Optimal Grade Transitions in a Gas Phase Polyethylene Reactor

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Using gas-phase technology many grades of polyethylene can be produced in a single reactor. For a series of three polyethylene products, model-based dynamic optimization is used to determine optimal grade changeover policies. Optimal manipulated variable profiles are determined for hydrogen and butene feed rates, reactor temperature setpoint, gas bleed flow, catalyst feed rate, and bed level setpoint. It is shown that large transitions in melt index are hampered by slow hydrogen dynamics, and that the time required for such a transition can be reduced by manipulating the temperature setpoint and the bleed stream flow. Reduction of the bed level and catalyst feed rates during changeovers can significantly reduce the quantity of off-specification polymer produced. It is demonstrated that melt index and density are not sufficient to characterize the properties of polymer produced during grade transitions, and that the shape of the cumulative copolymer composition distribution is very sensitive to the grade changeover policy used. Optimal transition policies should not be implemented without feedback control. Disturbances and model mismatch can result in product property trajectories which deviate significantly from the nominal optimal trajectory.

Introduction

In industrial settings, polyethylene grade specifications are generally quoted in terms of melt index (*MI*) and density (ρ) (ASTM, 1990), rather than molecular weight and comonomer content. It is essential to produce polyethylenes with a given *MI* and ρ because different polyethylene applications such as injection and roto-molded products, wire coating and film, require different properties. The *MI* and ρ of polyethylene are associated with both processing and end-use characteristics. *MI* is related to the rheological processing properties of the polymer as well as impact strength, stress crack resistance, tensile strength, and elasticity. ρ is related to stiffness, tensile strength, heat resistance, hardness, permeability, transparency, impact strength and flexibility (Foster, 1990). So that many types of polyethylene can be produced in a single reactor, grade transitions from one *MI* and ρ specification to the next are required. The frequency and magnitude of grade changes is determined by both prices and market demand. In industrial gas phase polyethylene reactors, the residence time of the polymer in the reactor is generally from 3 to 5 hours (Choi and Ray, 1985). Since grade changeovers can be made every few days, the potential for producing large amounts of off-specification polymer is large.

Although grade changeovers are of considerable economic importance to the polyolefin industry, very little information on this topic can be found in the literature. Sinclair (1987) has outlined some practical aspects of the grade transition problem, and Ramanathan and Ray (1991) have simulated nonoptimal grade transition strategies for two fluidized bed polyolefin reactors in series. Ramanathan and Ray determined that the catalyst feed rate, hydrogen feed rate, and bleed flow rate are important variables for accomplishing rapid grade transitions. However, no systematic study of grade changeovers has been performed. In this article, optimal open-loop policies for accomplishing grade changeovers are determined using dynamic model-based optimization. The models employed were developed by McAuley et al. and have been published elsewhere (McAuley et al., 1990; McAuley and MacGregor, 1991; McAuley, 1992).

First, the goals of the study are introduced, followed by a

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Table 1. Polyethylene Grades Considered in Transition Study

Grade	Scaled Melt Index Target	Scaled Density Target
A	0.2	9
B	0.16	13
C	2.4	13

review of dynamic optimization techniques. A brief process description is given and the issues involved in formulating and solving the optimal grade transition problem are then discussed. Optimal grade transition trajectories are shown for a typical progression of grade changes. Finally, the problems associated with implementing optimal off-line transitions without feedback are demonstrated. Since the transitions studied in this article pertain to actual polyethylene grades produced in an industrial reactor, the results are scaled so as to not reveal confidential operating conditions. All scaling is consistent with that study used by McAuley and MacGregor (1991).

Goals of the optimal grade transition study

The goals of this optimization study are:

- To formulate a set of dynamic optimization problems for grade transitions involved in producing a typical series of polyethylene products. The products studied are shown in Table 1. The specific transitions studied are $A \rightarrow B$, $B \rightarrow C$, $C \rightarrow B$, and $B \rightarrow A$. This set of transitions represents a production schedule which might be followed in an industrial reactor. Changeovers $A \rightarrow B$ and $B \rightarrow A$ involve a small change in the *MI* specification and a relatively large density transition. In transitions $B \rightarrow C$ and $C \rightarrow B$, a large change in *MI* is required but the desired density remains constant.
- To solve the optimization problems in the previous paragraph in order to determine optimal policies for manipulating the reactor inputs and to determine the types of optimal *MI* and ρ trajectories achievable.
- To determine the effects of problem formulation on the optimal solution. The factors considered include: the set of manipulated variables used to accomplish the changeover, the bounds on the manipulated variables, and the tuning of the objective function.
- To determine which of the optimal trajectories might be desirable for on-line implementation.

In order to accomplish these goals, a thorough understanding of both current dynamic optimization techniques and reactor operating strategies is required.

Dynamic Optimization Techniques and Applications

Dynamic systems modelled by nonlinear differential/algebraic equations (DAEs) arise in many aspects of chemical engineering. Optimization of these dynamic models is commonly used to solve kinetic parameter estimation problems (Biegler et al., 1986) and optimal control problems (Bryson and Ho, 1970; Ray, 1981; Farber and Laurence, 1986). Such optimization problems are more difficult to solve than steady state nonlinear programming (NLP) problems, because some of the equality constraints are given by differential equations.

An example of a typical optimal control problem for a dynamic system is shown below:

$$\min_{\underline{u}(t)} \; F(\underline{u}(t), \underline{x}(t)) \quad t \in [t_0, t_f]$$

$$\text{s.t.} \quad \underline{c}(\underline{u}(t), \underline{x}(t)) = \underline{0} \tag{1}$$

$$\dot{\underline{x}}(t) = \underline{f}[\underline{u}(t), \underline{x}(t)] \tag{2}$$

$$\underline{x}(t_0) = \underline{x}_0 \tag{3}$$

$$\underline{u}_* \leq \underline{u}(t) \leq \underline{u}^* \tag{4}$$

$$\underline{x}_* \leq \underline{x}(t) \leq \underline{x}^* \tag{5}$$

where

F = objective function
$\underline{c}$ = vector of algebraic equality constraints
$\underline{x}(t)$ = vector of state variables
$\underline{f}$ = vector of state derivatives
$\underline{u}(t)$ = vector of manipulated variables
$\underline{u}_*, \underline{u}^*$ = lower and upper bounds on manipulated variables
$\underline{x}_*, \underline{x}^*$ = lower and upper bounds on state variables.

The optimizer must choose the manipulated variable profile $\underline{u}(t)$ to minimize the performance index $F(\underline{x}(t), \underline{u}(t))$ so that the constraint Eqs. 1 and 2 are obeyed and the manipulated variables and state variables do not move beyond the bounds 4 and 5.

Biegler (1990) divides the solution methods for optimal control problems into three basic categories: iterative methods based on variational calculus; sequential nonlinear programming methods which use an embedded model; and simultaneous nonlinear programming methods. These methods are discussed below.

Variational methods involve the extension of analytical solution techniques for small design problems to iterative algorithms based on variational conditions. Variational methods include the well-known control vector iteration algorithms (Bryson and Ho, 1975) that are based on Pontryagin's maximum principle. According to Biegler (1990), variational methods require excessive model and adjoint equation evaluations and are effective only when applied to the simplest optimal control problems.

