Simultaneous Design, Scheduling, and Optimal Control of a Methyl-Methacrylate Continuous Polymerization Reactor

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This work presents a mixed-integer dynamic optimization (MIDO) formulation for the simultaneous process design, cyclic scheduling, and optimal control of a methyl methacrylate (MMA) continuous stirred-tank reactor (CSTR). This article makes two specific contributions. The first consists of incorporating process dynamics into grade transitions to determine changeover times and profiles, as opposed to using fixed changeover times as in previous works dealing with design, scheduling, and dynamic optimization. A second contribution is that the steady states that describe each polymer grade are left as functions of decision variables, which has not been done in the integration of design, scheduling, and dynamic optimization. Also, this work incorporates uncertainty in product demands. The corresponding mathematical formulation includes the differential equations that describe the dynamic behavior of the system, resulting in a MIDO problem. The differential equations were discretized using the simultaneous approach, based on ortogonal collocation on finite elements, rendering a mixed integer non-linear programming (MINLP) problem, where a profit function is to be maximized. The objective function includes product sales, some capital and operational costs, inventory costs, and transition costs. The optimal solution to this problem involves design decisions: flow rates, feeding temperatures and concentrations, equipment sizing, variables values at steady state; scheduling decisions: grade productions sequence, cycle duration, production quantities, inventory levels; and optimal control results: transition profiles, durations, and transition costs. The problem was formulated and solved in two ways: as a deterministic model and as a two-stage stochastic programming problem with hourly product demands as uncertain parameters described by discrete distributions. *AIChE J,* 54: 3160–3170, 2008
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Introduction

Design, scheduling, and control of a chemical process are complex problems which are usually approached independently. Typically, the design phase is carried out first, and

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scheduling and control problems are solved once the process design has been solved. In the first step, the design is carried out with certain goals regarding capacity, profitability, environmental and safety concerns, etc., whereas in a later step scheduling and control problems are solved during process operation, usually with the objective of minimizing costs or maximizing profit. This approach results in the loss of certain degrees of freedom due to the sequential solution of the three problems, which in turn might render suboptimal results for the overall process synthesis.[1] For this reason, the simultaneous solutions of design and control,[2–4] scheduling and design,[5,6] and scheduling and control problems,[7–14] have been the subject of some works. However, there is very little work[15,16] on the simultaneous solution of the three problems.

Determination of the optimal equipment dimensions and steady state operating conditions as part of an independent design phase has the risk of resulting in poor operability conditions, and inadequate process control, due to the decreased degrees of freedom. In previous works[3,4] the problem of simultaneously determining some process design variables, steady states and control structures has been addressed, and its solution has been put into practice in processes involving grade transitions in polymerization reactors. Another recent work by Asteasuain et al.[2] is relevant for the present work, because it deals with the simultaneous process and control system design of a multigrade continuous polymerization reactor. The design problem concerns the determination of process equipment, control structures, and tuning parameters, as well as the choice of reaction initiator. An important difference from the present work is that Asteasuain et al. did not consider scheduling decisions at all, whereas in this article a cyclic scheduling model is explicitly incorporated in the formulation. From the perspective of the present work, it should be remarked that the steady states that correspond to the different grade producing operations are also determined as part of the design problem. Simultaneously, optimal transition trajectories between those steady states are also evaluated as part of the control problem.

Simultaneous design and scheduling is also a common problem in the process systems engineering literature. A detailed review involving scheduling and design of batch processes is available elsewhere.[5] Optimizing highly nonlinear and nonconvex processes poses many challenges, especially because many local optimal solutions can be present. Heo et al.[6] address this problem using an evolutionary design method that performs a search near the optimal solution found by adding equipment units to the resulting configuration. However, the rigorous global solution to the design and scheduling problem in nonlinear, nonconvex problems remains a major challenge.

The robustness and flexibility of a process design is of major concern to process engineers. One common approach in practice is to over-design so as to guarantee feasibility of operating conditions for many possible scenarios. Obviously this approach has the disadvantage of producing suboptimal solutions for the expected range of values of the uncertain process conditions. Two main approaches have been used for the solution of process design under uncertainty[17]: the so-called deterministic and stochastic approaches. The first one involves the discretization of the uncertain parameters, and the solution of a multiperiod problem, where each uncertain realization scenario corresponds to a different period. The problem of optimal design under uncertainty is studied elsewhere,[5] and a solution based on the multiperiod technique is proposed. In the stochastic approach the optimization of an expected value function based on distribution functions of the uncertain parameters is undertaken using two or multi-stages stochastic programming formulations.[18,19] In the family of stochastic formulations another approach is the so-called probabilistic or chance constraint framework,[20–22] that has not received full consideration from the process system engineering community. In this latter approach, rather than considering the optimization of an expected value function, the idea is to compute optimal conditions under which a given constraint has the maximum probability to be met. Presently, there are no works comparing the advantages and weakness of each approach when dealing with uncertainty. Using a two-stage stochastic programming approach for dealing with discrete uncertainty, we address in the present work the simultaneous design, scheduling, and control of polymerization reactors under uncertainty. Because the formulation presented in this article is nonconvex, one can only guarantee feasibility for the scenarios generated by the set of values for the uncertain parameter, namely, the product demands. The ideas of robust optimization and its extensions, as presented by Ben-Tal et al.,[23] represent an option to handle ranges for uncertain parameters, instead of only discrete points, however, they usually rely on the assumption of convexity. Also, the numerical solution of the problem presented in this paper is already very computationally demanding, therefore we consider the use robust optimization techniques, as the ones just cited, to be a future step. For these reasons we will say that the uncertainty approach given in this papers results in a locally optimal solution for some specific, although very different, values of product demands as opposed to saying it is the global optimal solution for all uncertain demand realizations within a certain range.

The topic of simultaneous scheduling and control (or dynamic optimization) is the subject of recent works: Flores-Tlacuahuac and Grossmann,[9] Nystrom et al.,[10,11] Prata et al.,[12] and Terrazas-Moreno et al.[7] A comprehensive literature review on the subject literature can be found in a recent paper by our research group.[7] The basis of all solution methods is the discretization of the differential equations that describe dynamic behavior, and the addition of the resulting non-linear algebraic equations into a scheduling formulation resulting in MINLP problems.

