SIMULTANEOUS DESIGN AND CONTROL OF POLYMERIZATION REACTORS

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Abstract: Chemical engineering science has recognized the necessity of integrating process design and control; however, few steps have been taken in this direction in polymer science. In this work, a Mixed-Integer Dynamic Optimization approach is used for the simultaneous design and control of a styrene polymerization reactor. Our goal is to design the process and its control system in order to produce two polymer grades, which are defined in terms of the number average molecular weight (Mn). The process design involves reactor and initiator selection, and the two steady state operating points. The control system consists of a feedforward-feedback control scheme, which is designed to achieve optimal grade transition operation. The control system design includes optimal pairings between controlled and manipulated variables and controller's tuning parameters for PI feedback controllers, and the best trajectories of the feedforward controllers.

Keywords: Simultaneous design and control; grade transition optimization; polymerization reactor; mixed-integer dynamic optimization.

INTRODUCTION

Polymer synthesis and modification is a very important industry, producing nearly 200 million tons per year of a variety of polymers. Materials produced vary from high-volume resins sold at approximately one dollar per kilogram to high-priced specialty polymers at several thousand dollars per kilogram. During the past years, increased costs of energy, more stringent environmental regulations, and intense worldwide competition have motivated strong interest in optimizing plant designs and operating conditions.

Polymers have many application areas, and each area needs different specifications. In order to fulfill these requirements, different grades of the same polymers are usually produced. Continuous plants commonly manufacture these grades in the same equipment by switching the operating points. This operation, called grade transition or grade changeover, may be performed rather frequently so as to satisfy the changing market demands. Therefore, the minimization of off-specification product during grade transition and the transition time is essential for a lucrative process. This is why, in addition to steady-state optimization, intense research has been performed regarding optimal grade transition operation of polymerization reactors. For instance, McAuley and McGregor (1992) developed optimal transition policies among three polyethylene grades in a gas-phase reactor. Using dynamic optimization they calculated the best profiles of the input variables.

They also presented a very interesting analysis of different objective functions for the grade transition optimization. Takeda and Ray (1999) developed optimal transition policies for polyolefin loop reactors, comparing results with and without constraints in the state variables. Cervantes et al. (2002) carried out an open loop optimization of grade transitions in a low-density polyethylene plant. They calculated optimal profiles of butane feed and purge streams in order to minimize transition time. However, the usual approach in these studies is to analyze the grade transition between steady-states that are fixed in advance, assuming that some criteria, like steady-state optimization, has been used to determine them. Although some works combined steady-state optimization with optimal grade transition operation (Yi et al., 2003), these topics were treated sequentially, and therefore the influence of the optimal steady-states on the grade transition was not analyzed. The more interesting problem of studying the effect of the steady-states on the optimal transition policies has rarely been explored. In this situation it would be possible to find a sub-optimal, though still reasonable steady state, which allowed a more convenient grade changeover, resulting in a better process performance as a whole.
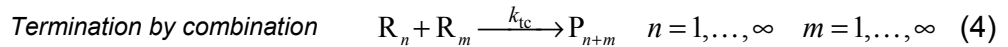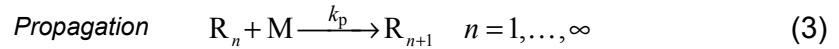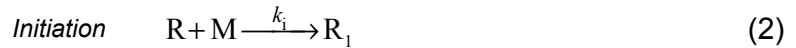
Optimal transition policies, which minimize economic loss during grade changeovers while keeping product quality within desired standards, can only be implemented with a control system that guarantees well-controlled operating conditions. Polymerization processes show several features that make process control a challenging task, such us high non-linearity, complex flow and heat-transfer dynamics, and a strong dependence of molecular properties on operating conditions. This has motivated plentiful work about control of polymerization reactors. Different control systems have been proposed, from classical PID controllers to modern non-linear model predictive control (NLMPC) schemes (Embiricu et al., 1996). A well-designed control system that ensures a safe operation envelope is extremely important for plant operation in general, and specially for grade changeovers. For instance, it is common to perform overshoots or undershoots aiming to reduce the transition time, which could lead to process runaway if they are not properly controlled. This is why several authors combined grade transition optimization with process control (i.e. Chatzidoukas et al., 2003; Wang et al. 2000; Na and Rhee, 2002; Bindlish and Rawlings, 2003; BenAmor et al., 2004). In most of these works, however, a sequential approach has been used to deal with process design and process controllability. For instance, Wang et al. (2000) calculated off-line optimal transition policies for an ethylene slurry polymerization reactor, and then applied a NLMPC to implement these policies in face of uncertainties in model parameters. Na and Rhee (2002) used a multivariable NLMPC to track set points that had been previously determined in a styrene solution polymerization.

