure 1. It should be noted that the time constants of the models identified are dependent on the profile of the input used to obtain the transition due to process nonlinearity. However, in practice, a step change in the input is seldom used. For a better representation of the nonlinear system, an input profile that approximates the actual closed-loop input profile should be used. This motivates the closed-loop identification of the linear models of the transitions.

In the closed-loop identification scheme, a PI controller was used along with the nonlinear model described by Eq. 1. This controller was used to generate closed-loop data consisting of step responses in the set point for the identification. The closed-loop transfer function for a first-order system with a PI controller is given as follows

$$y = \frac{K_m K_c(\tau_I s + 1)}{(\tau_m s + 1)\tau_I s + K_m K_c(\tau_I s + 1)} r$$

Simplifying the above as a sum of two first-order transfer functions

$$y = \left[\frac{g}{\tau_g s + 1} + \frac{h}{\tau_h s + 1}\right] r$$

yields closed-loop response in the time domain for a step change in the reference (R)

$$y(t) = gR(1 - e^{-t/\tau_g}) + hR(1 - e^{-t/\tau_h})$$

where g, h, τ_g, and τ_h are functions of τ_I, K_m, K_c, and τ_m. The gain of the process model can be determined from open-loop data as the gain of the transition is not affected by the identification scheme (closed-loop vs. open-loop) used. Thus, only the time constant of the first-order model was fitted to the closed-loop response of the nonlinear model. The time constants were observed to depend on the specific controller employed. In this study, the controller that results in the fastest response without constraint violation was used in the simulations to generate the data. The resulting time constants are shown in Table 2.

In order to evaluate the cost associated with a particular transition, an IMC controller was designed using a first-order filter with a time constant of lambda (λ) (Morari and Zafiriou, 1989). The following notation is introduced to calculate the closed-loop response of a particular transition (P) under the regulation of an IMC controller based on a process model (M). The transition and the process model are exact first-order processes with gain K_p and K_m, respectively, and time constants τ_p and τ_m, respectively. If there is no mismatch between the transition model (M) and the linear plant (P), then the closed-loop response to a step change in the reference is first-order with the time constant lambda.

In the case of plant-model mismatch ($M \neq P$), the closed-loop transfer function is

$$y = \frac{\tau_m s + 1}{\frac{K_m \lambda \tau_p}{K_p} s^2 + \frac{K_m \lambda + K_p \tau_m}{K_p} s + 1} r$$

which can be simplified into a sum of first-order transfer functions

$$y = \left[\frac{p}{\tau_1 s + 1} + \frac{q}{\tau_2 s + 1}\right] r$$

The corresponding time domain solution for a step input of magnitude R for the closed-loop system with an IMC con-

Table 2. Transition Gain and Time Constants

Transition	Gain (kg·h)/(kmol·m^3)	Time Const. (h)	Transition	Gain (kg·h)/(kmol·m^3)	Time Const. (h)
AB	−2.789e5	0.250	*BA*	−2.789e5	0.163
AC	−4.371e5	0.304	*CA*	−4.371e5	0.240
AD	−6.058e5	0.404	*DA*	−6.058e5	0.178
BC	−1.010e6	0.241	*CB*	−1.010e6	0.231
BD	−1.464e6	0.249	*DB*	−1.464e6	0.210
CD	−2.659e6	0.229	*DC*	−2.659e6	0.234

troller is

$$y(t) = pR(1 - e^{-t/\tau_1}) + qR(1 - e^{-t/\tau_2})$$

where p, q, τ_1, and τ_2 are functions of τ_p, K_m, K_p, τ_m, and lambda.

Transition Costs

In this section, three definitions of the cost of a grade transition are introduced. These costs are related to the "difficulty" of a particular grade transition and take into account in some fashion the economic loss (off-specification material) that results during a grade transition. However, it should be noted that these costs do not account for input constraint violations, although that issue is addressed in the next section. The three costs were calculated for all possible transitions in the polymerization reactor. Three models of the plant (with different time constants to represent the range) were considered in each case to study the effect of the choice of the transition model. The costs were also calculated for three different values of the filter time constant (λ) in order to study the effect of varying λ. The optimal schedules obtained based on the costs alone are shown in Tables 3, 4, and 5.