The simultaneous solution of design, scheduling, and optimal control has been studied very little. The present work has the objective of simultaneously determining the optimal solution of these problems for a continuous polymerization reactor, operating under a cyclic schedule assumption, and for which the simultaneous dynamic optimization (SDO) technique is used.[24] Uncertainty in grade demand is handled in one of the two case studies presented using a two-stage stochastic programming formulation. Two similar works are those presented by Bhatia and Biegler,[15,16] in which the dynamic optimization for batch design and scheduling is solved. However, there are important differences between the present work and the two works by Bhatia and Biegler. In this work we consider the dynamic optimization of grade transitions, which means that the changeover times and costs in the scheduling formulation are functions of decision variables. Bhatia and Biegler use the aggregated scheduling formulation of Birewar and Grossmann[25] in which changeover times are not dynamically modeled. Another difference is that as this work involves a continuous reactor, and not a batch reactor, the steady states that determine operating conditions for each polymer grade, as well as the initial and final points for grade transitions, are decision variables.

This article is organized as follows. In a first part, the problem is defined, detailing all assumptions, and the optimization formulation is developed. This formulation is based on previous work by our research group.[7] In a second part two case studies are presented: the first one assumes deterministic values for all parameters, whereas the second includes different scenarios depending on the realization of grade demand uncertainty from a set of possible discrete values. Finally, conclusions and future research directions are presented.

Problem Definition

A given number of polymer grades, specified in terms of molecular weight distributions are to be manufactured using an industrial reaction system. The present work is concerned with simultaneously determining the design for the reaction process, the cyclic manufacturing operation, and the control profile during grade transitions that feature optimality conditions. Because no process design is known a priori, the process steady states corresponding to different grade production conditions must be determined as part of the solution. The problem is solved using a mixed integer dynamic optimization (MIDO) approach in which the economic profit is to be maximized. The objective function includes the following terms: sales, inventory costs, transition costs, capital costs, and steady state operation costs. The design parameters are the reactor and jacket volumes, the feed and cooling water flow rates and their respective temperatures, as well as the monomer and initiator feed stream concentrations. The steady states describing each polymer grade are also determined as part of the design. On the other hand, the schedule is described by the sequencing of grades, the production mix, the duration of the production periods, and the overall cycle duration. Finally, the control decisions involve the optimal grade transitions and their duration, during which the initiator flow rate is the manipulated variable.

The formulation includes certain assumptions that are worth mentioning: (a) inventory, raw material, equipment, and utilities costs are deterministic parameters; (b) no model mismatch or process perturbations are considered; (c) polymer production is bounded between the minimum amount to satisfy grade demand, and an upper bound on this quantity, since in almost all cases it is possible to sell a certain amount of overproduction, especially when dealing with polymer products with high demand; (d) all grades are produced only once during the production cycle; (e) once a grade has been produced it is stored and depleted until the end of the cycle; and (f) once a production wheel is finished it is immediately and indefinitely repeated; grade inventories allow the constant consumption of a product until it is produced again, so that no product shortages occur. Note also that the mathematical model, as presented, assumes that the set of differential equations that describes the dynamic behavior of the system, accurately models the process over all the range of conditions used. We think that this is a reasonable assumption under many circumstances. For instance, the model presented in the case study has been previously used under similar conditions, and it will be assumed to correctly approximate the polymerization process under the relevant conditions.

Although the problem formulation involves many significant simplifications, the need for a robust process design able to deal with uncertainty in some parameters is not overlooked. In this work uncertainty in scheduling parameters, namely product demands, is handled through a two-stage stochastic multiperiod formulation.

Design, Scheduling and Control MIDO Formulation

The problem is solved using a MIDO formulation based on the simultaneous scheduling and control (SSC) formulation proposed by our research group.[7] As in previous works,[7–9] the manufacturing operation is carried out in production cycles. The cycle time is divided into a series of slots. Within each slot two operations are carried out: (a) the production period during which a given product is manufactured around steady-state conditions, and (b) the transition period during which dynamic transitions between two products take place. The description of the formulation proposed in this work is divided according to the characteristics of its different sections (objective function, design, scheduling, and optimal control). The notation is listed in detail in the end of article.

Objective function

$$\max\Bigg\{\sum_{i=1}^{N_\mathrm{p}}\frac{C_i^\mathrm{p}W_i}{T_\mathrm{c}}-\alpha\frac{V^\beta}{at}-F\rho C_\mathrm{p}(T_\mathrm{in}-T_\mathrm{amb})C^{st}-F_\mathrm{cw}\rho_\mathrm{w}\Big(C^\mathrm{cw}+\frac{C_{\mathrm{p_{cw}}}(T_j^*-T_\mathrm{w})}{\lambda_{hv}}P_\mathrm{ew}C^\mathrm{mw}\Big)-\sum_{i=1}^{N_\mathrm{p}}\frac{C_i^\mathrm{s}(G_i-W_i/T_\mathrm{c})\Theta_i}{2}-\sum_{k=1}^{N_\mathrm{s}}\theta_k^tF_\mathrm{mon}C_\mathrm{min}MW_\mathrm{mon}\frac{C^r}{T_\mathrm{c}}-\left[\sum_{k=1}^{N_\mathrm{s}}\sum_{f=1}^{N_\mathrm{fe}}h_{fk}\theta_k^tC_{I\mathrm{in}}MW_{\mathrm{in}i}\sum_{c=1}^{N_\mathrm{cp}}F_{fck}^I\gamma_c\right]\frac{C^\mathrm{I}}{T_\mathrm{c}}\Bigg\} \quad (1)$$

The total process profit is given by the income of the manufactured products minus the sum of some capital costs, operation costs, inventory costs, and the product transition costs. All terms are calculated on an hourly basis or divided by the cyclic time (T_c) so that the objective function value corresponds to the cyclic hourly profit. The first term represents the amounts sold of each grade (W_i), times their respective prices (C_i^p) divided by cycle duration (T_c). The second, third, and fourth terms in the objective function represent the capital an operating costs related to design decisions. The second term corresponds to reactor costs, considering a four-year amortization,[2] where αV^β is a correlation of the equipment costs between 13 and 1315 gallons.[26] The denominator *at* provides the hourly cost corresponding to the above-mentioned amortization time. The third term is related to the costs of heating the feed stream from room temperature T_{amb} up to the desired feeding temperature T_{in}, where F is the feed stream flow rate, ρ is the feed stream density, and C_{p} is its specific heat. The fourth term quantifies the costs related to cooling water. $F_{\text{cw}}\rho_{\text{w}}C^{\text{cw}}$ is the cost of supplying cooling water to the reactor. $\frac{Cp_{\text{cw}}(T_j^*-T_{\text{w}})}{\lambda_{\text{hv}}}P_{\text{ew}}C^{\text{mw}}$ represents the cost of the cooling water lost during cooling tower operation, where $C_{\text{p}_{\text{cw}}}$ is the specific heat of water, T_j^* is an expected average temperature of the jacket, T_{w} is the room temperature of water, λ_{hv} is the latent heat of vaporization, P_{ew} is an average fractional loss of water due to vaporization and finally, C^{mw} is the unit cost of cooling water.