If the manipulated variable profile, $\underline{u}(t)$, is discretized or expressed as a polynomial or piecewise constant function, the optimal control problem can be solved sequentially as an NLP. This control parameterization approach is advantageous in that standard nonlinear optimization algorithms can be used to determine the parameters $\underline{p}$ required to specify $\underline{u}(t)$ (Ray, 1981). A diagram outlining this approach is shown in Figure 1. First, an initial set of parameters, $\underline{p}$, is used to construct the manipulated variable trajectories $\underline{u}(t)$. These trajectories provide input to the dynamic model which is integrated to determine the resulting trajectories of the state variables. Next, the performance index, J, is calculated from the state trajectories. The optimizer chooses a new set of parameters and the process is repeated until the optimum is reached within a specified tolerance. The number of iterations required to obtain a suitable solution can be greatly reduced if accurate sensitivity

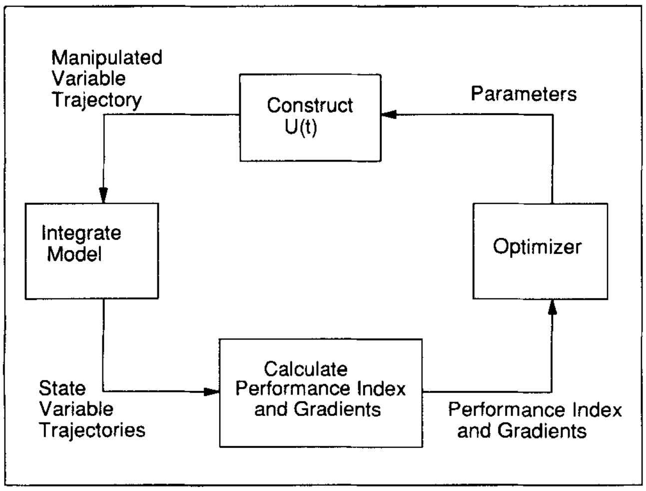

Figure 1. Embedded model approach to dynamic optimization.

information is provided to a gradient based optimizer. Sensitivities can be determined by integrating a set of adjoint equations along with the model differential equations (Leis and Kramer, 1988). The major disadvantages of embedded model techniques are that bounds on state variables as shown in Eq. 5 are difficult to handle (Beigler, 1990) and the optimal solution to the original problem is not obtained if $\underline{u}(t)$ is poorly parameterized (Ray, 1981). Recently, these problems have been studied by Goh and Teo (1988) and by Chen and Hwang (1990). Sequential approaches have been very successful in solving large-scale dynamic optimization problems (Sargent and Sullivan, 1979; Mujitaba and Macchietto, 1988).

In simultaneous nonlinear programming methods, both the manipulated variable profile and the state equations are parameterized to form an NLP problem with only algebraic equation constraints. This type of formulation makes the handling of bounds on state variables relatively simple (Li and Biegler, 1988; Eaton and Rawlings, 1990; Tjoa and Biegler, 1991). However, simultaneous approaches lead to much larger NLPs than embedded model methods and extreme care must be taken in the parameterization step to ensure that an accurate algebraic representation of the solution to the differential equations is obtained. As yet simultaneous optimization and integration approaches have been used only to solve small dynamic optimization problems, but they provide a promising research area for the future (Biegler, 1990).

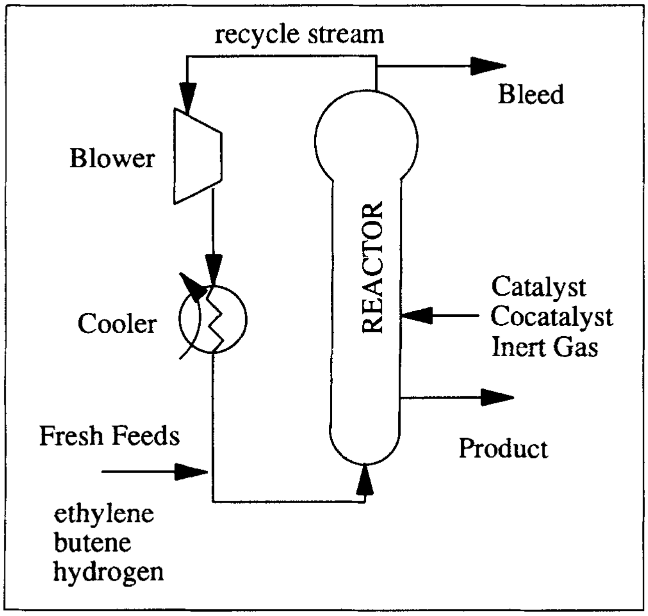

Figure 2. Gas-phase polyethylene reactor system.

Process Description

In fluidized-bed polyethylene reactors, the copolymerization of ethylene and α-olefin comonomers is carried out using a heterogeneous Ziegler-Natta or supported metal oxide catalyst (Burdett, 1988). A schematic diagram of this reactor system is shown in Figure 2. In this study, the feed to the reactor comprises ethylene, butene, hydrogen, and nitrogen. These gases provide the fluidization and heat-transfer media, and supply reactants for the growing polymer particles. The fluidized particles disengage from the reactant gas in the expanded top section of the reactor. The unreacted gases are combined with fresh feed streams and recycled to the base of the reactor. Since the reaction is highly exothermic, heat must be removed from the recycle gas before it is returned to the reactor. The conversion per pass through the bed is very low, making the recycle stream much larger than the fresh feed streams. Because polymer particles in the fluidized bed are mixed well and the conversion per pass is low, gas composition and temperature are essentially uniform throughout the bed. To regulate the quantity of polymer in the bed, the product discharge valve near the base of the reactor opens periodically and the fluidized product flows into a surge tank. The unreacted gas is recovered from the product which proceeds downstream for further processing and distribution. A small gas bleed stream is removed from the system to prevent the accumulation of inerts and impurities in the gas phase.

Polymerization reactions involving transition metal catalysts occur very quickly compared with the time scale of the gas-phase and solid-phase reactor dynamics. Under the assumption of uniform gas composition and temperature, all of the polymer made during a short time interval at a specific type of catalyst site is similar in structure because it is produced under the same reaction conditions. The composition and molecular weight distributions of the polymer produced during this short time period are referred to as instantaneous properties, whereas the molecular weight and composition distributions of the total polymer in the fluidized bed are cumulative properties. The instantaneous melt index and density, MI_i and ρ_i, are influenced by the reactor temperature and the composition of the gas phase. The rate at which the cumulative polymer properties, MI_c and ρ_c, change in response to a change in the instantaneous polymer being produced depends on the residence time of the solid-phase.

The Optimal Grade Transition Problem

When formulating an optimal grade transition problem, one must understand which features distinguish a good grade transition from a bad one, and also know the relative importance

Table 2. Scaled Manipulated Variables and Their Bounds

Manipulated Variable	Scaled Lower Bound	Scaled Upper Bound
Butene feed rate	0	1
Hydrogen feed rate	0	1
Reactor temperature setpoint	−7	8
Reactor vent valve position	0	1
Catalyst feed rate	0	1
Bed level setpoint	−1	1

of the competing goals embodied in the notion of an *optimal* policy. A desirable grade transition policy is one which:

a) drives the product properties to their new target values in a short period of time, producing only a small quantity of off-specification polymer.

b) ensures that the reactor operates safely during the changeover. Excursions above the sticking temperature of the polymer and disruptions of fluidization, heat transfer and mixing in the bed cannot be tolerated.

c) results in economically desirable steady-state reactor conditions at the end of the transition. Reactor temperature, bed level, polymer production rate, and gas bleed rate should all settle at pre-specified final values.

d) does not adversely affect the quality or consistency of the on-specification polymer product in the reactor at the end of the transition period.

One important question related to a) above is:

> Which is more desirable, reducing the *quantity* of off-specification material produced, or reducing the *time* required to reach the new property target?

The answer to this question depends on economic conditions. During periods of high market demand, it may be better to adopt a policy which produces more off-specification polymer, but reaches the new target faster. Conversely, in periods of low demand, a policy which produces less off-target material at the expense of a longer transition time may be preferable.