Table 3. Squared Error Cost for all the Schedules

Transition Model in IMC	$\frac{\lambda}{\tau_m}$	ABCDA	ABDCA	ACBDA	ACDBA	ADBCA	ADCBA
$\tau_m = 0.21$ (DB)	1.0	0.602	0.515*	0.882	0.520	1.00	0.741
	5	0.682	0.556*	0.966	0.556	1.00	0.722
	10	0.697	0.5631*	0.982	0.5633	1.00	0.720
$\tau_m = 0.18$ (DA)	1.0	0.527	0.473*	0.805	0.484	1.00	0.754
	5.0	0.637	0.532*	0.920	0.534	1.00	0.754
	10.0	0.670	0.549*	0.954	0.550	1.00	0.725
$\tau_m = 0.40$ (AD)	1.0	0.594	0.520*	0.865	0.527	1.00	0.750
	5.0	0.678	0.555*	0.958	0.557	1.00	0.730
	10.0	0.695	0.562*	0.978	0.563	1.00	0.722

*Denotes optimal schedule.

Table 4. Settling Time Cost for All the Schedules

Transition Model in IMC	$\frac{\lambda}{\tau_m}$	ABCDA	ABDCA	ACBDA	ACDBA	ADBCA	ADCBA
$\tau_m = 0.21$ (DB)	1.0	0.958	0.987	0.789	1.00	0.761*	0.935
	5	0.952	0.995	0.805	1.00	0.795*	0.943
	10	0.953	0.998	0.807	1.00	0.803*	0.948
$\tau_m = 0.18$ (DA)	1.0	0.703	0.718	0.600*	0.768	0.842	1.00
	5.0	0.954	0.991	0.788	1.00	0.760*	0.925
	10.0	0.952	0.993	0.800	1.00	0.785*	0.937
$\tau_m = 0.40$ (AD)	1.0	0.970	0.981	0.851	1.00	0.812*	0.928
	5.0	0.956	0.995	0.816	1.00	0.806*	0.945
	10.0	0.954	0.998	0.813	1.00	0.808*	0.949

*Denotes optimal schedule.

Table 5. Envelope Time Cost for All the Schedules

Transition Model in IMC	$\frac{\lambda}{\tau_m}$	ABCDA	ABDCA	ACBDA	ACDBA	ADBCA	ADCBA
$\tau_m = 0.21$ (DB)	1.0	0.933	0.971	0.886	1.00	0.853*	0.922
	5	0.919	0.987	0.885	1.00	0.883*	0.922
	10	0.918	0.990	0.887*	1.00	0.891	0.927
$\tau_m = 0.18$ (DA)	1.0	0.713	0.722	0.692*	0.784	0.910	1.00
	5.0	0.925	0.980	0.876	1.00	0.850*	0.912
	10.0	0.919	0.984	0.880	1.00	0.871*	0.917
$\tau_m = 0.40$ (AD)	1.0	0.937	0.960	0.926	1.00	0.890	0.885*
	5.0	0.920	0.986	0.902	1.00	0.890*	0.924
	10.0	0.921	0.990	0.897*	1.00	0.900	0.928

*Denotes optimal schedule.

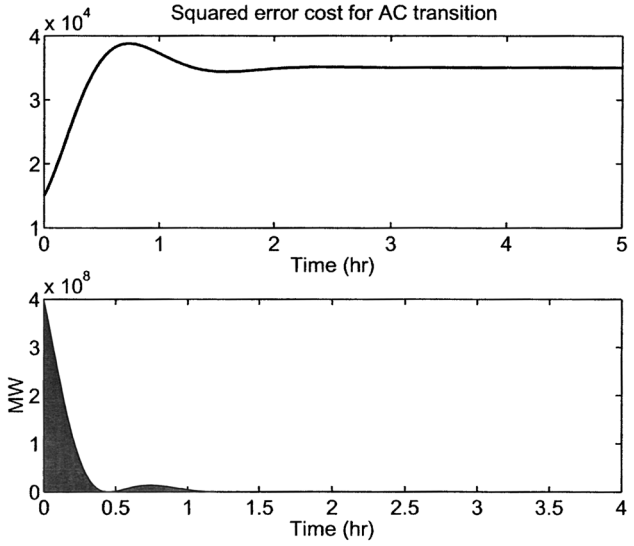

Figure 2. Squared-error cost.

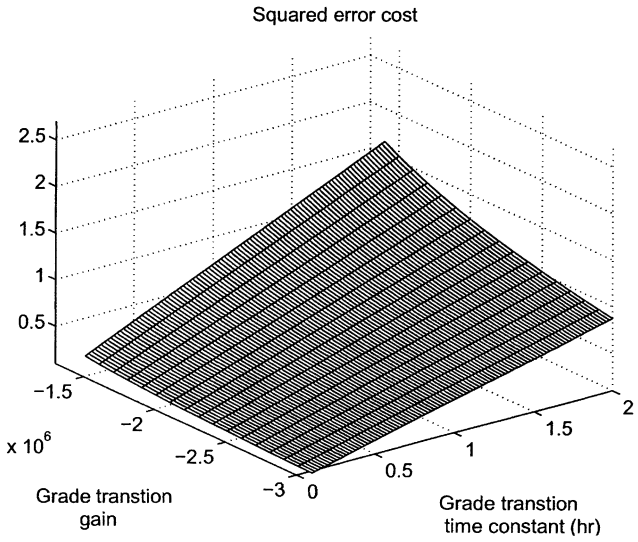

Figure 3. Various squared error costs with the gain and time constant of the transition model with AD transition as linear model in the IMC structure.