The remaining terms correspond to inventory and transition costs, as explained in detail in a previous work.[7]

1. Design formulation.

a) Bounds on design variables

b) The CSTR and process variables were bounded around the nominal values reported by Silva-Beard et al.[27]

c) Steady States

$$0 = f^n(x_{\text{ss}}^1, \ldots, x_{\text{ss}}^n, u_{\text{ss}}^1, \ldots u_{\text{ss}}^m, \mathbf{p}), \quad \forall n \tag{2}$$

Equation 2 represents the dynamic model equations set to zero, denoting a steady state. Variables x_{ss}^n and u_{ss}^n represent the values of the system states and manipulated variables at steady state, whereas **p** stands for the design parameters.

The variables selected as design variables strongly influence both capital and operating costs. In our formulation we assume that capital costs are mainly related to reactor volumes. On the other hand, operating costs are mainly driven by cost of raw materials (flow rate and temperature of monomer and initiator) and auxiliary services (cooling water flow rate and temperature).

2. Scheduling formulation.

The scheduling formulation has been described in detail in previous works,[7,9] except for Eq. 4b. This equation establishes an upper bound on production (U^{p}, chosen as one and half times the minimum demanded quantity). It is assumed that some considerable (but not unlimited) amount of product can be sold, over the minimum demand to be satisfied.

a) Product assignment

$$\sum_{k=1}^{N_s} y_{ik} = 1, \quad \forall i \tag{3a}$$

$$\sum_{i=1}^{N_p} y_{ik} = 1, \quad \forall k \tag{3b}$$

where y_{ik} is a binary variable to denote whether product i is produced at slot k

b) Amounts manufactured

$$W_i \geq D_i T_{\text{c}}, \quad \forall i \tag{4a}$$

$$W_i \leq U^p D_i T_{\text{c}}, \quad \forall i \tag{4b}$$

$$W_i = G_i \Theta_i, \quad \forall i \tag{4c}$$

$$G_i = F_i^o C_{\text{m0}} \frac{MW_{\text{monomer}}}{1000}, \quad \forall i \tag{4d}$$

c) Processing times

$$\theta_{ik} \leq \theta^{\max} y_{ik}, \quad \forall i, k \tag{5a}$$

$$\Theta_i = \sum_{k=1}^{N_s} \theta_{ik}, \quad \forall i \tag{5b}$$

$$p_k = \sum_{i=1}^{N_p} \theta_{ik}, \quad \forall k \tag{5c}$$

e) Timing relations

$$t_k^{\text{e}} = t_k^{\text{s}} + p_k + \theta_k^t, \quad \forall k \tag{6a}$$

$$t_k^{\text{s}} = t_{k-1}^{\text{e}}, \quad \forall k \neq 1 \tag{6b}$$

$$t_k^{\text{e}} \leq T_{\text{c}}, \quad \forall k \tag{6c}$$

$$t_{fck} = (f-1)\frac{\theta_k^t}{N_{fe}} + \frac{\theta_k^t}{N_{fe}}\gamma_c, \quad \forall f, c, k \tag{6d}$$

3. Dynamic optimization formulation.

To address the optimal control part, the simultaneous approach[24] for addressing dynamic optimization problems was used in which the dynamic model representing the system behavior is discretized using the method of orthogonal collocation on finite elements.[28,29] According to this procedure, a given slot k is divided into a number of finite elements. Within each finite element an adequate number of internal collocation points is selected. Using several finite elements is useful to represent dynamic profiles with nonsmooth variations. Thus, the set of ordinary differential equations comprising the system model, is approximated at each collo-

Table 1. Objective Function Parameters

α* = 688.351
β* = 0.75
at (hr/4 years) = 35040
$\rho^{\dagger}$ (kg/m^3) = 866
$Cp^{\dagger}$ [kJ/(kg K)] = 2
T_{amb} (K) = 298
$C^{\text{st}\ddagger}$(\$/kJ) = 8.22 × 10^{-6}
$\rho_{\text{w}}^{\dagger}$ (kg/m^3) = 1000
$Cp_{\text{cw}}^{\ddagger}$ (kJ/kg K) = 4.2
$\lambda_{\text{hv}}^{\ddagger}$ (kJ/kg) = 2417
$P_{\text{ew}}^{\ddagger}$ = 0.3 × 10^{-2}
T_j* (K) = 340
$C^{\text{mu}\ddagger}$ (\$/kg) = 2.23 × 10^{-2}
MW_{mon} (kg/kg mol) = 100.20
$C^{r\S}$ (\$/kg) = 1.5
MW_{ini}§ (kg/kg mol) = 164.21
$C^{I\P}$ (\$/kg) = 11

*Adapted from Matches 2007.[26]
†Silva-Beard et al.[27]
‡Turton et al.[33]
§Ref. 34
¶Asteasuain et al.[2]

Table 2. pMMA Grade Information

	Grade A	Grade B	Grade C	Grade D	Grade E
Desired MW (kg/kg mol)	15,000	20,000	25,000	35,000	45,000
Demand (kg/hr)	1.6	1.4	1.0	0.8	0.6
Price ($/kg)	1.20	1.30	1.50	1.60	1.65
Inv. Cost [$/hr kg)] 10^{-3}	1.20	1.50	1.60	1.60	1.65

cation point leading to a set of nonlinear equations that must be satisfied.

a) Dynamic mathematical model discretization

$$x^n_{fck} = x^n_{o,fk} + \theta^t_k h_{fk} \sum_{l=1}^{N_{cp}} \Omega_{lc} \dot{x}^n_{flk}, \quad \forall n, f, c, k \tag{7}$$