The sequential methodology does not consider the strong interaction existing between process design and its operability. Process control is an inherent property of its design, and has a great influence on process economics. The necessity of incorporating control aspects in the early stages of process design has been recognized in other fields of chemical engineering (Bansal et al., 2002), but polymer engineering science is now making its first efforts in this direction. One of these works is that of Chatzidoukas et al. (2003), who performed a simultaneous control structure selection and grade transition optimization in a gas-phase olefin polymerization reactor. However, they did not include equipment design and steady state operating conditions in their optimization problem

In this work a Mixed – Integer Dynamic Optimization (MIDO) approach is applied to the simultaneous design and control of a continuous stirred tank reactor (CSTR) for styrene polymerization. Process design includes reactor unit and peroxide initiator selection, and the steady-state operating points for producing two polymer grades. At each steady-state, the only specification is the polymer number average molecular weight (Mn). The control system is designed to achieve an optimal transition between grades. It consists of a feedforward-feedback multivariable scheme. With polymer grades as the only specifications, the process and the control system are designed simultaneously to achieve optimal grade transition operation. The control system design includes optimal pairings between controlled and manipulated variables and controller's tuning parameters for PI feedback controllers, and the best control trajectories of the feedforward controllers.

PROCESS DESCRIPTION AND MATHEMATICAL MODEL

Figure 1 represents the process studied in this work, the solution polymerization of styrene in a jacketed CSTR. Reactor inputs consist of styrene monomer, initiator and solvent streams at the feed temperature T_f; polystyrene, solvent and unconverted monomer and initiator compose the reactor effluent, at temperature T. Water is used to cool the reactor. The mathematical model used in this work is based on the one published by Russo and Bequette (1998), which comprises the following kinetic mechanism:

$$\text{Peroxide decomposition} \qquad \text{I} \xrightarrow{\ k_d\ } 2\,\text{R} \qquad\qquad (1)$$

$$\text{Initiation} \qquad \text{R} + \text{M} \xrightarrow{\ k_i\ } \text{R}_1 \qquad\qquad (2)$$

$$\text{Propagation} \qquad \text{R}_n + \text{M} \xrightarrow{\ k_p\ } \text{R}_{n+1} \quad n = 1,\ldots,\infty \qquad\qquad (3)$$

$$\text{Termination by combination} \qquad \text{R}_n + \text{R}_m \xrightarrow{\ k_{tc}\ } \text{P}_{n+m} \quad n = 1,\ldots,\infty \quad m = 1,\ldots,\infty \qquad (4)$$

where I is the peroxide initiator, R is the initiation radical, M is styrene monomer, R_n is a macroradical of chain length n and P_n is a polymer molecule of chain length n; k_d, k_i, k_p and k_{tc} are the kinetic constants of initiator decomposition, initiation, propagation and termination, respectively. Monomer thermal initiation and gel effect are neglected in this model. Assuming quasi steady-state of radicals and constant physical properties of the reaction mixture, the differential equations resulting from the mass and energy balances are:

$$\text{Initiator} \qquad \frac{dI}{dt} = \frac{1}{V}\left(Q_i I_f - QI\right) - k_d I \qquad\qquad (5)$$