Squared error cost

The squared error cost is defined to be the integrated square of the error over the time window of a grade transition. As the closed-loop response for the identified linear transition model is known, the integral of the squared error (Figure 2) can be calculated analytically as follows

$$J_y = \int_0^\infty (y - y_{ss})^2 dt = \frac{p^2R^2\tau_1}{2} + \frac{2pqR^2\tau_1\tau_2}{\tau_1+\tau_2} + \frac{q^2R^2\tau_2}{2} \quad (2)$$

The squared error costs penalizes transitions with a large change in the molecular weight due to the second-order dependence of the cost on the reference change (R). In polymerization systems, this cost does not translate to economic benefit, although the squared error cost is often used as a measure of controller performance. The squared error cost was calculated for the different combinations of the controller model (M) and lambda. The results are shown in Figure 3. The squared error cost increased with an increase in the process time constant and decreased with increase in the magnitude of the process gain. This is a result of the sluggishness at larger values of time constant and the smaller process gain. It can be observed from Table 3 that transitions from A to D are penalized heavily by the squared error cost and do not appear frequently in the optimal schedule. The squared error cost penalizes transitions that involve large reference changes as the model/controller time constant is increased. The effect of increasing the filter time constant has an equivalent effect. The squared error cost would penalize transitions that are fast but involve a large change in the process variable.

Settling time cost

The settling time cost is calculated as the time taken for the process variable to reach and stay within 5% of the final value (depicted in Figure 4). Mathematically, the settling time t_s is expressed as follows

$$y(t) = pR(1 - e^{-t/\tau_1}) + qR(1 - e^{-t/\tau_2})$$
$$t > t_s \; |y(t) - R| \; < 0.05R$$

Settling time cost is another popular performance metric of closed-loop control systems. Bounds on the output are specified depending on the tolerance towards variability in the product. This is, however, closer to the economic cost of a transition in terms of the amount of off-spec material formed. It is also noted that the settling time cost also does not penalize transitions based on the magnitude of the reference change. The variation of the settling time cost with respect to the gain and the time constant of the transition model is

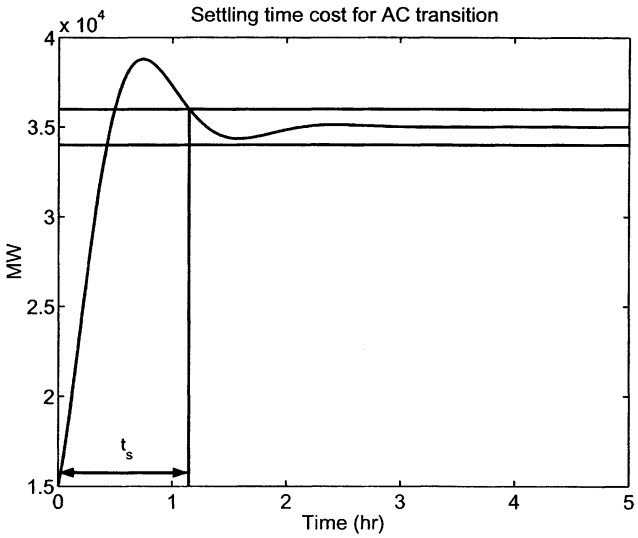

Figure 4. Settling time cost.

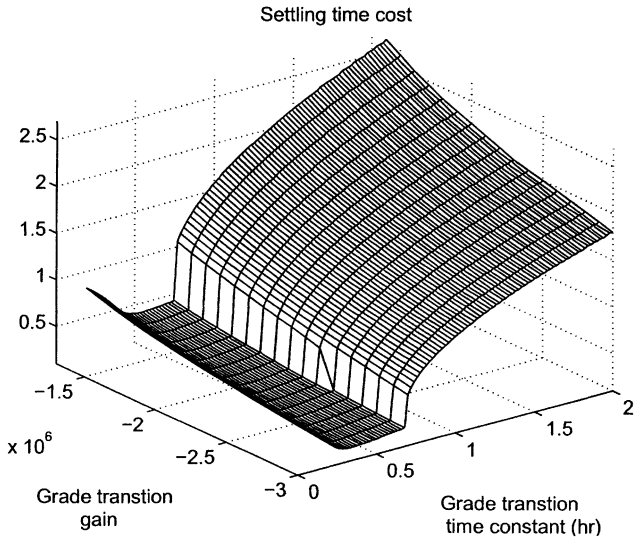

Figure 5. Various settling time costs with the gain and time constant of the transition model with AD transition as linear model in the IMC structure.