Also note that in the present formulation the length of all finite elements is the same and computed as

$$h_{fk} = \frac{1}{N_{\text{fe}}} \tag{8}$$

b) Continuity constraint between finite elements

$$x^n_{o,fk} = x^n_{o,f-1,k} + \theta^t_k h_{f-1,k} \sum_{l=1}^{N_{\text{cp}}} \Omega_{l,N_{cp}} \dot{x}^n_{f-1,l,k}, \quad \forall n, f \geq 2, k \tag{9}$$

c) Model behavior at each collocation point

$$\dot{x}^n_{fck} = f^n(x^1_{fck}, \ldots, x^n_{fck}, u^1_{fck}, \ldots u^m_{fck}), \quad \forall n, f, c, k \tag{10}$$

d) Initial and final controlled and manipulated variable values at each slot:

$$x^n_{\text{in},k} = \sum_{i=1}^{N_p} x^n_{\text{ss},i} y_{i,k}, \quad \forall n, k \tag{11}$$

$$\bar{x}^n_k = \sum_{i=1}^{N_p} x^n_{\text{ss},i} y_{i,k+1}, \quad \forall n, k \neq N_s \tag{12}$$

$$\bar{x}^n_k = \sum_{i=1}^{N_p} x^n_{\text{ss},i} y_{i,1}, \quad \forall n, k = N_s \tag{13}$$

$$u^m_{\text{in},k} = \sum_{i=1}^{N_p} u^m_{\text{ss},i} y_{i,k}, \quad \forall m, k \tag{14}$$

$$\bar{u}^m_k = \sum_{i=1}^{N_p} u^m_{\text{ss},i} y_{i,k+1}, \quad \forall m, k \neq N_s - 1 \tag{15}$$

Table 3. CSTR Design Variable Results

$F = 0.390$ m^3/h
$F_{\text{cw}} = 0.010$ m^3/h
$C_{\min} = 0.767$ kg mol/m^3
$C_{I\text{in}} = 10.000$ kg mol/m^3
$T_{\text{in}} = 344.8$ K
$T_{\text{w0}} = 298.0$ K
$A = 15.120$ m^2
$V = 2.073$ m^3
$V_0 = 0.415$ m^3

Table 4. pMMA Steady State Results

	Grade A	Grade B	Grade C	Grade D	Grade E
C^m (kg mol/m^3)	0.4162	0.4749	0.5216	0.6070	0.6760
$C^I \times 10^3$ (kg mol/m^3)	1.5064	0.9056	0.5833	0.2195	0.0661
T^R (K)	348.1	347.3	346.7	345.7	344.8
Q^I (10^4 m^3/h)	1.1486	0.6598	0.4105	0.1455	0.0419
X (%)	0.4574	0.3809	0.3199	0.2089	0.1186
MW (kg/kg mol)	15,200	20,200	24,800	34,800	44,800

$$\bar{u}^m_k = \sum_{i=1}^{N_p} u^m_{\text{ss},i} y_{i,1}, \quad \forall m, k = N_s \tag{16}$$

$$u^m_{1,1,k} = u^m_{\text{in},k}, \quad \forall m, k \tag{17}$$

$$x^n_{o,1,k} = x^n_{\text{in},k}, \quad \forall n, k \tag{18}$$

$$x^n_{\text{tol},k} \geq x^n_{N\text{fe},Nc,k} - \bar{x}^n_k, \quad \forall n, k \tag{19}$$

$$-x^n_{\text{tol},k} \leq x^n_{N\text{fe},Nc,k} - \bar{x}^n_k, \quad \forall n, k \tag{20}$$

e) Lower and upper bounds on the decision variables

$$x^n_{\min} \leq x^n_{fck} \leq x^n_{\max}, \quad \forall n, f, c, k \tag{21a}$$

$$u^m_{\min} \leq u^m_{fck} \leq u^m_{\max}, \quad \forall m, f, c, k \tag{21b}$$

f) Smooth transition constraints

$$u^m_{f,c,k} - u^m_{f,c-1,k} \leq u^c_{\text{cont}}, \quad \forall m, k, c \neq 1 \tag{22}$$

$$u^m_{f,c,k} - u^m_{f,c-1,k} \geq -u^c_{\text{cont}}, \quad \forall m, k, f, c \neq 1 \tag{23}$$

$$u^m_{f,1,k} - u^m_{f-1,N\text{fe},k} \leq u^f_{\text{cont}}, \quad \forall m, k, f \neq 1 \tag{24}$$

$$u^m_{f,1,k} - u^m_{f-1,N\text{fe},k} \geq -u^f_{\text{cont}}, \quad \forall m, k, f \neq 1 \tag{25}$$

$$u^m_{1,1,k} - u^m_{\text{in},k} \leq u^f_{\text{cont}}, \quad \forall k \tag{26}$$

$$u^m_{1,1,k} - u^m_{\text{in},k} \geq -u^f_{\text{cont}}, \quad \forall k \tag{27}$$

Equations 22–27 force the change between adjacent collocation points and finite elements to be within a certain acceptable range.

Two-stage stochastic programming approach for uncertainty in demand

Generally speaking, scheduling and optimal control problems, because of their nature, are able to handle uncertainties

Table 5. Scheduling Variables at the Optimal Solution

Product	Process T (h)	Production (kg)	Trans T (h)	T start (h)	T end (h)
A	95.25	1307.34	14.21	0	109.47
E	137.32	490.25	1.74	109.57	248.52
D	104.16	653.67	1.26	248.52	353.95
C	85.07	817.08	2.58	353.94	441.59
B	100.06	1143.92	3.07	441.59	544.73

The objective function value is $ 2.32/hr and 544.7 h of total cycle time.