$$\text{Monomer} \qquad \frac{dM}{dt} = \frac{1}{V}\left(Q_m M_f - QM\right) - k_p M \lambda_0 \qquad\qquad (6)$$
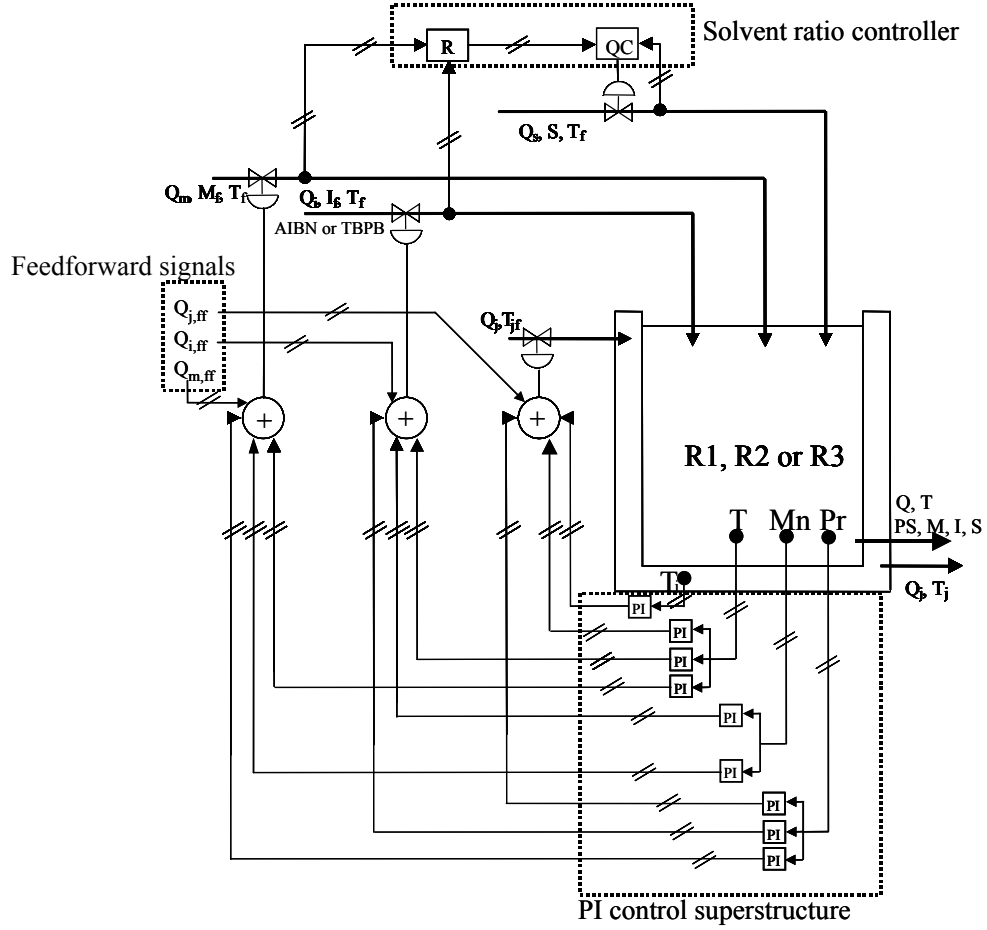
Figure 1. Polymerization reactor scheme.

Reactor temperature

$$\frac{dT}{dt} = \frac{Q}{V}\left(T_{\mathrm{f}} - T\right) + \frac{\left(-\Delta H_{\mathrm{r}}\right)}{\rho Cp} k_{\mathrm{p}} M \lambda_0 - \frac{UA}{\rho CpV}\left(T - T_{\mathrm{j}}\right) \qquad (7)$$

Jacket temperature

$$\frac{dT_{\mathrm{j}}}{dt} = \frac{Q_{\mathrm{j}}}{V_{\mathrm{j}}}\left(T_{\mathrm{j\,f}} - T_{\mathrm{j}}\right) + \frac{UA}{\rho_{\mathrm{j}} Cp_{\mathrm{j}} V_{\mathrm{j}}}\left(T - T_{\mathrm{j}}\right) \qquad (8)$$

0th order moment of the polymer molecular weight distribution

$$\frac{dM_0}{dt} = \frac{1}{2} k_{\mathrm{tc}} \lambda_0^2 - \frac{Q}{V} M_0 \qquad (9)$$

1st order moment of the polymer molecular weight distribution

$$\frac{dM_1}{dt} = k_{\mathrm{tc}} \lambda_0^2 + k_{\mathrm{p}} M \lambda_0 - \frac{Q}{V} M_1 \qquad (10)$$

where

$$\lambda_0 = \sqrt{\frac{2 \, \text{efic} \, k_\text{d} I}{k_\text{tc}}} \tag{11}$$

In the present model, monomer conversion (x), polymerization rate (Pr) and polymer number average molecular weight (Mn) are calculated according to Eqs. (12) – (14), respectively.

$$x = \frac{M_1}{M + M_1} \tag{12}$$

$$\text{Pr} = k_\text{p} M \lambda_0 \tag{13}$$

$$\text{Mn} = \text{Mw}_\text{M} \frac{M_1}{M_0} \tag{14}$$

In eqs (5) – (14), M, I, and λ_0 are the monomer, initiator, and global radical concentrations; T and T_j are the reactor and jacket temperatures; M_0 and M_1 are the 0th and 1st order moments of the polymer chain length distribution; Q_i, Q_m, Q_s, and Q_j are the flow rates of initiator, monomer, solvent and coolant. The total flow rate Q is the sum of the feed streams. Subscript f denotes feed conditions. The initiator decomposition efficiency is variable "efic", and Mw_M is the monomer molecular weight.