shown in Figure 5. The settling cost variation with the transition gain is generally monotonic, although it passes through a minimum with respect to the time constant. A sharp increase in the cost around a transition time constant of 0.75 h occurs as a result of an overshoot pushing the molecular weight outside the 5% envelope. Optimal schedules for various controller models and the filter time constant based on the settling time cost are also shown in Table 4. Unlike the squared error costs, settling time cost does not penalize transitions that are fast, but involve a large change in the molecular weight. Transitions with a higher time constant are penalized more by settling time cost for increase in the model time constant. The effect of increasing filter time constant is an increase in the cost of all the transitions. In this case, the schedule ADBCA is the optimal schedule for most combinations of the filter time constant and the model time constant except the case where the model DA and a filter time constant ratio $\lambda/\tau_m = 1$ is used. Since the controller is aggressive, this results in an overshoot and increase in the cost, as the design corresponds to the area where the sharp increase in the cost is seen in Figure 5.

Envelope time cost

The envelope time cost is defined as the time during which off-spec product is formed (depicted in Figure 6). Since it is assumed that the production rate is constant, this cost refers to the time after which the process variable leaves the region of specification for the first grade until the time when it enters the region of specification for the second grade and stays within that region. The acceptable tolerance is defined as 5% of the desired molecular weight. Mathematically, this can be formulated as follows

$$t > t_1 \quad y(t) > 1.05y_1 \quad \text{if} \quad R > 0$$

$$t > t_1 \quad y(t) < 0.95y_1 \quad \text{if} \quad R < 0$$

$$t > t_2 \quad 0.95y_2 < y(t) < 1.05y_2$$

$$\text{Cost} = t_{\text{env}} = t_2 - t_1$$

The dependence of the envelope time cost on the transition time constant and gain are shown in Figure 7. The characteristics seen in the figure are similar to those of the settling time cost, except that the sharp increase in the cost occurs at a time constant of 1.25 h. This is due to the definition of the envelope cost that allows for a larger range of acceptable molecular weight ($\pm 5\%$ of the actual value). The time during which the process variable stays within the bounds of the ini-

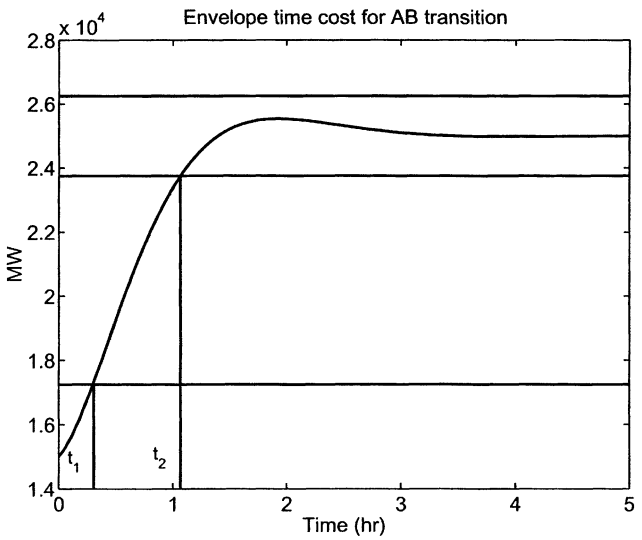

Figure 6. Envelope time cost.

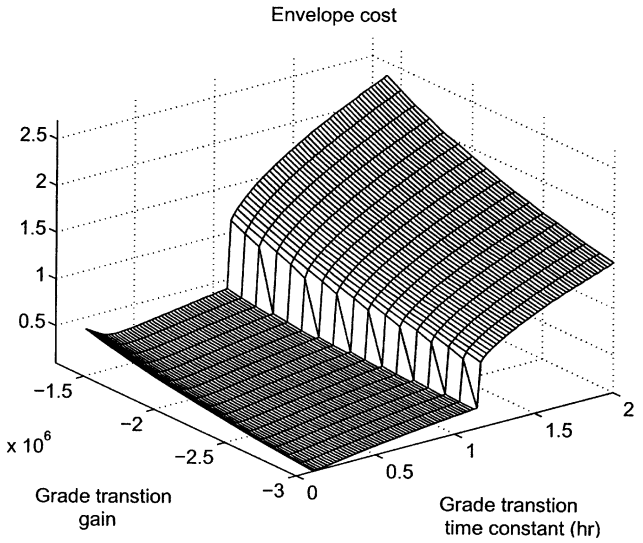

Figure 7. Various envelope time costs with the gain and time constant of the transition model with AD transition as linear model in the IMC structure and with B and D as initial and final points for transition, respectively.