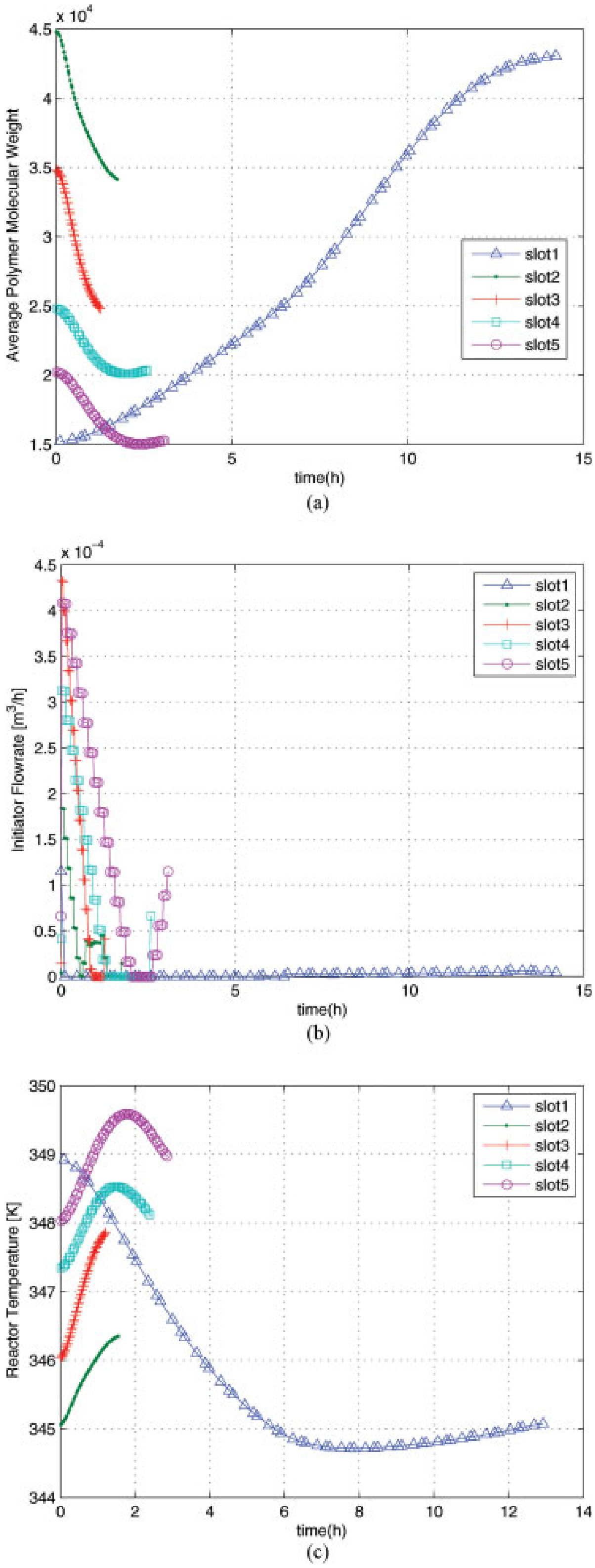

Figure 1. Dynamic transitions in the pMMA CSTR, obtained through deterministic procedures.

(a) Average molecular weight, (b) manipulated variable, and (c) reactor temperature. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Table 6. Contributions to the Objective Function for the Deterministic Example

Objective Function Term	Contribution ($/hr)
Sales	11.27
Reactor (4 yr amortization)	2.22
Feed stream heating	0.26
Cooling water	1.32
Inventories	2.63
Offspec during transitions	2.53

from one scheduling period to the next. In other words, if uncertainties are present at the beginning of each scenario, and remain fixed throughout it, then the scheduling and the optimal control problems can be solved once for each scenario to accommodate each uncertainty realization. On the other hand, the design problem can only be solved once, and the design variable values, obtained from the solution cannot be changed throughout the different scenarios. In this work we assume that product demands are subject to uncertainties that are expressed as discrete distributions for hourly product demands, which give rise to the different scenarios. The simultaneous design, scheduling, and optimal control problem is then solved as a two-stage stochastic programming problem, in which the scheduling and optimal control are selected in stage 2 for each scenario. The context of uncertainty used in this article is similar to the perfect information context presented by Bhatia and Biegler,[16] in which once a design is carried out, changes in scheduling and optimal control can be made from scenario to scenario, based on the fact that complete (perfect) information about demand uncertainties is resolved before every cycle begins.

An important assumption must be made at this point to be able to use the proposed two-stage stochastic programming approach. In cyclic scheduling, products are consumed constantly throughout the cycle, and part of every product inventory carries over into the next cycle, until production of the relevant product begins again. In this context, changing the schedule order of production may cause product shortages if the production period of this product begins later in the new cycle than in the previous one. In this work it is assumed that a schedule switch caused by a change in demand scenario (if necessary) happens only once in a large number of cycles. In fact, the number of cycles is assumed to be large enough such that shortages that might occur during schedule switches need not be modeled in the formulation.

The two-stage stochastic programming formulation used in this work is similar to that used by Bhatia and Biegler,[16] and it has the following form:

$$\begin{aligned} &\max \sum_{q=1}^{N\text{ds}} \omega_q \phi_q(x_q, u_q, \text{sc}_q, d, \theta_q) \\ &\text{s.t.} \\ &\qquad h_q^z(x_q, u_q, \text{sc}_q, d) = 0 \\ &\qquad g_q^z(x_q, u_q, \text{sc}_q, d) \leq 0 \\ &\qquad h_q^{sc}(\text{sc}_q, d, \theta_q) = 0 \\ &\qquad g_q^{sc}(\text{sc}_q, d, \theta_q) \leq 0 \\ &\qquad h^d(d) = 0 \\ &\qquad d_{\min} \leq d \leq d_{\max} \\ &\qquad u_q, x_q \in Z, \text{sc}_q \in \text{SC}, d \in D, \theta_q = (\theta_q^1 \ldots \theta_q^{N\text{ds}}) \end{aligned} \tag{28}$$

Table 7. Demand Scenarios in Example 2

	Grade A	Grade B	Grade C	Grade D	Grade E	Probability
Demand scenario 1 (kg/h)	1.6	1.4	1.0	0.8	0.6	0.30
Demand scenario 2 (kg/h)	1.6	1.4	1.0	0.8	0.9	0.20
Demand scenario 3 (kg/h)	1.6	1.4	0.5	0.8	0.6	0.20
Demand scenario 4 (kg/h)	1.6	1.4	0.5	0.8	0.9	0.15
Demand scenario 5 (kg/h)	4.8	1.4	0.5	0.8	0.9	0.15

The set q, corresponds to each different demand scenario, and ω_q, is the probability that a demand scenario q will occur. Optimal control state variables and manipulated variables are designated as x_q and u_q, respectively, sc_q are scheduling variables, d are design variables, and θ_q represents the uncertain parameters, in this case the product demands. Different scenarios have different scheduling and optimal control solutions, but are linked by a fixed set of design variables.

Case Studies

In the following section the proposed formulation is used to solve the simultaneous design, scheduling and optimal control of a MMA polymerization reactor, where different polymer grades are produced. First, the problem is solved as a deterministic problem. In a second case, uncertainty in three of five polymer grade demands is taken into account, and the problem is solved using a two-stage stochastic programming formulation.

MMA polymerization

The MMA polymerization system used in this article is described by Silva-Beard et al.[27] The polymerization reactions take place in a CSTR. The variables that correspond to the reactor design are bounded around the nominal values used in the above-mentioned work.[27] The desired average molecular weight distributions are 15,000, 20,000, 25,000, 35,000, and 45,000, which are the only parameters defined, because the determination of the variables that describe the steady states corresponding to each grade are left as decision variables for the optimization.