Control system

The control system is composed by a multivariable feedforward-feedback control scheme (see Figure 1), plus a ratio controller. Reactor and jacket temperatures, polymerization rate and Mn are considered as possible controlled variables. The variables that could be manipulated in this reactor are monomer, initiator and coolant flow rates. Solvent flow rate is attached to the initiator and monomer flow rates through a ratio controller, which keeps a constant solvent volume fraction of 50%. Feedforward controllers are used for property control (Mn), and feedback PI controllers for reactor and jacket temperatures, polymerization rate and Mn control. The overall action on each manipulated variable is composed by the feedforward signal plus the action of the PI loops in which that variable is involved (see Figure 1). For this work it was established that feedforward controllers must manipulate all control efforts, but optimal pairing between manipulated and controlled variables for the PI controllers must be determined. The allowed alternatives are shown in the PI superstructure presented in Figure 1.

The equation that describes the control action on the manipulated variables is

$$U_i = U_{i,ff} + \sum_{j=1}^{4} K_{i,j} \left[\left(Y_{j,set} - Y_j \right) + \frac{1}{\tau_{i,j}} \int_0^t \left(Y_{j,set} - Y_j \right) dt' \right] \tag{15}$$

In this equation, U_i is the i-th manipulated variable ($U_1 = Q_j$, $U_2 = Q_i$, $U_3 = Q_m$), and Y_j is the j-th controlled variable ($Y_1 = T$, $Y_2 = T_j$, $Y_3 = Mn$, $Y_4 = Pr$); $Y_{j,set}$ is the set point of the Y_j variable. $U_{i,ff}$ stands for the feedforward controller's action. The summation represents the addition of the signals of all possible PI loops.

In order to account for operative constraints on the manipulated variables, the following saturation function was included:

$$U_i = \begin{cases} U_{i,max} & if \quad U_{i,max} < U_i \\ U_i & if \quad U_{i,min} \le U_i \le U_{i,max} \\ U_{i,min} & if \quad U_i < U_{i,min} \end{cases} \tag{16}$$

Eq. (16) was smoothed as shown by Eq. (17).

$$U_i = 0.25 \Big[\left(U_i - U_{i,min} \right) \tanh \left(\xi \left(U_i - U_{i,min} \right) \right) + U_i + U_{i,min} \Big] \\ \Big[\tanh \left(\xi \left(U_{i,max} - U_i \right) \right) + 1 \Big] + 0.5 U_{i,max} \Big[\tanh \left(\xi \left(U_{i,max} - U_i \right) \right) + 1 \Big] \tag{17}$$

Parameter ξ determines the "smoothness" of the expression defined by Eq. (17). The greater ξ is, the more Eq. (17) resembles Eq. (16). In this work we used $\xi = 10^6$. Finally, Eq. (18) is used to determine the solvent flow rate so as to obtain the required solvent volume fraction of 50%

$$Q_s = Q_i + Q_m \tag{18}$$

DESIGN PROBLEM

Continuous polymer plants usually alternate between the productions of several polymer grades. In this work, however, we will focus on the grade transition operation between two polystyrene grades, called grades A and B. These grades will be defined by their number average molecular weight. The process and control system will be simultaneously designed to minimize off-specification product during grade transition from grade A to B. At the same time, dynamic feasible operation in terms of product specifications and process constraints must be achieved.

Process design includes the selection of optimal reactor size, initiator, and steady-state operating points. The control system design will provide optimal trajectories for the

feedforward controllers, the "best" pairings between controlled and manipulated variables for the PI controllers, as well as the PI controllers' tuning parameters.