tial value is not taken into account by the settling time cost. Thus, if the objective is minimization of the off-spec product, the time during which the process variable is out of the specifications reflects the economic cost (envelope cost). Therefore, the optimal schedules obtained using this cost (Table 5) are considered for further analysis. The envelope time cost increases with a decrease in the magnitude of K_m for most of the transitions. Also, the cost increases with an increase in τ_m, and for transitions with lower time constants, this increase is pronounced. Increasing the filter time constant also increases the envelope cost as the response is slower. Thus, at higher λ, the optimal schedules include the AC transition instead of the AD transition when the models chosen for the controller design are DB and AD. The primary reason for the difference between this cost and the settling time cost is that the bounds on the molecular weight are broader as discussed above.

Screening Based on Controllability Analysis

In this section, screening tools are introduced for eliminating transitions which violate input constraints and that display excessive variations in the molecular weight. These screening tools are proposed based on the controllability analysis from robust control theory (Skogestad and Postlethwaite, 1996). Once the cost of the various transitions are obtained as described in the previous section, the screening tools can be used to take into account the presence of input constraints and variations in the molecular weight.

Elimination based on constraint violation

In calculating the cost associated with each transition, constraints on the inputs have not been considered in the analysis of the linear system. In this section, an approach is discussed to incorporate constraint violations to determine the optimal transition schedule. Since the objective during the transition is reference tracking, the limitations on the allowable bandwidth due to input constraints is considered. To achieve acceptable control up to a frequency ω_r of the reference signal, it is required that

$$|G| > |R_s| - 1 \qquad \forall \omega \le \omega_r$$

where G is the transfer function of the plant and R_s is reference scaling ratio. Thus, ω_r can be calculated for the transition problem to yield

$$\omega_r = \frac{\sqrt{K_p^2 - (R_s - 1)^2}}{(|R_s| - 1)\tau_p}$$

The bandwidth of the controller designed in the previous section can also be calculated by considering the sensitivity function (S)

$$|S(j\omega_b)| = \frac{1}{\sqrt{2}}$$

Solving for ω_b in the equation above, one can obtain the following expression for the bandwidth

$$\omega_b = \sqrt{\frac{-b - \sqrt{b^2 - 4ac}}{2a}}$$

where a, b, and c are defined as

$$a = -K_m^2 \lambda^2 \tau_p^2$$

$$b = (K_m \lambda + K_p \tau_m)^2 - 2K_m K_p \lambda \tau_p - 2K_c^2 \lambda^2$$

$$c = K_p$$

Comparing the controller's bandwidth with the maximum allowed bandwidth from the acceptable control analysis under input constraints provides an indication of the possibility of constraint violations. For cases where $\omega_b > \omega_r$, there exist certain frequency ranges of the reference signal where constraints are violated. For this study, transitions which did not satisfy $|G| < |R_s| - 1$ at $\omega = 0$ were also considered as transitions that would violate the input constraints, and the corresponding transition was eliminated from consideration in the optimal schedule. The scaling used in this section is critical in determining whether a transition violates input constraints. The scaling was chosen to make sure that the transitions that violated the input constraints also violated the frequency domain criteria. The transitions that are likely to violate input

Table 6. Optimal Schedules Based on Envelope Costs Considering the Effect of Input Constraints

Transition Model	$\frac{\lambda}{\tau_m}$	Transitions Violating Input Constraints	Optimal Schedule	Violation Under Uncertainty	Optimal Schedule
$\tau_m = 0.21$ (DB)	1.0	—	*ADBCA*	*AC*, *AD*	*ABCDA*
	5.0	—	*ADBCA*	—	*ADBCA*
	10.0	—	*ACBDA*	—	*ACBDA*
$\tau_m = 0.18$ (DA)	1.0	*AC*, *AD*	*ABCDA*	*AB*, *AC*, *AD*	—
	5.0	—	*ADBCA*	*AC*, *AD*	*ABCDA*
	10.0	—	*ADBCA*	*AD*	*ACBDA*
$\tau_m = 0.40$ (AD)	1.0	*AC*, *AD*	*ABCDA*	*AB*, *AC*, *AD*	—
	5.0	—	*ADBCA*	*AD*	*ACBDA*
	10.0	—	*ACBDA*	—	*ACBDA*