Deterministic approach

Under this situation, all problem parameters are considered deterministic. Equations 1–27 are used directly to solve the simultaneous design, scheduling, and optimal control of the MMA polymerization CSTR. Information about the parameters embedded in the objective function and desired grades is shown in Tables 1 and Table 2, respectively. Results were obtained using the MINLP solver DICOPT,[30] based on the outer approximation algorithm[31] through the GAMS modeling system. The problem consisted of 5000 continuous variables and 25 binary variables, and its solution took 1855 CPU s in a 2.86 GHz machine with 2 GB of RAM memory. The solution was found after four major iterations of the outer approximation algorithm, the NLP solver used was conopt3 and the MIP solver was cplex. The time spent solving the NLPs represented 97% of the total solution time, whereas the MIP problem took the remaining 3%. Tables 3 and 4 show the values of all design variables at the optimal solution point. Table 5 contains the scheduling variables that describe the optimal cycle, including hourly profit, whereas Figures 1a–1c show the optimal dynamic profiles during grade transitions. Table 6 shows the different contributions of each term in the objective function.

It is interesting to notice how the largest contribution to the costs are design related. This indicates that any decision taken to decrease the design costs would involve an undesirable trade-off in the transition and inventory costs. For instance, a smaller reactor or feed stream flow rate would decrease the design costs, but the production rate would necessarily be smaller, which in turn would increase the cycle time and inventory costs.

On the other hand, the resulting optimal schedule (AEDCB) is dominated by transitions between grades that have similar molecular weights, occurring in the direction of higher molecular weight to lower molecular weight, except of course, for the A–E transition, required at the beginning of the cycle. We have analyzed this type of transitions in detail in previous works.[7,8] From a dynamic point of view, transitions between grades with similar molecular weights are fast, since they involve similar steady state operating conditions (see Table 4). A long transition is allowed to occur to permit all other transitions to be performed between similar grades.[7] Another important dynamic behavior is the shutting down of initiator feed stream. Because the AIBN initiator is expensive, transitions that involve shutting down initiator flow rate to the reactor result in little AIBN wasted during transitions. As a final observation, it is interesting to see that the resulting dynamic operation does not involve a

Table 8. CSTR Design Variable Results in Example 2

$F = 0.431$ m^3/h
$F_{cw} = 0.0100$ m^3/h
$C_{min} = 0.809$ kg mol/m^3
$C_{Iin} = 10.000$ kg mol/m^3
$T_{in} = 344.87$ K
$T_{w0} = 298.00$ K
$A = 15.370$ m^2
$V = 2.125$ m^3
$V_0 = 0.425$ m^3

Table 9. pMMA Steady State Results in Example 2

	Grade A	Grade B	Grade C	Grade D	Grade E
C^m (kg mol/m^3)	0.4413	0.5045	0.5547	0.6487	0.7181
$C^I \times 10^3$ (kg mol/m^3)	1.4945	0.9047	0.5851	0.2112	0.0653
T^R (K)	348.93	348.04	347.34	346.02	345.05
$Q^I \times 10^4$ (m^3/h)	1.2798	0.7336	0.4553	0.1529	0.0450
X (%)	0.4545	0.3764	0.3143	0.1981	0.1124
MW (kg/kg mol)	15,200	20,200	24,800	35,200	44,800

Table 10. Scenario by Scenario Results Using the Two-Stage Stochastic Programming Formulation

Scenario	Sequence	Cycle Time	Trans. Time	Sales	Design Costs	Inventory Costs	Trans. Costs
1	$A \to E \to D \to C \to B$	542	20.97	11.27	3.87	2.69	2.69
2	$A \to E \to D \to C \to B$	546	20.97	12.01	3.87	2.80	2.67
3	$A \to B \to C \to D \to E$	652	27.74	10.14	3.87	2.92	2.92
4	$A \to E \to D \to C \to B$	561	20.97	10.88	3.87	2.60	2.60
5	$A \to E \to D \to C \to B$	598	21.86	14.24	3.87	2.96	2.50

The weighted objective function is 2.25 \$/h. Scenario profits, sales, and costs are in \$/h; cycle and total transition times are in hours.

Table 11. Scheduling and Control Results Using the Deterministic Design

Scenario	Sequence	Cycle Time	Trans. Time	Sales	Design Costs	Inventory Costs	Trans. Costs
1	$A \to E \to D \to C \to B$	554	22.86	11.27	3.80	2.67	2.48
2	$A \to E \to D \to C \to B$	556	22.86	11.27	3.80	2.68	2.47
3	$A \to E \to D \to C \to B$	562	22.86	10.14	3.80	2.45	2.45
4	$A \to E \to D \to C \to B$	580	22.86	10.61	3.80	2.58	2.37
5	$A \to E \to D \to C \to B$	627	22.86	12.07	3.80	2.76	2.19

The resulting profit using the same probabilities (weights) as in the two-stage stochastic programming formulation, is 2.23 \$/hr. Scenario profits, sales, and costs are in \$/h; cycle and total transition times are in hours.

significant temperature change, approximating an isothermal process.

Two-stage stochastic programming approach for different demand scenarios

In the second example uncertainty is introduced in the hourly demands of grades A, C, and E. In real life operations, uncertain demand is a continuous quantity, which can usually be described by a probabilistic distribution, but in this work, uncertainty in grade demand is handled through a set of discrete values which represent different demand scenarios. The problem is solved by using a two-stage stochastic programming approach for optimal design under uncertainty,[5] in which each period represents a different demand scenario, and where the objective function represents a weighted sum of the different possible scenarios. These scenarios are independent from each other, except for the set of design variables that remain constant throughout all of them.[16] The rigorous procedure for flexibility analysis would call for a second step in which the optimal design is tested all over the uncertain demand parameters domains.[5] The critical feasibility points would then be included as part of the finite set of possible values for the uncertain parameters, and solved within the multiscenario formulation, generating an iterative procedure. This procedure will not be included in this paper. Also the noncovexity of the problem results in the fact that no flexibility analysis involving discrete realizations of the uncertain demand will be truly rigorous. As mentioned in the introduction, there are some alternatives for robust optimization under uncertainty,[23] but they will not be used in this article because they greatly depend on the convexity assumption, and because of the added computational demand of those approaches, on top of an already demanding problem. However we recognize that this limitation should be addressed in future works. Since the discretized demand values include significant variations from the nominal point, we can still say that the problem is locally solved for very different uncertain parameter realizations, and analyze the solution as such. The application of large scale MINLP algorithms[32] could allow a for some interesting possibilities, listed later in this article.

The example described below involves five different demand scenarios where low and high demand values for grades C and E are combined (demands for grades B and D remain constant), generating four scenarios. An extreme demand combination involving a significant change in demand for grade A generates the fifth scenario. Throughout this section of the article, the results for the multiscenario formulation will be shown, and a comparison against the deterministic formulation will be carried out.