In this study, it is assumed that the desired steady-state conditions for the next grade, which are required in item c) are known, either from experience, or from the solution to a separate steady-state optimization problem. Whenever the optimal steady-state conditions change due to economic decisions, the optimal dynamic grade transition policies will also change. While items b) and c) above are straightforward, d) is not as obvious. An additional question which must be asked when formulating the optimal transition policy problem is: How much overshoot in instantaneous *MI* and ρ should be used to bring the cumulative properties to their targets quickly?

The answer to this question depends on the use to which the polymer will be put, and on the importance of consistency in the molecular weight and composition distribution in that application.

Knowing the measured values of cumulative *MI* and ρ is not sufficient to give a complete prediction of the properties of a linear polyethylene sample. *MI* and ρ are only reflections of an average molecular weight and average composition of the copolymer. The breadths of the molecular weight and composition distributions also affect polymer properties. A continuous gas phase reactor operating at steady state with a given catalyst produces polymer with a certain *MI* and ρ and a fixed molecular weight and composition distribution. However, during grade transitions, the old polymer contained in the reactor is mixed with new instantaneous polymer produced at different conditions, leading to potential broadening of both the molecular weight and composition distributions. While the *MI* and ρ of this transition material may be within the specifications of a certain commercial grade of polyethylene, the properties of the transition polymer can differ substantially from those of polyethylene with the same *MI* and ρ produced under steady-state reactor conditions. Therefore, grade transition policies which cause excessive overshoots in instantaneous *MI* and ρ should be avoided. To illustrate this point, the effect of different levels of instantaneous density overshoot on the copolymer composition distribution is investigated later in this article.

Many issues must be considered when formulating dynamic optimization problems to study grade transitions. The manipulated variables available for on-line control and their associated bounds must be known, as well as any constraints on state variables in the dynamic model. Choosing an objective function can be a difficult task; the implications of the objective function structure and tuning on reactor operability, economics and product quality should be considered.

Manipulated variables and their bounds

The variables which are manipulated in this study to obtain optimal grade transitions are shown in Table 2 along with lower and upper bounds. The butene feed rate, hydrogen feed rate, and reactor vent position affect product properties by changing the gas composition in the reactor. The catalyst feed rate and the quantity of polymer in the bed influence the production rate and the solid phase time constant, thereby affecting the rate at which cumulative *MI* and ρ change in response to changes in the instantaneous properties. The upper bounds on the gas feed and catalyst feed rates are fixed by the physical size of valves and catalyst injection equipment. The temperature setpoint must remain above the lower limit to ensure adequate catalyst activity, and below the upper limit to prevent sticking of the polymer particles. The vent position is held below its upper bound to prevent excessive bleeding of gas from the reactor. The mass of polymer in the bed must remain between the limits shown to ensure proper fluidization and mixing in the bed. The scaled bounds in Table 2 are indicative of the types of limits encountered in industrial gas phase polyethylene reactors. The actual values of the bounds encountered by specific industrial reactors depend on the grades of polymer being produced and on the physical design of the reactor.

An additional variable which could be manipulated by the optimizer is the feed rate of nitrogen to the reactor. Nitrogen addition could be used to increase the pressure in the reactor, and thereby flush other gas phase components out of the reactor in the bleed stream. This action would have much the same effect as opening the bleed valve. Since the bleed valve position is already included as a manipulated variable in the optimization study, nitrogen feed flow manipulations have not been considered.

Objective function and constraints

Integral quadratic objective functions are commonly used both in process control designs and in dynamic optimization problems. The reason for their popularity is that they are an effective and simple way of penalizing deviations from targets over the time period of interest. Perhaps the simplest objective which could be conceived for the grade transition trajectory problem is to minimize $F(\underline{u})$ where:

$$F(\underline{u}) = \int_{t_0}^{t_f} \{ w_1 (\ln MI_c - \ln MI_{sp})^2 + w_2 (\rho_c - \rho_{sp})^2 \} dt \qquad (6)$$

t_0 is the time at which the grade transition begins and t_f is a time in the future, well beyond the end of the changeover, when the reactor will have reached steady state. w_1 and w_2 are weighting factors related to the relative costs of deviations of MI_c and ρ_c from their respective target values, MI_{sp} and ρ_{sp}. Consistent with previous model development work (McAuley and MacGregor, 1991), the objective function in Eq. 6 penalizes deviations of the logarithm of MI_c from setpoint rather than raw MI_c deviations. As a result, the same percentage error in cumulative melt index is penalized equally, regardless of the level of MI_c.

Minimization of this objective function will result in a transition policy which satisfies item a) in the list of desirable features. As long as t_f is chosen to be sufficiently large, MI_c and ρ_c will be forced toward their setpoints and maintained there at steady state. By satisfying the bounds given in Table 2, item b) will also be satisfied. However, without further penalties or constraints, the solution to this simple problem will not necessarily meet criteria c) and d). Some means is required to ensure that the final steady state is an economically desirable one and that the resulting molecular weight and composition distributions at the end of the grade transition are not too broad.

Constraints or penalties on model states can be incorporated in several ways. Hard bounds can be defined for functions of the state variables, or penalty terms can be added to the objective function to ensure that no constraints are violated by the optimal solution. Since broad molecular weight and composition distributions can lead to undesirable product properties, excessive overshoots of the instantaneous MI and ρ cannot be allowed during a transition, even though they can assist in quickly bringing MI_c and ρ_c to their target values. Two alternative approaches are discussed below which could be used to force the optimizer to consider the trade-off between fast transitions and narrow distributions. They are specification of hard bounds on MI_i and ρ_i, and the use of quadratic penalty terms in these variables in the performance index.

Consider a melt index transition from an initial value MI_0 to a new, higher target value. An upper allowable limit on the instantaneous melt index, MI_i^* could be specified so that during the transition, the instantaneous MI is forced to have values less than or equal to this upper limit:

$$MI_i(t) \le MI_i^* \qquad (7)$$

Expression 7 could be included as a constraint in the optimization problem. Formulation of the problem in this way would mean that if $MI_i^* = 25$ dg/min, then a sustained instantaneous melt index of 24.9 dg/min would be acceptable in the optimal solution, but an infinite penalty would be placed on an instantaneous melt index of 25.1 dg/min, for even a short time. While this type of hard constraint makes sense for the bounded manipulated variables, it may not be the best description of the desire to trade-off fast transitions against the formation of low molecular weight tails. This type of state variable constraint is also difficult to handle using an embedded model technique, so a more complex simultaneous solution approach might be in order.

A second method of handling the trade-off between fast transitions and narrow molecular weight distributions involves the addition of a quadratic penalty function to the original performance index $F(\underline{u})$. An objective function of the form:

$$J = F(\underline{u}) + \int_{t_0}^{t_f} \{ w_3 (\ln MI_i - \ln MI_{sp})^2 + w_4 (\rho_i - \rho_{sp})^2 \} dt \qquad (8)$$

penalizes large deviations of the instantaneous MI and ρ from their targets, including deviations beyond the desired upper limit. The relative importance of the original performance index, involving the cumulative properties, and the importance of limiting the tails of the molecular weight and composition distributions, is influenced by the choice of the weighting factors, w_3 and w_4. The quadratic penalty function in Eq. 8 results in a smoothly increasing penalty on instantaneous polymer properties which deviate from the target, and is easily handled using an embedded model approach.