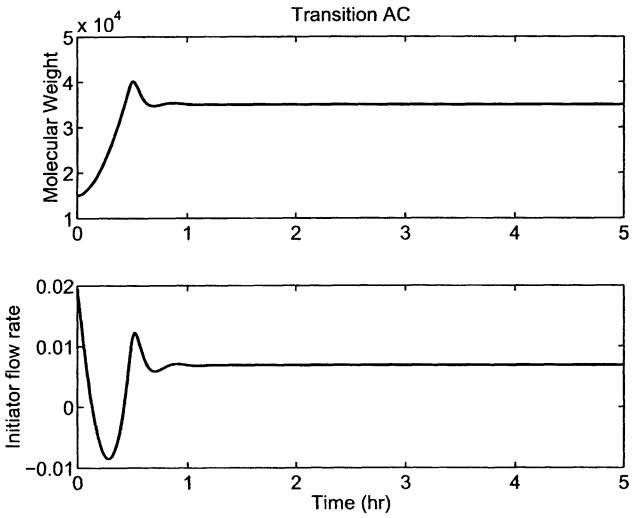

Figure 8. Input constraint violation for the AC transition, when $\lambda = 0.18$ hr, and the controller is based on the DA transition model.

constraints are identified from the analysis presented here as shown in Table 6. Figure 8 depicts the results of the simulation with the nonlinear process model for the case, where the transition was screened using the procedure described in this section. Thus, this screening procedure identifies transitions that could violate input constraints, which can then be verified by simulation (Figure 8). In this article, all the transitions identified by this procedure were found to violate the input constraints.

Elimination based on total variation

The total variation is defined as the sum of the deviation of the extrema in the process variable from the final steady-state value and can also be calculated as the integrated absolute area of the impulse response. Total variation is an indicator of the degree of oscillations in the response. Total variation (TV) can also be bounded as follows (Skogestad and Postlethwaite, 1996)

$$M_T \le TV \le (2n+1)M_T$$

Here, M_T refers to the frequency domain peak of $T(j\omega)$, the complementary sensitivity function, and n is the order of the complementary sensitivity function. This can be easily evaluated in closed form as compared to the total variation and is used as the measure of the degree of oscillations. Thus, higher the value of M_T, higher is the degree of variations in the response. The frequency at which the T is a maximum (ω_T) can be found as a solution to a quadratic equation. For the grade transition problem, T is determined to be

$$|T(j\omega)| = \frac{K_p\sqrt{1+\tau_m^2\omega^2}}{\sqrt{\left(K_p - K_m\tau_p\lambda\omega^2\right)^2 + \left[\omega\left(K_p\tau_m + K_m\lambda\right)\right]^2}}$$

Differentiating the above equation with respect to ω and equating the derivative to zero and solving for ω_T, one obtains

$$\omega_T = \sqrt{\frac{-q-\sqrt{q^2-4pr}}{2p}}$$

where p, q, and r, are defined as

$$p = -K_m^2\lambda^2\tau_p^2\tau_m^2$$

$$q = -2K_m^2\lambda^2\tau_p^2$$

$$r = -\left[K_p^2\lambda^2 + 2K_mK_p\lambda(\tau_m - \tau_p)\right]$$

If M_T is greater than a critical value, this would result in excessive variations, and, thus, the corresponding transition can be eliminated. In considering the effect of total variation, M_T was calculated and if this was found to be greater than 1.05, the transition was eliminated. Transition AD violated this consideration when $\lambda/\tau_m = 1$ and $\tau_m = 0.17$ as the resulting controller was aggressive. However, the optimal schedule based on the envelope cost does not include the AD transition for the particular choice of the filter time constant and the model.

Minimum Transition Time

In this section, the minimum time required for a grade transition without violating the input constraints is calculated for the linear models of all the grade transitions. This is formulated as an optimization problem (Eq. 3), where the free variable in the optimization is the filter time constant. A particular transition is assumed to be the model for the controller design. The closed-loop response of the molecular weight and the initiator flow rate is analytically obtained and a weighted sum of the ratio of the envelope time cost to the model time constant, and the ratio of the filter time constant to model time constant is chosen as the objective function. Then, the scalar optimization problem is solved to obtain the minimum transition time for all the transitions and is used to determine the optimal schedule shown in Table 7. The optimal schedule is determined for different transition models in the IMC structure

$$\min_{\lambda} J(\lambda) = w_1\frac{t_{\text{env}}}{\tau_m} + w_2\frac{\lambda}{\tau_m}$$

$$\text{s.t. } 0 \le u(t) \le 0.1 \text{ m}^3/\text{hr} \quad \forall t \in \left[t_0, t_f\right] \tag{3}$$

where t_{env}/τ_m is related to the off-specification product cost normalized for the different controller models, λ/τ_m is an indicator of the speed of response of the closed-loop, and $u(t)$ is the initiator flow rate.