The different demand scenarios are detailed in Table 7. To efficiently solve the multiscenario formulation, it is initialized with the independent solutions to each demand scenario.[16] In other words, each scenario is solved as a deterministic problem, and the different solutions are passed on to initialize the two-stage stochastic programming problem. The multiscenario problem was solved using the MINLP solver DICOPT,[30] based on the outer approximation algorithm[31] through the GAMS modeling system. The problem consisted

Table 12. Scheduling and Control Results Using the Two-Stage Stochastic Programming Design

Scenario	Sequence	Cycle Time	Trans. Time	Sales	Design Costs	Inventory Costs	Trans. Costs
1	$A \to E \to D \to C \to B$	542	20.93	11.27	3.87	2.68	2.68
2	$A \to E \to D \to C \to B$	554	20.93	12.01	3.87	2.83	2.62
3	$A \to E \to D \to C \to B$	570	20.93	10.14	3.87	2.55	2.55
4	$A \to E \to D \to C \to B$	560	20.93	10.88	3.87	2.59	2.59
5	$A \to E \to D \to C \to B$	590	20.93	14.25	3.87	2.92	2.46

The weighted objective function is 2.41 \$/h. Scenario profits, sales, and costs are in \$/h; cycle and total transition times are in hours.

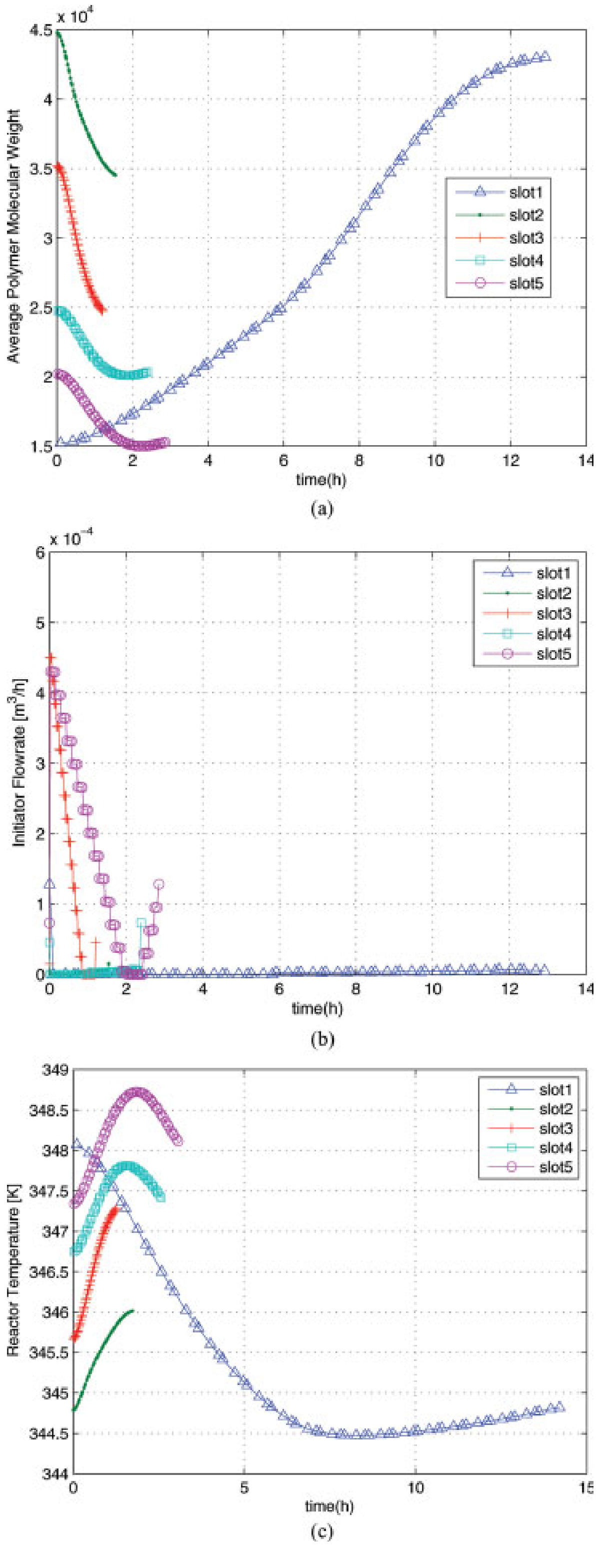

Figure 2. Dynamic transitions in the pMMA CSTR, obtained by simultaneous scheduling and optimal control, using as fixed design the one obtained in the multiperiod example.

(a) Average molecular weight, (b) Manipulated variable, and (c) Reactor temperature. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

of 24,704 continuous variables and 125 binary variables. The solution took 87,676 CPU s (~24 h) on a 2.86 GHz machine with 2 GB of RAM memory, using a full space solution approach (i.e. no decomposition optimization technique was used). The solution was found after two major iterations of the outer approximation algorithm, the NLP solver used was conopt3 and the MIP solver was cplex. The time spent solving the NLPs represented 21% of the total solution time, whereas the MIP problem took 79%. Tables 8 and 9 show the values of all design variables at the optimal solution. Table 10 show the objective function value and other relevant values for the description of each period solution, within thve two-stage stochastic programming formulation.

As shown in Tables 3 and 8 the differences in terms of the CSTR design variables are in the feed stream flow rate, monomer concentration and reactor size (which in turns determines the area and volume of the jacket). However, the steady states determined through both approaches are very similar. The first scenario of the two-stage stochastic programming approach, corresponds to the deterministic problem. The solutions found by both approaches for the same scenario show different sequences, cycle durations and slightly different distribution of costs as shown in Table 10. The hourly profit of this particular scenario is lower in the two-stage stochastic programming solution than in the deterministic solution. However, size and nonconvexity of both problems are different, and as with every nonlinear, nonconvex problem, local optimal points are present. A way to compare both solutions in similar conditions was necessary. The main expected advantage of the two-stage stochastic programming formulation over the deterministic solution is a more robust design. In some cases a certain design found to be optimal for a deterministic problem might not be feasible for all expected conditions. Being this the case, a relevant comparison would involve comparing the deterministic design vs. the two-stage stochastic programming design, using the same problem conditions. This means that design variables found through both methods could be fixed and the same scheduling and optimal control problem could then be solved using both designs. The results shown in Tables 11 and 12 correspond to the proposed approach: they are the result of using as fixed designs those found by the deterministic and two-stage stochastic programming approaches, and solving each period independently as a scheduling and optimal control problem. The solution to the first example in this article (the original deterministic problem) was used as initialization point for all scenarios and for both designs. In this comparison it is evident that the design obtained from the two-stage stochastic programming formulation performs better than the one obtained by using the deterministic approach. It is worth noticing that in both cases the production scheduling is the same in all scenarios. The main differences are found in total transitions durations and cycle times. In Figures 1a–2c one can see that most transitions have similar durations, except for the transition corresponding to slot 3 for both cases (in both cases this transition corresponds to a $D \rightarrow C$ transition). Cycle time differences can be attributed to faster transitions and to faster process rates in the two-stage stochastic programming formulation. A good summary of how the two-stage stochastic programming approach compares against the deterministic approach is presented in