Depending on market conditions, the steady-state production of a given grade of polyethylene is associated with economically optimal settings for temperature, vent flow rate, bed level and catalyst feed rate. While these variables can and should be allowed to deviate from their desired values in the short run, the long-term tendency of the control system should be to drive these variables toward the desired positions. Only two degrees of freedom, the hydrogen and butene feed rates are required to achieve the desired polyethylene properties at steady state. Thus, the extra manipulated variables can be forced to settle near the desired values without causing offset in the product properties. The following simple quadratic penalty terms will make certain that T_{fsp}, the final steady-state temperature setpoint, is driven to its desired value T_{des}, and that the bleed value position, v_p, settles at the desired value, v_{pdes}:

$$w_5 (T_{fsp} - T_{des})^2 + \int_{t_0}^{t_f} w_6 (v_p - v_{pdes})^2 dt \qquad (9)$$

No integration of the first penalty term in Eq. 9 is required because both T_{fsp} and T_{des} are constants which do not change with time, whereas, the deviation of the vent position is penalized over the entire duration of the transition. Costs associated with leaving the temperature setpoint near its limits for several hours are minimal. However, it is important to ensure that the bleed valve does not unnecessarily remain near its limits for a sustained period of time. Excessive venting is expensive, and leaving the valve closed for a long period of time can result in the accumulation of poisons in the system. The weighting factors w_5 and w_6 can be used to weight the relative importance of moving toward the desired settling positions of manipulated variables against minimizing the other terms in the objective function.

If only the butene and hydrogen feed rates, the reactor temperature, and the vent position are used as manipulated variables, the effects on production rate during the grade transition are relatively minor. In this case, an objective function containing terms from expressions 6, 8 and 9 leads to all of the desired features of a good grade transition. If, however, the catalyst feed rate and the bed level are also manipulated, marked changes in production rate can occur. Thus, when the catalyst feed rate and bed level are included as manipulated variables, the objective function should be amended to account for changing production rate and its potential implications on the desirability of grade transition policies.

Production of off-specification polymer results in a cost or, alternatively, a loss of potential profit for the polyethylene producer. Polymer which does not fall between the specification limits of commercial grades must be sold at a discount, because there is little market for it. There are also costs associated with polymer which is within specification limits but which is off-target. Customers prefer the polyethylene they purchase to have consistent properties both within a shipment and between successive shipments. Inconsistent polymer can cause increased processing equipment setup costs and can ultimately lead to loss of market share for the polyethylene producer.

Taguchi (1986) suggests the use of quadratic loss functions for associating actual costs with deviations of product properties from their targets. Assuming that C, the cost associated with poor quality for a unit mass of polymer produced in the reactor, is a quadratic function of both cumulative and instantaneous properties:

$$C = a_1(\ln MI_c - \ln MI_{sp})^2 + a_2(\rho_c - \rho_{sp})^2 + a_3(\ln MI_i - \ln MI_{sp})^2 + a_4(\rho_i - \rho_{sp})^2 \qquad (10)$$

The coefficients, a_i, are weighting factors denoting the relative costs of deviations in the respective polymer properties. For an entire grade transition, then, the total cost of off-target production is:

$$\int_{t_0}^{t_f} P_R C\,dt = \int_{t_0}^{t_f} P_R\{a_1(\ln MI_c - \ln MI_{sp})^2 + a_2(\rho_c - \rho_{sp})^2 + a_3(\ln MI_i - \ln MI_{sp})^2 + a_4(\rho_i - \rho_{sp})^2\}\,dt \qquad (11)$$

where P_R is the instantaneous polymer production rate. An objective function which minimizes the cost of off-specification production, while ensuring an economically desirable final temperature setpoint, bleed position, bed level (B_w), and production rate is:

$$\int_{t_0}^{t_f} P_R C\,dt + w_5(T_{fsp} + T_{des})^2 + w_7(B_{wfsp} - B_{wdes})^2 + \int_{t_0}^{t_f}\{w_6(v_p - v_{pdes})^2 + w_8(P_R - P_{Rdes})^2\}\,dt \qquad (12)$$

At the beginning of a grade transition, when the polymer properties are far from target, the first term in the performance index dominates, and the optimizer will take action to simultaneously bring the properties closer to their setpoints and to reduce the production rate so that little off-specification polymer is produced. Near the end of the transition, when the product properties are close to their targets, the first term in the objective function will be small relative to the final term, so that the optimizer will choose the manipulated variables to achieve the desired steady state production time.

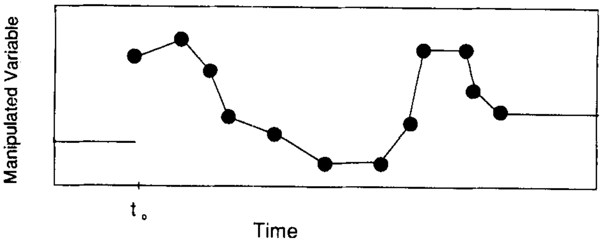

Figure 3. Parameterization of the manipulated variable trajectories.

Method of solution

Since hard constraints on state variables are not required in the problem formulation, an embedded model approach has been adopted. The manipulated variable profiles are parameterized by approximating the optimal policies as a series of ramps. Other commonly used parameterization techniques include approximation of the manipulated variable trajectories by a series of steps, or by a polynomial expression. In the current study, the ramp approximation was chosen because it can approximate many different functions with only a few decision variables. As shown in Figure 3, the decision variables chosen by the optimizer are the values of the manipulated variable trajectories at the end points of the ramps. For each manipulated variable, the trajectory is specified by 12 decision variables. Three different sets of switching times corresponding to the end-points of the ramps were chosen arbitrarily and are shown in Table 3. Since the $A \rightarrow B$ and $B \rightarrow A$ transitions require less than ten time periods to attain steady state, a final switching time of seven units from the start of the transition is appropriate. $B \rightarrow C$ and $C \rightarrow B$ transitions require approximately 15 and 18 time periods, respectively, so that larger final switching times are required. In all of the transitions, a final time, t_f, of 60 time periods is used in the objective function calculations. Some steady-state segments have been removed from graphs of the results so that more attention can be focussed on the first 20 to 30 time periods of each transition.

A commercial nonlinear programming package, MINOS 5.1 (Murtagh and Saunders, 1987) was used to solve for the optimal decision variables. A set of adjoint equations was integrated, along with the model equations and the objective function, in order to supply the optimizer with accurate gradient information.

Results

Policy I: hydrogen and butene feed rates as manipulated variables

The simplest optimal grade changeover policy is one in which only the hydrogen and butene feed rates are manipulated to accomplish the transition. Such a changeover is shown in Figure 4. Note that MI is plotted on a log scale, and that all other variables are plotted on standard linear scales. The objective

Table 3. Switching Times Used to Parameterize Manipulated Variable Trajectories

Transition	Switching Times [Scaled Time Units]											
$A \rightarrow B$, $B \rightarrow A$	0	0.33	0.67	1	1.5	2	2.5	3	4	5	6	7
$B \rightarrow C$	0	1	2	3	4	5	6	7	8	9	10	11
$C \rightarrow B$	0	1	2	3	4	6	8	10	12	14	16	18

function resulting in this set of trajectories is Eq. 8, wherein weights w_1 to w_4 are 1.0, 0.04, 0.25 and 0.01, respectively. Using these weighting factors, a deviation of 1% in *MI* and of 0.05 scaled density units are penalized equally. In addition, deviations in instantaneous properties are penalized half as much as similar cumulative property deviations. The $A \rightarrow B$ transition in Figure 4 begins at time period 5, followed by $B \rightarrow C$ at period 25, $C \rightarrow B$ at period 55 and $B \rightarrow A$ at period 85. The $A \rightarrow B$ transition involves a small downward change in *MI* from 0.2 to 0.16 scaled units, and a large density change from 9 to 13 units. This transition is accomplished by turning off the butene feed for several time periods, and then moving to the steady-state position of 0.40. Some oscillations in the hydrogen feed rate are used to bring *MI* to its new setpoint. Note that the final settling positions of the hydrogen feed rate and concentration are very near to their positions before the transition. At steady state the grade change is mainly achieved by the reduction in butene concentration which causes *MI* to decrease and ρ to increase.