Process design variables

Two of the process design items involve discrete decisions. One of them is the polymerization reactor. The design of this unit is limited because of equipment availability. Only three alternatives are possible, whose features are listed below:

R1	R2	R3
V = 2000 L	V = 3000 L	V = 3500 L
V_j = 2208 L	V_j = 3312 L	V_j = 3864 L

The other discrete decision is the initiator type. Through an appropriate initiator selection, it is possible to enhance reactor performance to increase production, achieve certain molecular properties or improve controllability. With the approach used in this work, it is possible to provide any finite number of initiator alternatives, and then model the selection of one or more initiators. In this work, the initiators allowed are azobis(isobutyronitrile) (AIBN) and tert-butyl peroxybenzoate (TBPB), and only one of them may be selected. AIBN is more reactive than TBPB. Initiator selection is modeled by means of binary variables (y_{AIBN} and y_{TBPB}). These variables are employed to select the pre-exponential factor and the activation energy of the initiator decomposition constant corresponding to the chosen initiator:

$$k_d = A_d e^{(-E_d/RT)} \tag{19}$$

$$A_d = A_{AIBN} y_{AIBN} + A_{TBPB} y_{TBPB} \tag{20}$$

$$E_d = E_{AIBN} y_{AIBN} + E_{TBPB} y_{TBPB} \tag{21}$$

$$y_{AIBN} + y_{TBPB} = 1 \tag{22}$$

y_{AIBN} and y_{TBPB} take the value of 1 if the corresponding initiator is selected, or 0 otherwise. The integer constraint represented by Eq. (22) is used to specify the selection of one of the initiators.

The other process design variables are the operating temperatures T, T_j and T_f, and the flow rates Q_j and Q_i at both steady-states. T_{jf} and Q_m are known in advance, and Q_s is determined by Q_m and Q_i as shown by Eq. (18). Process model equations, product specifications (Mn is known at each steady-state) and other process restrictions result in

only three degrees of freedom among the mentioned steady-state design variables for the optimization problem.

Control system design variables

The control system design includes calculating the optimal profiles of the feedforward signals ($U_{i,\text{ff}}$ in Eq. (15)). These are calculated by the optimizer as series of piecewise constant values, in order to optimize the design objective function. For the PI controllers, design variables involve the selection of the optimal parings between controlled and manipulated variables, the controllers´ tuning parameters ($K_{i,j}$ and $\tau_{i,j}$ in in Eq. (15)) and the set points of the controlled variables ($Y_{j,\text{set}}$ in Eq. (15)). The latter are treated as piecewise constant optimization variables, while $K_{i,j}$ and $\tau_{i,j}$ are considered as time invariant. The selection of the matching between controlled and manipulated variables is modeled by setting the following constraint to the gains of the PI controllers:

$$K^{lb}_{i,j} y_{i,j} \leq K_{i,j} \leq K^{ub}_{i,j} y_{i,j} \tag{23}$$

The binary optimization variable $y_{i,j}$ takes the value of 1 if the i-th manipulated variable is matched with the j-th controlled variable, or 0 otherwise. In the latter case, Eq. (23) forces the controller gain to be zero, and hence the action of that control loop disappears. The control superstructure would yield 2^{12} = 4096 control alternatives, identified by the 12 binary variables that represent the possible combinations between the 4 controlled variables and the three manipulated variables. However, as can be seen in Figure 1, some of these pairings were disregarded in advance, based on process knowledge and previous simulations:

- Controlling T_j manipulating Q_i ($y_{2,2}$ = 0)

- Controlling T_j manipulating Q_m ($y_{3,2}$ = 0)

- Controlling Mn manipulating Q_j ($y_{1,3}$ = 0)

The multivariable scheme considered in this work allows any controlled or manipulated variable to be involved in more than one loop simultaneously. The lengths of the time intervals for the piecewise constant control variables are also considered as optimization variables.

Product specifications and process constraints

As mentioned before, grade specifications, defined in terms of the polymer Mn, must be satisfied at steady-states. The number average molecular weight of grade A is Mn_A = 50000 g/mol, and that of grade B is Mn_B = 40000 g/mol. Besides, monomer conversion at steady-state must satisfy the constraints shown by Eq. (24)

$$0.18 \leq x_A, x_B \leq 0.50 \qquad (24)$$

The lower limit represents an acceptable limit for profitable production, while the upper bound was selected to avoid high viscosities in the reaction mixture.