The results presented in Table 7 show that the transition time is dependent on the transition model used in the controller design. The dependence of the minimum transition

Table 7. Cost of the Schedules Based on the Minimum Transition Time

Transition Model	ABCDA	ABDCA	ACBDA	ACDBA	ADBCA	ADCBA
$\tau_m = 0.21\ (DB)$	0.720*	0.746	0.722	0.758	0.939	1.00
$\tau_m = 0.18\ (DA)$	0.801	0.784*	0.847	0.859	1.00	0.979
$\tau_m = 0.40\ (AD)$	0.905	0.766	1.00	0.768	0.799	0.585*

time on the weights (w_1 and w_2) is minimal, as the schedules that occur when the weights are changed have almost the same cost. This approach is an alternative to the costs described in the previous sections. Here, the dependence on the filter time constant is eliminated through the optimization procedure. Although calculation of this cost requires higher computational time in comparison with the costs in the previous section, this explicitly accounts for the input constraints.

Analysis in the Presence of Uncertainty

Uncertainty characterization

The analysis presented in the previous sections considered the nominal linear first-order models of all the grade transitions. However, this representation is not exact due to the nonlinearities present in the process and other variables in practice. Analysis in the previous sections also suggests the importance of the process gain and the time constant in determining the cost of the transitions. In this section, an effort has been made to address this issue of uncertainty. Uncertainty in the gain and the time constant of the linear model of the transition is assumed to be $\pm 5\%$ and $\pm 10\%$, respectively. Techniques from uncertainty analysis in robust control theory are used to identify the transitions that violate input constraints under uncertainty (Skogestad and Postlethwaite, 1996). This uncertainty is characterized by an upper bound on the magnitude of the relative error between the perturbed and the nominal plant ($(G_p - G)/G$), using an uncertainty weight as shown in Figure 9. The uncertainty weight is identified as

$$w_I(s) = \frac{0.070s + 0.052}{0.39s + 1} \tag{4}$$

Evaluation of transition costs and controllability analysis under uncertainty

All of the costs presented in the previous sections were determined for various sets of the perturbations. The worst case of the perturbations was then used to calculate the optimal schedule. It was found that the squared error, the settling time, and the envelope cost formulations yielded an optimal schedule that did not change with the perturbations.

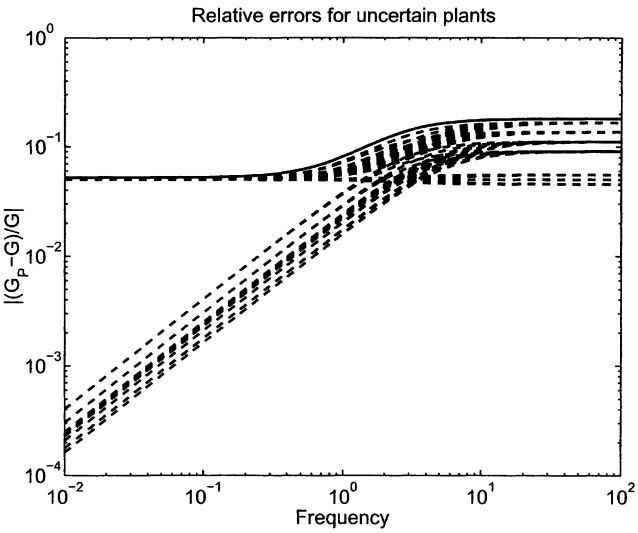

Figure 9. Uncertainty characterization for perturbations in the gain and the time constant of the linear model.

For the controller model and the specified closed-loop time constant, the worst case cost was typically the nominal model for most of the transitions, and, thus, did not affect the optimal schedule. The minimum transition time is the same as the nominal case, when the model for the controller is chosen as AD or DA. However, when the model chosen is DB, the optimal schedule is different (See Table 8). Here, uncertainty causes the worst case cost of the trasition AB to increase relative to the AC transition. Thus, the transition AB is eliminated in the optimal schedule.