Overshoots in the instantaneous *MI* and ρ are used to bring the cumulative properties quickly to their new targets. With the weighting factors w_3 and w_4 both set to zero, the size of these overshoots is much larger than in Figure 4. If deviations in MI_i and ρ_i are not penalized, the maximum value of ρ_i attained during the $A \rightarrow B$ transition is 20 scaled density units, compared with only 16 units in Figure 4. Such a large deviation of ρ_i from the set point can lead to undesirable properties of the polymer leaving the reactor between time periods 7 and 13. Even though the cumulative polymer appears to be on target, it is a mixture of instantaneous polymer with scaled ρ_i ranging from 9 to 20, and will have different physical properties from polymer produced at steady state with a scaled density of 13 units. By changing the values of w_3 and w_4, optimal trajectories can be found which give the desired trade-off between overshoots in the instantaneous properties and the time required to achieve each grade changeover.

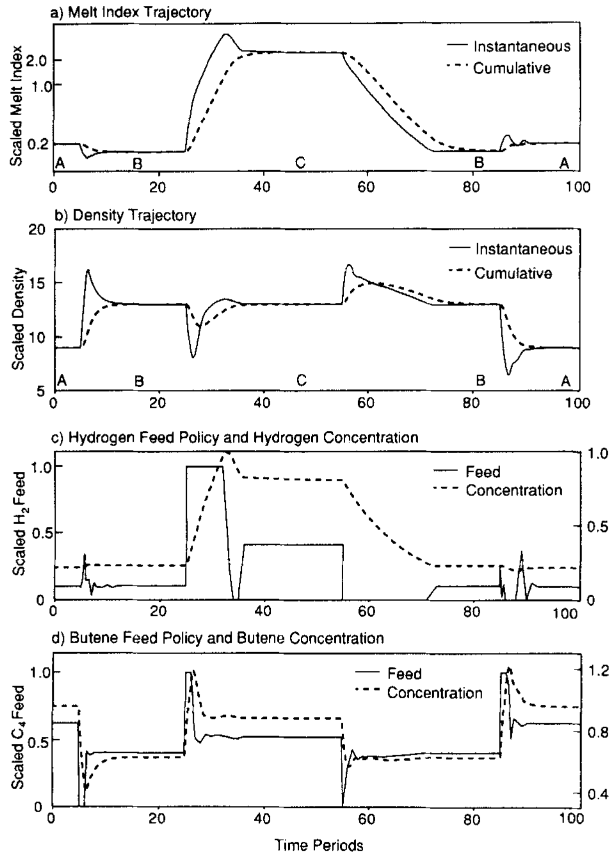

Figure 4. Optimal transition policy I.

Butene and hydrogen feed rates are manipulated variables.

The $B \rightarrow C$ transition, beginning at time period 25, involves a large change in *MI* from 0.16 to 2.4 units, and no change in the density setpoint. The optimizer accomplishes this transition by initially increasing both the hydrogen and butene feed rates to their upper bounds in order to increase *MI*. This action causes the density to deviate significantly from its setpoint. The accompanying overshoot in instantaneous *MI* results in broadening of the molecular weight distribution.

An important facet of the grade changeover problem is revealed in Figure 4. During the $B \rightarrow C$ transition, the butene concentration responds rapidly to the step in the butene feed rate, whereas the response of the hydrogen concentration to the hydrogen feed rate change is much more sluggish. In the $C \rightarrow B$ transition which begins at time period 55, the hydrogen concentration response associated with the downward step in the hydrogen feed rate is even more sluggish than the response to the upward step. This slow change in the hydrogen concentration is responsible for the slow *MI* response. The optimal trajectories and manipulated variable policies for the upward and downward steps are very different, reflecting the inherent nonlinearity of the quality control problem.

In the $B \rightarrow A$ transition, beginning at time period 85, the grade change is accomplished primarily through an increase in the butene concentration. During this transition, the scaled density decreases to seven units. Without a penalty on instantaneous density deviations, ρ_i drops even further to five units. This high level of comonomer incorporation may be unacceptable, depending on the product quality requirements of the customer.

While improving the instantaneous property trajectories, the penalties on MI_i and ρ_i deviations do result in considerably longer transition times and in the production of more cumulative polymer which deviates from the *MI* and ρ targets. A summary of the changeover times and amounts of off-target material produced for the transition policies studied is given in Table 4. To calculate the quantity of off-specification polymer produced, the following criterion was used. Prime pol-

Table 4. Comparison of Optimal Transition Policies

	Manipulated Variables		Transition Time and Quantity of Off-Spec.			
			$A \rightarrow B$	$B \rightarrow C$	$C \rightarrow B$	$B \rightarrow A$
Policy I	H,B	Time	4.1	11.8	24.1	4.1
		Mass	4.237	11.717	24.499	4.389
Policy I $w_3 = w_4 = 0$	H,B	Time	2.0	10.9	24.1	2.4
		Mass	2.043	10.845	24.492	2.594
Policy II	H,B,T,V	Time	3.6	9.5	17.5	4.1
		Mass	4.240	10.576	16.043	4.649
Policy II High H_2 Bound	H,B,T,V	Time		9.0		
		Mass		10.149		
Policy II 11 period discretization	H,B,T,V	Time			33.3	
		Mass			33	
Policy III	H,B,T,V,C,W	Time	3.6	10.0	17.1	3.7
		Mass	3.666	9.484	9.510	3.878

ymer was defined as any material with both MI_c within ±5% and ρ_c within ±0.25 scaled density units of one of the target grade specifications. All other polymer was categorized as off-prime. Similarly, the transition time is the time interval commencing when the polymer first left the specification range of the previous grade, and lasting until the cumulative properties entered, and stayed within, the specification range of the new target material. Obviously, this method of segregating good polymer from off-target material does not include any criterion for judging the breadth or shape of the molecular weight or composition distribution, and, as such, is not being promoted as a means of classifying prime and nonprime polymer to sell to customers. These results are merely tabulated as one means of comparing the grade transitions resulting from different types of problem formulations.

To illustrate this point, a series of composition distributions for the polymer produced before and after the $B \rightarrow A$ grade changeover are shown in Figures 5 and 6. In Figure 5, the steady-state composition distributions for both grades A and B are shown. These composition distributions are bimodal due to the presence of two different types of active sites on the catalyst (McAuley et al., 1990). One site produces high molecular weight polymer chains with low comonomer incorporation, and the other produces lower molecular weight polymer with a higher level of comonomer incorporation. Near the end of the changeover, at time 89.5, MI_c and ρ_c of the polymer in the reactor are within the specification limits used in Table 4. However, as shown in Figure 6, the cumulative composition distribution of the polymer is very different from that of grade A polymer produced at steady state. With $w_3 = 0.25$ and $w_4 = 0.001$, as in Figure 4, the cumulative composition distribution at time 89.5 is tetramodal instead of bimodal. Some of the old polymer produced before the start of the changeover still remains in the reactor, and has been mixed with the new instantaneous polymer produced during the changeover. If instantaneous property deviations are not penalized ($w_3 = w_4 = 0$), then a much larger overshoot in instantaneous density is optimal. For this case the cumulative composition distribution at time 89.5 is broader, and contains a large tail of copolymer with high comonomer incorporation. This high comonomer tail may lead to unacceptable product performance, even though the average composition of the copolymer is within the specification limits.