In order to avoid significant monomer thermal initiation, upper bounds for the reactor temperature must be set. Those bounds were selected as 100 ºC and 110 ºC for the steady-state and the grade transition operations, respectively. Another important point to consider is that this type of process usually presents steady-state multiplicity. In order to exclude low conversion steady-states, a lower bound of 70 ºC for the steady-state reactor temperature was selected. Steady-state temperatures for production of both polymer grades (A and B) and reactor temperature during transition must then verify Eqs. (25) and (26), respectively

$$70\,^{\circ}\text{C} \leq T_A, T_B \leq 100\,^{\circ}\text{C} \qquad (25)$$

$$T(t) \leq 110\,^{\circ}\text{C} \qquad (26)$$

Besides, an upper limit for the jacket temperature at any time was selected so as to keep a safety margin with respect to the boiling point of water, as shown in Eq. (27).

$$T_j(t) \leq 95\,^{\circ}\text{C} \qquad (27)$$

Notice that reactor and jacket temperature constraints (Eqs. (26) and (27)) during grade transition are path constraints. This class of constraint was dealt with by converting them into end-point constraints, following the procedure reported by Bansal et al. (2002).

Additional process restrictions involve monomer flow rate at steady-states and cooling fluid inlet temperature, which are fixed at 0.105 L s^{-1} and 22ºC, respectively. The feed temperature is not known in advance, but it should be the same at both steady states. An upper bound for this variable was set in order to keep it within the typical values reported in the literature, as shown by Eq. (28).

$$T_f \leq 67\,^{\circ}\text{C} \qquad (28)$$

Additional process restrictions involve monomer flow rate at steady-states and cooling fluid inlet temperature, which are fixed at 0.105 L s^{-1} and 22 ºC, respectively. The feed temperature is not known in advance, but it should be the same at both steady states.

Objective function

The objective function for the simultaneous process and control system design is shown by Eq. (29).

$$Gt = \int_0^{t_f} \left(Mn_B - Mn(t) \right)^2 dt \qquad (29)$$

where Mn_B is the number average molecular weight of grade B. An objective function like Eq. (29) not only minimizes an off-specification property, but also the transition time because the final transition time (t_f) is treated as an additional optimization variable (Chatzidoukas et al., 2003).

OPTIMIZATION PROBLEM FORMULATION

The simultaneous process – control system design that has been presented constitutes a Mixed-Integer Dynamic Optimization (MIDO) problem, which can be posed as follows

$$\min_{u(t),z,d,y} Gt\left(x_d(t_f), x_a(t_f), z, u(t_f), y, d, p \right)$$

$$s.t.$$

$$h_d\left(\dot{x}_d(t), x_d(t), x_a(t), z, u(t), y, d, p \right) = 0$$

$$h_a\left(x_d(t), x_a(t), z, u(t), y, d, p \right) = 0$$

$$h_0\left(x_d(0), x_a(0), z, u(0), y, d, p \right) = 0$$

$$h_y(y) = 0 \qquad (30)$$

$$g_e\left(\dot{x}_d(t_f), x_d(t_f), x_a(t_f), z, u(t_f), y, d, p \right) \le 0$$

$$g_q(z, d, y, p) \le 0$$

$$u^{lb} \le u(t) \le u^{ub}$$

$$z^{lb} \le z \le z^{ub}$$

$$y \in \{0,1\}^{11}$$

$$d \in D$$

h_d and h_a are the model differential – algebraic system, h_0 is the set of initial conditions and h_y is the set of pure integer equalities; g_e and g_q are end-point and time-invariant inequalities, respectively, and D is a set of three discrete values representing allowed reactor sizes. The set h_a includes the model differential equations set to zero, in order to define both steady-states. $U(t)$ is the set of time-varying optimization variables (7 elements), z is the set of time-invariant decision variables (29 elements), y is a vector of 11 binary

Table 1. Process optimal design.

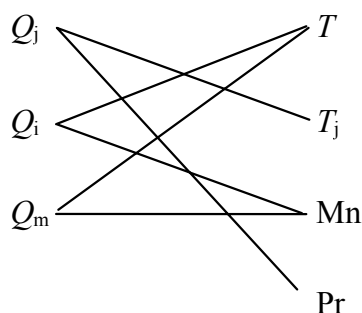| Reactor Unit: R1 (2000 L)		Initiator: AIBN
	Grade A	Grade B
T	100ºC	100ºC
T_f		66ºC
T_j	54ºC	45ºC
Q_j	0.079 L s^{-1}	0.138 L s^{-1}
Q_i	2.51 10^{-3} L s^{-1}	3.48 10^{-3} L s^{-1}
Conversion	33%	37%

Figure 2. Optimal pairing between manipulated and controlled variables.

variables, and d is a discrete variable (reactor volume); $x_d(t)$ are the differential state variables, $x_a(t)$ are the algebraic variables and p are the model parameters.