Using the controllability analysis to screen transitions based on input constraints, the minimum allowable bandwidth for reference tracking is obtained for the perturbed model as shown below

$$G_p(s) = G(s)(1 + w_I \Delta_I)$$

where Δ_I is the scalar normalized perturbation. Controllability analysis for reference tracking requires

$$|G_p| > |R_s| - 1 \quad \forall \omega \le \omega_{rm} \quad \& \quad \forall \Delta_I \text{ s.t. } |\Delta_I| \le 1$$

Table 8. Cost of the Schedules Based on the Minimum Transition Time in the Presence of Uncertainty

Transition Model	ABCDA	ABDCA	ACBDA	ACDBA	ADBCA	ADCBA
$\tau_m = 0.21\ (DB)$	0.728	0.751	0.720*	0.757	0.950	1.00
$\tau_m = 0.18\ (DA)$	0.671	0.651*	0.883	0.878	1.00	0.990
$\tau_m = 0.40\ (AD)$	0.897	0.771	1.00	0.768	0.800	0.584*

As the minimum of G_p occurs when $\Delta_t = -1$, the minimum allowable bandwidth (ω_{rm}) for reference tracking is obtained by examining the following inequality

$$|G(1-w_I)| > |R_s| - 1 \qquad \forall \omega \le \omega_{rm}$$

The maximum bandwidth of the controller for the perturbed plant can be obtained by the following analysis. The sensitivity function for the perturbed plant and the definition of the controler bandwidth are as follows

$$|S_p| = \left| \frac{1}{1 + GK(1 + w_I \Delta_I)} \right|$$

$$\left| S_p(j\omega_{mb}) \right| = \frac{1}{\sqrt{2}}$$

The perturbation that leads to the maximum bandwidth for control (ω_{mb}) is $\Delta_I = +1$ and the bandwidth can be calculated by solving the above equation. However, unlike the nominal case, the equation is of a higher order than a quadratic and an analytical solution is not possible. Thus, whenever $\omega_{mb} > \omega_{rm}$, constraint violation can occur at certain frequency ranges. The analysis incorporating uncertainty reveals several transitions that violate the input constraints, and these are summarized in the Table 6.

The complementary sensitivity function (T_p) for the perturbed case and the optimization problem associated with obtaining the peak value of $T_p(M_T)$ is detailed below

$$M_T = \max_{\omega, \Delta_I} \left| \frac{GK(1 + w_I \Delta_I)}{1 + GK(1 + w_I \Delta_I)} \right|$$

$$\text{s.t. } \Delta_I = re^{i\theta} \qquad |\Delta_I| = r \le 1$$

Here, unlike the nominal case, an analytical solution for M_T is not possible, and, thus, a constrained optimization problem with ω and Δ_I as the free variables was solved to obtain M_T. It was found that no additional transitions were eliminated relative to the nominal case.

Conclusions

In this article, a scheme for optimal control-relevant scheduling of the grade transitions is presented. The effect of nonlinearities is considered through the use of separate linear models for each transition and a single linear controller. Various transition costs are employed to quantify the grade transitions. The envelope time cost reflects the economic cost of the off-spec product. However, input constraints are not considered in this cost. The minimum transition time cost is also directly related to the cost of the off-spec product and takes into account the input constraints, and is independent of the controller.

Insights from robust control theory are used to derive an heuristic to screen transitions. This heuristic is based on frequency domain criteria that are related to input constraint violation and the degree of variations in the response. A preliminary screening tool that accounts for input constraints and the variability in the response is computed, given a linear model of the transition and a linear controller. This can be used to analyze the transitions in an efficient manner, as most of the calculations described in earlier sections are straightforward, often yielding analytical expressions. Thus, these approaches can be applied to large-scale problems involving several grades. The minimum transition time calculation involves a greater computational cost, but would be significantly faster than solving the rigorous nonlinear programming problem. The scheme is demonstrated on an isothermal polymerization reactor with a single input and an output. The effect of uncertainty in scheduling the transitions has also been addressed in this article. It was found that uncertainty had an important effect on certain aspects such as constraint violations, while in some others (total variation) it had a minimal effect.

The analysis in the article does not include several important aspects of the scheduling problem such as inventory management and the market demand for different grades. A rigorous solution including all the details would result in an MINLP formulation. Difficulties associated with solving such MINLP problems are well recognized (Shah et al., 1993; Orcun et al., 2001). In this context, the heuristics that were presented in this article could be used along with a modified MINLP approach to search over the subset of all possible solutions in a rigorous fashion. These heuristics provide insight into identifying the fundamental limiting behavior for certain "difficult" transitions (transitions that violate input constraints or display excessive overshoot). Such an approach could combine effectively fundamental insights and the rigor of a programming approach to yield an efficient algorithm-engineered solution to the optimal grade transition scheduling problem.

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