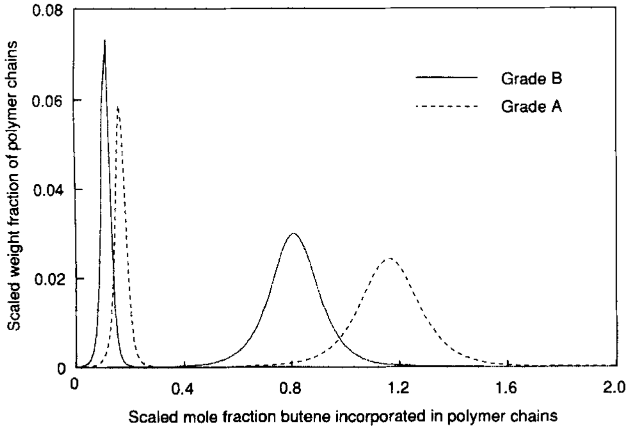

Figure 5. Steady state copolymer composition distribution for Grades A and B.

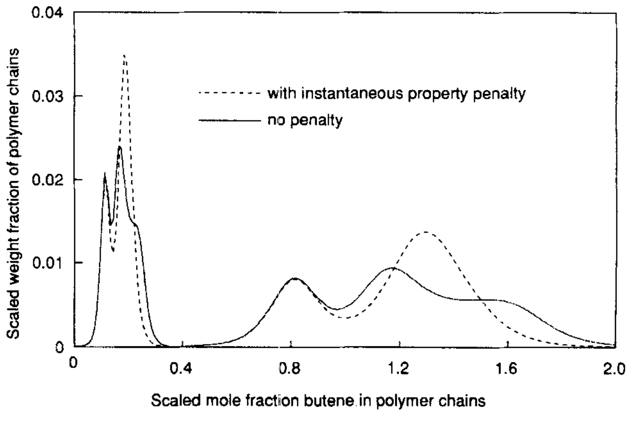

Figure 6. Cumulative composition distribution of the copolymer in the reactor at time period 89.5.

Effect of penalizing instantaneous product property deviations from target.

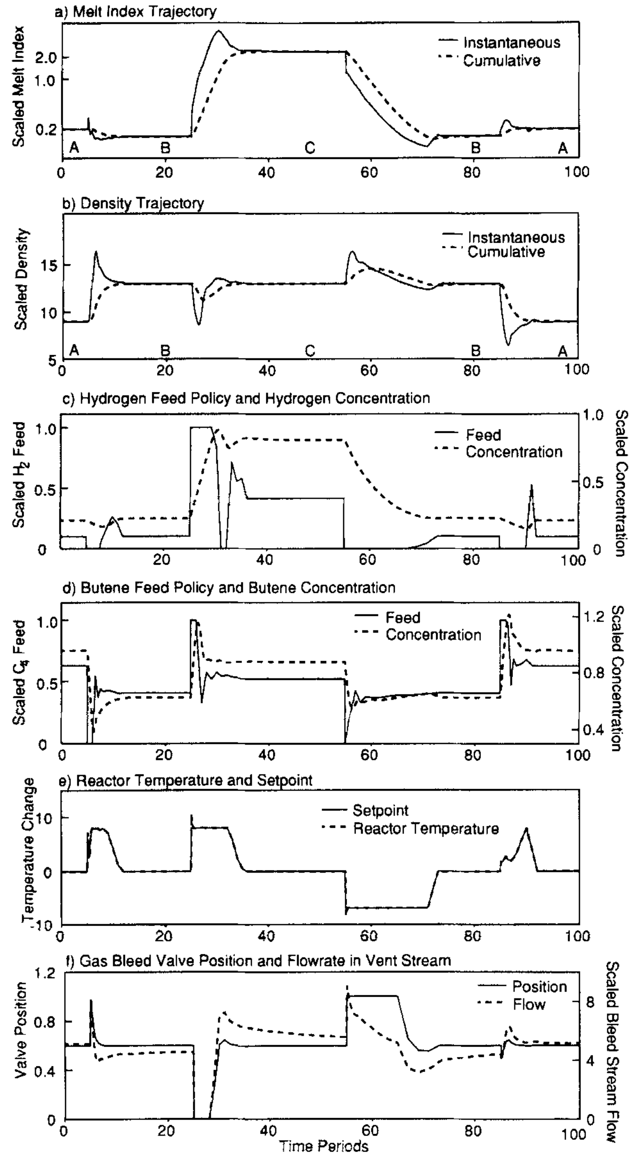

Figure 7. Optimal transition policy II.

Effect of including temperature setpoint and bleed valve position as manipulated variables.

Policy II: benefits of manipulating reactor temperature and bleed valve position

In this set of transitions, the reactor temperature setpoint and bleed valve position are included in the set of manipulated variables, along with the hydrogen and butene feed rates. Expression 9, with $w_5 = 12$ and $w_6 = 0.125$, is added to the objective function, so that the temperature and bleed valve position settle at or near their desired final values. The density trajectories in Figure 7 are very similar to those of Figure 4. The greatest benefits of manipulating the temperature and bleed valve are observed in the *MI* trajectories. As shown in Figure 7, the response of the reactor temperature to setpoint changes is very fast. One potential problem with these temperature responses is the temperature overshoot. If the $B \rightarrow C$ transition is unacceptable because the initial temperature spike might lead to particle sticking and agglomeration, then the bound on the first temperature setpoint decision variable should be reduced by several degrees and the optimization repeated. The fast changes in temperature result in equally fast changes in MI_i, making temperature a desirable manipulated variable for *MI* control during grade transitions.

A peculiar result shown in Figure 7 is that both the $A \rightarrow B$ and $B \rightarrow A$ transitions make use of an increase in the reactor temperature above the initial value. One explanation of why this action is optimal is that a higher temperature leads to a higher production rate and a smaller solid phase residence time. This smaller residence time allows for a faster changeover of cumulative properties in the reactor.

During the $B \rightarrow C$ transition, the optimizer closes the vent for 3 time periods in order to increase the rate of hydrogen accumulation in the reactor. As a result, the hydrogen concentration in Figure 7 climbs more quickly than in Figure 4. Hence, MI_i rises more quickly and reaches a slightly higher maximum value. The grade transition wherein venting is most beneficial is $C \rightarrow B$. The optimizer holds the vent position at its upper limit for ten time periods during the changeover. Opening the vent allows hydrogen in the reactor to escape, causing the hydrogen concentration to fall more quickly than in Policy I. As a result, the duration of the grade transition is reduced to 17.5 time periods. Although the polymer produced between time periods 73 and 78 is prime according to the definition used in Table 4, it may have slightly different physical properties than polymer produced after time period 80.

Use of bleed stream manipulations has very little benefit for transitions $A \rightarrow B$ and $B \rightarrow A$. Perhaps both venting and temperature setpoint changes should be reserved for grade transitions involving a large change in *MI*.

Sensitivity of the $B \rightarrow C$ transition to the maximum hydrogen feed rate

One of the bounds imposed on the optimization problem, which could be changed by a design change in the plant, is the upper bound on the hydrogen feed rate. A larger valve would allow more hydrogen to flow into the reactor in a shorter period of time. To assess the potential benefit of such a change, Policy II was rerun with the upper hydrogen feed rate bound increased by 11.1%. The optimal policy is similar to that in Figure 7, except that the hydrogen concentration and MI_i climb faster, resulting in a faster transition, less off-target material, and a higher overshoot in MI_i. The resulting savings in off-spec production and in transition time are shown in Table 4.

Effect of manipulated variable discretization

Since the manipulated variable profiles have been parameterized as shown in Figure 3, the grade transitions determined in this study are actually slightly suboptimal. The true optimal manipulated variable trajectories which would minimize the objective function are curves rather than a series of ramps. The reason that the ramp approximation was adopted is that the resulting optimization problem is much easier to solve than that involving determination of the true optimal curves for the manipulated variables. While approximation of the true optimal solution could be improved by finer discretization of the manipulated variable policies, addition of more decision variables makes solution of the optimization problem more time consuming. Each additional decision variable increases the number of degrees of freedom considered by the optimizer, but the main reason for the increase in solution time is that more adjoint equations must be added to the model integration stage so that the required gradient information can be provided to the optimizer. Since a set of 11 ramps joining 12 points is capable of approximating a great many curves, no more decision variables were added to the optimization problem.