Additional constraints were also included involving controlled and manipulated variables, and time derivatives for the states. These constraints ensured that the target operating point (where grade B is produced) was actually reached. The resulting MIDO was solved with gPROMS/gOPT package (Process Systems Enterprise Ltd.).

RESULTS AND DISCUSSION

The optimal process design is shown in Table 1. As may be seen, the smallest reactor and the faster initiator were selected. Besides, the process was designed to operate at the highest allowed temperature at both steady-states. It should be noted that constraints on the feed temperature and monomer conversion are satisfied.

The optimal PI control structure is schematized in Figure 2, while the corresponding optimal values for the controllers' gains and integral times are shown in Figure 3. Figure 4 shows the polymer Mn and the Mn set point trajectories. It can be seen that the optimally

$$K = \begin{bmatrix} \cdots & K_{1,2} = 7.95 \times 10^{-3} \dfrac{L/s}{K} & \cdots & K_{1,4} = -416.15 \dfrac{L/s}{g/s} \\ K_{2,1} = 7.96 \times 10^{-6} \dfrac{L/s}{K} & \cdots & K_{2,3} = -2.63 \times 10^{-5} \dfrac{L/s}{g/mol} & \cdots \\ K_{3,1} = -7.96 \times 10^{-6} \dfrac{L/s}{K} & \cdots & K_{3,3} = 2.38 \times 10^{-5} \dfrac{L/s}{g/mol} & \cdots \end{bmatrix}$$

$$\tau = \begin{bmatrix} \cdots & \tau_{1,2} = 114286 s & \cdots & \cdots \\ \cdots & \cdots & \tau_{2,4} = 114286 s & \cdots \\ \tau_{3,1} = 1.90 \times 10^{6} s & \cdots & \tau_{3,4} = 988468 s & \cdots \end{bmatrix}$$

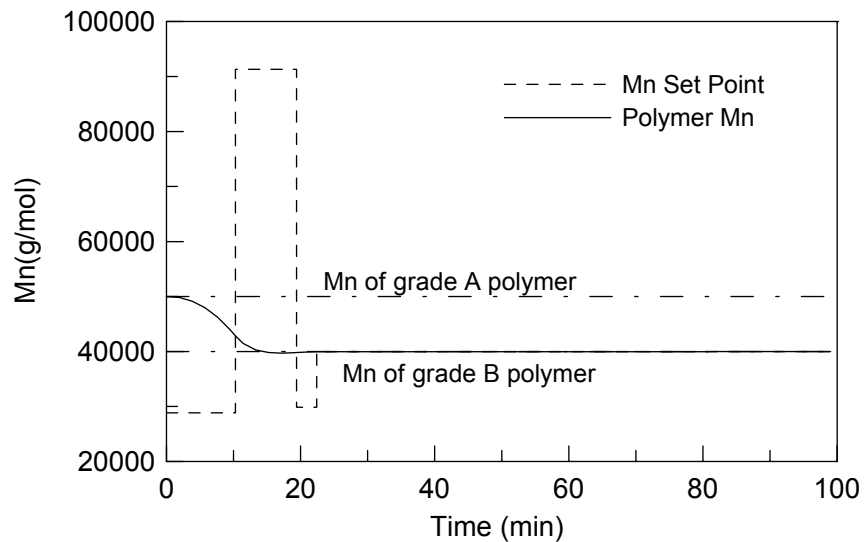**Figure 3**. Optimal values of the controllers' gains and integral times.

Figure 4. Time profiles of the polymer Mn and the Mn set point.

designed control system drives Mn to grade B specification in approximately 15 minutes, a very short time in comparison with the reactor residence time of 2.5 h. As this property is kept almost constant thereon, the amount of off-specification product is minimal. The optimal profile of the Mn set point resulted in a low value at the beginning of the transition, where a rapid descent of this property is needed. Afterwards, the set point rises when the Mn is about to reach the target value, probably to minimize the undershoot, and then settles at grade B Mn.

Figure 5 depicts reactor temperature and reactor temperature set point. Please note the difference in the time scales with respect to Figure 4. A rapid variation of the reactor temperature at the beginning of the transition is observed. This time coincides with the one needed to take the polymer Mn to the target value. Afterwards, the control system slowly takes reactor temperature to its set point value. It can be seen that the maximum reactor temperature of 110 ºC is never violated. Notice the long time needed to reach the steady state value of the reactor temperature, in comparison with the polymer Mn. It should
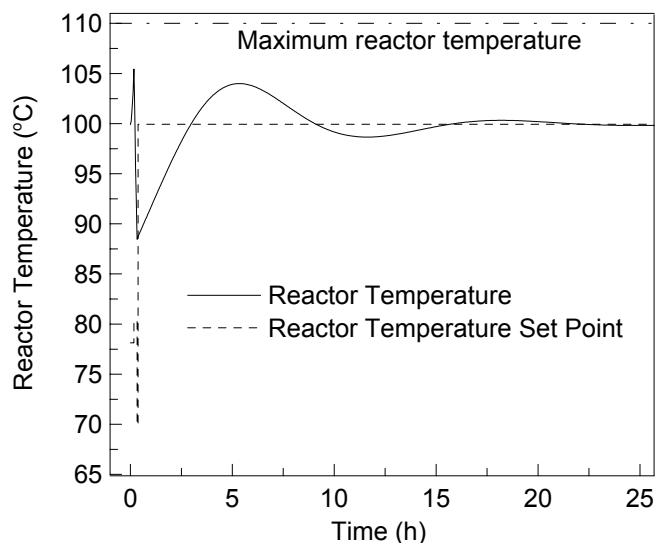
Figure 5. Reactor temperature and reactor temperature set point profiles.
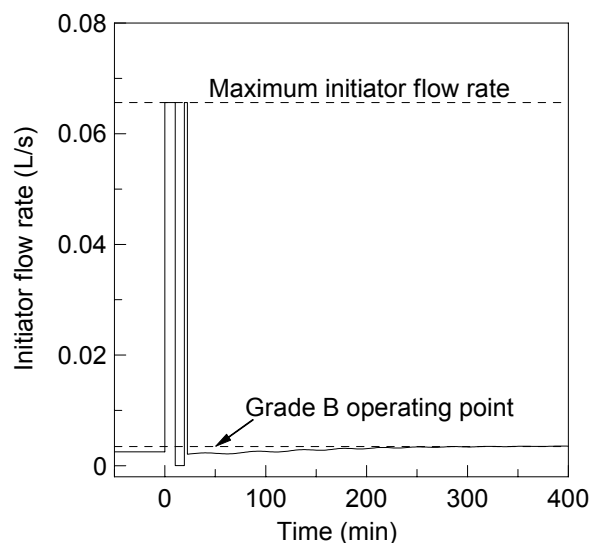

Figure 6. Initiator flow rate profile.

be remembered, however, that the design function consisted only in minimizing off-specification Mn. This long time recovery of the reactor temperature was the best way to fulfill this objective. A similar tendency was observed for the jacket temperature profile.

Figure 6 shows the time profile of one of the manipulated variables, the initiator flow rate. Notice that the grade transition starts at time 0. Sudden variations may be observed during the first 20 minutes, approximately the time needed to stabilize the polystyrene Mn at its target value. Then, this flow rate presents a slow approach to the steady-state operating point. The other manipulated variables show similar profiles. It should be mentioned that the sudden variations of flow rates are a common practice in grade transition operation.

CONCLUSIONS

In this work a Mixed-Integer Dynamic Optimization approach was successfully used for the simultaneous design and control of a solution styrene polymerization reactor. In this way, the strong interaction between process design and control was taken into account.

The process and the control system were optimally designed to achieve optimal transition operation between two polystyrene grades. Process design variables included discrete decisions (reactor and initiator type selections), as well as continuous operating variables (i.e. steady-state reactor temperatures and process flow rates).

A multivariable feedforward-feedback control scheme was optimally determined simultaneously with the process design. Design variables included discrete decisions (optimal pairing between controlled and manipulated variables), time-invariant continuous variables (PI controllers' tuning parameters) and piece-wise constant ones (optimal profiles for the feedforward controllers and PI set points). The optimal multiloop PI structure involved three manipulated variables that in combined action controlled four process variables. The optimal process and control system design allowed a grade transition with minimal off-specification polymer. At the same time, process constraints at steady-state and during grade transition were rigorously satisfied.

Future work will include steady-state economic objectives together with the transition optimization in the design objective. At the same time, multiple grade transition sequences and more realistic polymer grade specifications will be addressed.

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