A more important factor that can lead to significant suboptimality is the position of the decision variables in time. Optimal $B \rightarrow C$ and $C \rightarrow B$ transitions require approximately 10 and 20 time periods, respectively, for the reactor to reach a new steady state, whereas $B \rightarrow A$ and $A \rightarrow B$ transitions can be completed in less than 5 time periods. Therefore, different spacing of the switching variables in time is appropriate for each type of transition. The three sets of switching times shown in Table 3 were determined using an exploratory study of the sensitivity of the transition trajectories to switching times. Three general conclusions were obtained from the study. Firstly, fast changes in the manipulated variables tend to occur early in the transitions, so it is important that relatively frequent switching of the manipulated variables is allowed early in the changeovers. Secondly, placing extra switching points beyond the time when the reactor has already reached a new steady state has no effect on the trajectories obtained. Thirdly, the time corresponding to the final switching interval must be sufficiently large, compared with the time for the optimal trajectory to reach its new target. Otherwise, the resulting grade transition will take significantly longer and produce more off-specification material than the true optimal trajectory. To illustrate this phenomenon, the discretization policy normally used for the $B \rightarrow C$ transitions was used to optimize a longer $C \rightarrow B$ transition. Since the final switching time was now only 11 time periods beyond the start of the transition, the optimizer was unable to hold the hydrogen feed rate, the vent position and the temperature setpoint at their bounds for as long as required to give a good transition. As shown in Table 4, the total transition time was greatly extended from 17.5 to 33.3 time periods, and the quantity of off-specification polymer produced more than doubled. The reason for this increase in transition time is that, after period 11, the hydrogen feed rate was forced to its steady-state value, and the rate at which the melt index approached its target was determined by the slow dynamics of the falling hydrogen concentration. Moving the final switching points further ahead in time permits the optimizer to keep the hydrogen feed rate low longer, thereby achieving a transition policy closer to the true optimum.

Policy III: benefits of manipulating catalyst feed and bed level

In the transition policies discussed so far, no attempt is made to improve the grade changeovers by manipulating either the catalyst feed rate or the bed level setpoint. As a result, the production rate remains relatively constant, varying by only ±15% throughout the grade changeovers. In this section, the catalyst feed rate and the bed level are manipulated so that less off-specification polymer is produced early in the transitions, when the instantaneous product properties are far from their targets. Since the production rate can fluctuate wildly during such changeovers, the objective function in expression 12 has been adopted. Since the scaled production rate in Policies I and II always remained near unity, the values of a_1 to a_4 in expression 12 have been set equal to w_1 to w_4 in earlier objective functions. This choice of weighting factors results in the same trade-offs between MI and ρ and between cumulative and instantaneous properties as in the earlier optimization studies. In addition, the values of w_5 and w_6 are kept at 12 and 0.125, respectively, to ensure consistency with previous policies. w_7 and w_8, the penalty coefficients for the final bed level and for production rate deviations, have been set at 33.75 and 2.0, respectively. The optimal policies which result from this objective function are shown in Figure 8. The corresponding transition times and quantities of off-specification material are given in Table 4.

For the $A \rightarrow B$ transition, incorporating catalyst feed and bed level manipulations resulted in a similar transition time compared to that of Policy II, but in a 13.5% reduction in the quantity of off-specification product. The reduction in nonprime polymer results from a drop in the bed level and the initial catalyst feed rate, which causes a reduction in the production rate at the start of the transition. Also, dropping the reactor bed level allows more of the polymer initially in the bed to be classified within the product A grade specification, rather than having it remain in the reactor to be mixed with new instantaneous polymer. While the optimal trajectories for ρ_i and ρ_c are very similar to those in Figure 7, the melt index trajectories are very different. The instantaneous MI does not experience an initial upward spike as in Figure 7. The new optimal temperature profile, which involves a decrease in the temperature setpoint, rather than an increase, is responsible for this downward fluctuation in MI_i. The hydrogen feed profile is also very different from Policy II. The optimizer uses an increase, rather than a decrease, in hydrogen concentration during the transition in order to accomplish the changeover. As before, the steady-state hydrogen concentrations before and after the transition are nearly identical. Note that the production rate, bed level, and bleed valve position all settle at their final values. If one could tolerate a slightly longer transition time in exchange for the production of less off-specification material, then a slightly lower value of w_8, the coefficient of the production rate deviation term in the objective function, could be adopted. A smaller penalty on production rate deviations from setpoint would result in a lower catalyst feed rate and a lower production rate of off-specification material during the initial stages of the transition, when the butene concentration is too high.

Compared with Policy II, the $B \rightarrow C$ transition shown in Figure 8 results in a 10.3% reduction in the quantity of off-specification material produced, but in a 10% increase in transition time. The reason for the smaller amount of off-target polymer is that much of the Grade B polymer initially in the bed is dumped out at the start of the transition, rather than remaining inside to be blended with new instantaneous polymer. In addition, the production rate falls to about 70% of its steady-state level so that less polymer is produced when the instantaneous properties are far from the new target. The reason for the longer transition time is that the solid phase residence time in the reactor between periods 32 and 38 is larger than in Policy II because the bed level is climbing.

The $C \rightarrow B$ transition requires 17.1 time periods, which is

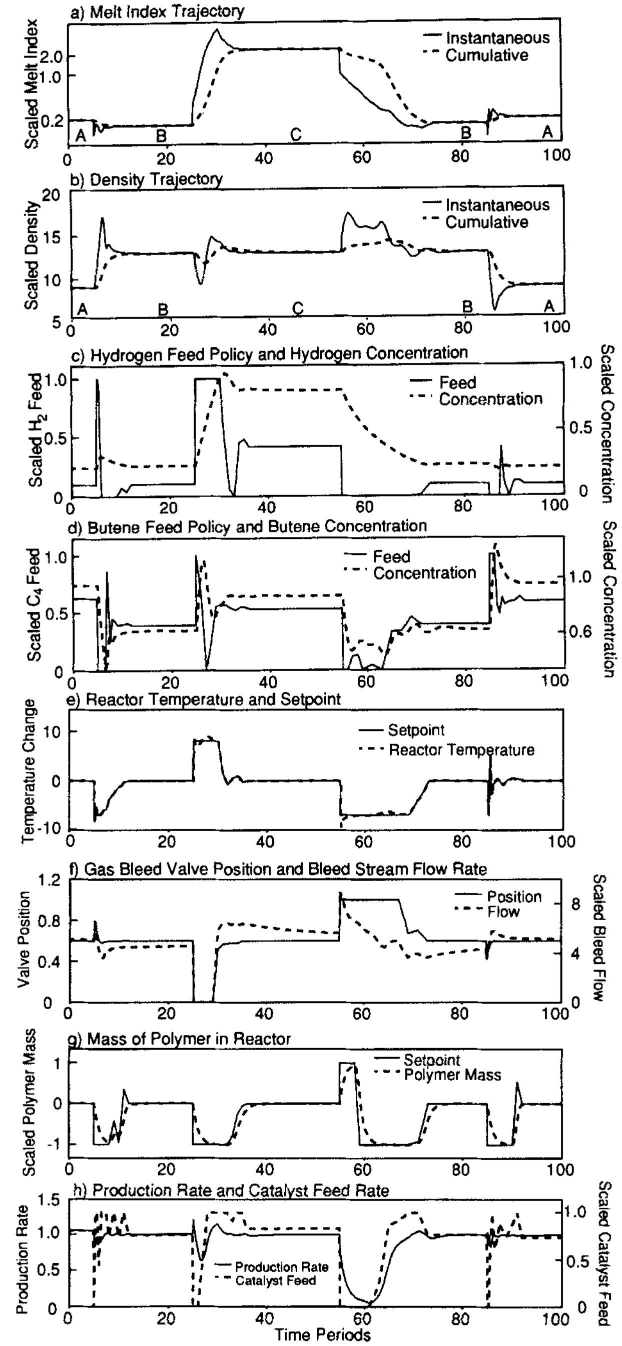

Figure 8. Optimal transition policy III.

Effect of including catalyst feed rate and bed level setpoint as manipulated variables.

marginally less time than in Policy II. However, the quantity of off-target material is reduced by over 40%. By shutting off the catalyst feed, the optimizer is able to almost stop the production of off-specification material while waiting for sufficient hydrogen to be vented from the reactor. During this transition, the optimal bed level policy in Figure 8 is somewhat unexpected. Instead of decreasing the bed level setpoint to its lower limit, the optimizer increases the bed level. This results in a very large solid phase residence time between periods 55 and 60 and in a very slow change in both ρ_c and MI_c. By keeping the bed level high and the production rate low, the optimizer is able to use a low butene concentration to reduce MI_i quickly, without producing a large deviation in the cumulative density. After several hours, some of this material is dumped from the reactor and new instantaneous polymer with properties nearer to the targets is used to refill the bed to the desired level. The $C \rightarrow B$ changeover policy in Figure 8 gives only a slight reduction in the objective function (<2%) compared with the more intuitive approach wherein the bed level is initially set to its lowest value. The type of policy determined by the optimizer is very sensitive to the relative values of a_1, a_2, a_3 and a_4 in the objective function. A smaller penalty on ρ_c, or a larger penalty on MI_c, can result in an optimal initial bed level setpoint at the lower, rather than the upper, bound. In either case, the reduction in production rate, while MI_i is moving toward the new target, is an effective means of reducing the quantity of off-specification polymer.

Manipulation of the catalyst feed and bed level for the $B \rightarrow A$ transition results in a significant reduction in both transition time and off-specification product. Since much of the old polymer in the reactor is dumped out early in the transition, less instantaneous polymer with properties at or beyond the new target values is required to bring the cumulative properties within the specification limits.

Implementation of optimal policies without feedback

When implementing an optimal grade transition policy online, it is essential to account for mismatch between the predictions of the model used in the optimization study and the true behavior of the plant. Otherwise, steady-state offset can occur between the desired MI and ρ, and the actual product properties achieved. Even if the model used to determine the optimal transition is an exact description of plant behavior at the time when the optimal policies are determined, small disturbances in catalyst properties and in impurity levels in the reactor can lead to mismatch during future changeovers.

The potential effects of model mismatch are illustrated in Figure 9, which shows the simulated open-loop implementation of optimal policy II for the $C \rightarrow B$ transition. At the beginning of the transition there is no mismatch, however, at time period 67, a new batch of catalyst is introduced into the catalyst feed stream. This catalyst batch has the same distribution of catalyst sites as the previous batch, but has 10% fewer active sites per unit mass of catalyst. As a result, the production rate begins to fall at period 67, and remains lower than that achieved with the nominal catalyst. The reduction in catalyst sites in the reactor leads to a lower butene consumption rate, and to an increase in the butene concentration in the reactor, compared to the nominal transition. The higher than optimal butene concentration results in a final scaled MI and ρ of 0.1716 and 12.455, respectively. Therefore, implementation of the optimal nominal policy without accounting for the catalyst site concentration mismatch results, not only in a suboptimal grade transition trajectory, but also in the production of off-specification polymer during the steady-state period following the transition. Feedback control actions during the grade changeover could prevent deviations from the nominal optimal product property trajectory, and, thereby, prevent the production of off-specification polyethylene. Appropriate feedback con-

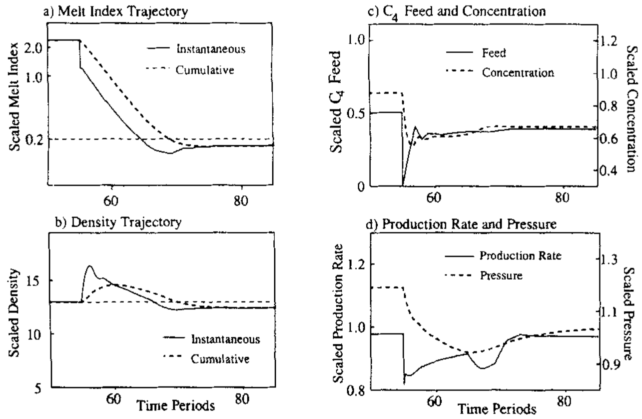

Figure 9. Implementation of the policy II $C \rightarrow B$ with step change in catalyst quality at time period 67.

trol strategies for on-line implementation of the optimal policies developed in this article are described by McAuley (1992).

Conclusions

A set of optimal grade transition trajectories has been determined for a series of grade changes between three commercially relevant polyethylene grades. It was concluded that:

1. An embedded model approach to dynamic optimization, using commercially available optimization software, provides a simple and effective method for solving dynamic optimization problems.
2. Use of an embedded model approach requires parameterization of the manipulated variable trajectories. If the parameterization chosen does not allow enough variation in the manipulated variable policy throughout the time interval when the transition occurs, then the solution to the parameterized problem may be very different from the solution to the true unparameterized optimization problem.
3. Quadratic penalty terms can be included in the objective function to prevent large undesirable overshoots in instantaneous *MI* and ρ, and to ensure that the reactor temperature, bed level, bleed rate and production rate settle at economically desirable levels.
4. Reactor temperature and gas vent rate are important manipulated variables for transitions which involve large changes in the *MI* target. Less benefit is realized during transitions dominated by a density change.
5. Large transitions in *MI* are hampered by the slow hydrogen dynamics in the gas phase. As a result, an 11% increase in the maximum allowable hydrogen feed rate leads to a significant reduction in the transition time required for a transition to lower melt index.
6. When the instantaneous polymer being produced is far from the target, decreasing the catalyst feed rate and the bed level in the reactor can be used to reduce the production rate of off-specification material during the initial stages of a grade transition.
7. The type of optimal manipulated variable profile determined can be very sensitive to small changes in the structure of the objective function and to the relative sizes of the weighting parameters, especially when many variables are manipulated to achieve the optimal trajectory.
8. Implementation of nominal optimal manipulated variable policies, without accounting for disturbances or model mismatch, can lead to product property trajectories which differ significantly from the associated nominal optimal property trajectories. Feedback control during grade changeovers is required to ensure that large quantities of off-specification material are not produced.

Acknowledgment

The authors thank A. N. Hrymak for his valuable suggestions, and the Natural Science and Engineering Research Council of Canada for financial support.

Notation

a_i = cost coefficient for deviation of property i from target
B_w = mass of polymer in the fluidized bed
$\underline{c}$ = vector of algebraic inequality constraints
C = cost per unit mass of polymer due to deviations from property targets
C_4 = butene
$\underline{f}$ = vector of functions describing state time derivatives
F = value of objective function
H_2 = hydrogen
J = objective function
MI, ρ = melt index and density
P_R = production rate
t = time
T = reactor temperature
$\underline{u}$ = trajectories of manipulated variables
$u_*, \underline{u}^*$ = lower and upper bounds on manipulated variables
v_p = valve position
w_i = objective function weighting factors
$\underline{x}$ = state variables in the dynamic model
$\underline{\dot{x}}$ = time derivatives of state variables
$\underline{x}_*, \underline{x}^*$ = lower and upper bounds on state variables

Subscripts

c = cumulative property
des = desired value
f = final value
i = instantaneous property
sp = setpoint
0 = initial value

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Manuscript received Feb. 11, 1992, and revision received May 5, 1992.