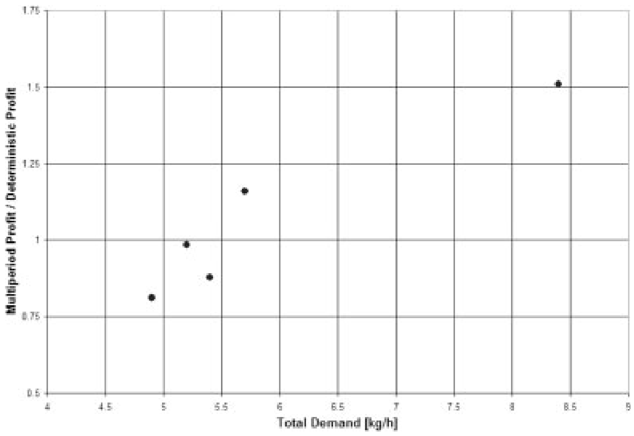

Figure 3. Relative performance two stage stochastic programming approach vs. deterministic approach.

Figure 3. From this figure one can see that there is a clear trend in which, as total hourly demand (summation over all polymer grades) increases, the two-stage stochastic programming approach performs better than the deterministic approach.

Conclusions

The optimization formulation presented in this article successfully addressed the simultaneous design (including steady state determination), cyclic scheduling, and control of a MMA polymerization reactor under deterministic and uncertain demand characteristics. Since chemical process design must be flexible and robust enough to accommodate for process uncertainties, a two-stage stochastic programming formulation which deals with demand uncertainties in the form of a finite set of values was proposed. This problem was solved, and interesting observations could be drawn from such a solution, and from its comparison vs. a deterministic approach. When the design variables (including the determined steady states) resulting from the two-stage programming solution, were fixed and different demand scenarios were solved independently, significantly better solutions than those provided using the deterministic design were found. The comparison was made using identical conditions (same constraints, objective function, solver and solver options, computer hardware, etc.), including the same initialization point.

This work represents another step in the simultaneous solution of process and grade design, scheduling, and optimal control. The next steps can take many directions: process design beyond reactor design, implementation of close-loop control schemes, inclusion of more complex scheduling models, solution of larger dynamic models by optimization decomposition techniques, parallel computing for scheduling and control, integration of planning, scheduling and control, inclusion of uncertainty in model and other market parameters, and/or continuous probability distributions for uncertain quantities based on stochastic optimization formulations, extension of most of the past research points to deal with batch plants. Recent developments and improvements of large scale MINLP problem[32] solvers further encourages the exploration of all these research possibilities.

Notation

Indices

Products, $i, p = 1,\ldots N_p$
Slots, $k = 1,\ldots N_s$
Finite elements, $f = 1,\ldots N_{fe}$
Collocation pointsc, $l = 1,\ldots N_{cp}$
System states, $n = 1,\ldots N_x$
Manipulated variables, $m = 1,\ldots N_u$
Demand scenarios, $q = 1,\ldots N_{ds}$

Decision Variables

y_{ik} = binary variable to denote if product i is assigned to slot k
p_k = processing time at slot k
t_k^e = Final time at slot k
t_k^s = start time at slot k
t_{fck} = time at finite element f and collocation point c of slot k
G_i = production rate
T_c = cyclic time (h)
x_{fck}^n = nth system state in finite element f and collocation point c of slot k
$\dot{x}_{flk}^n$ = value of nth state derivative with respect to time in finite element f and collocation point l of slot k
u_{fck}^m = mth manipulated variable in finite element f and collocation point c of slot k
W_i = amount produced of each product (kg)
θ_{ik} = processing time of product i in slot k
θ_k^t = transition time at slot k
Θ_i = total processing time of product i
$x_{o,fk}^n$ = nth state value at the beginning of the finite element f of slot k
$\bar{x}_k^n$ = desired value of the n-th state at the end of dynamic transition of slot k
$\bar{u}_k^m$ = desired value of the m-th manipulated variable at the end of dynamic transition of slot k
$x_{in,k}^n$ = nth state value at the beginning of dynamic transition of slot k
$u_{in,k}^n$ = mth manipulated variable value at the beginning of dynamic transition of slot k
$x_{ss,i}^n$ = nth state value at steady state of product i
$m_{ss,i}^m$ = mth manipulated variable value of product i
X_{fck} = conversion in finite element f and collocation point c of slot k
MWD_{fck} = molecular weight distribution in finite element f and collocation point c of slot k
T_{in} = monomer feed stream feeding temperature (K)
T_w = cooling water feeding temperature (K)
F_{mon} = monomer feed stream flow rate (m^3/h)
F_{cw} = cooling water flow rate (m^3/h)
C_{min} = monomer feed stream concentration (kmol/m^3)
$C_{I in}$ = initiator feed stream concentration (kmol/m^3)
V = reactor volume (m^3)
V_0 = jacket volume (m^3)
A = surface area for heat exchange (m^2)
z = control-related variables
sc = scheduling-related variables
d = design-related variables

Parameters

N_p = number of products
N_s = number of slots
N_{fe} = number of finite elements
N_{cp} = number of collocation points
N_x = number of system states
N_u = number of manipulated variables
N_{ds} = number of demand scenarios
D_i = demand rate (kg/h)
θ_q = uncertain parameters values at period q

α = pre-exponential factor of reactor volume-cost correlation (\$/m^3)
β = exponential factor of volume-cost correlation
at = number of hours in the four year amortization period (h)
C_i^p = price of products (\$/kg)
C_i^s = cost of inventory (\$/kg-hr)
C^r = cost of raw material (\$/lt of feed solution)
C^I = cost of initiator (\$/lt of feed solution)
C^{st} = cost of providing energy from steam (\$/kJ)
C^{cw} = cost of supplying cooling water (\$/kg)
C^{mw} = unit cost of replacing cooling water (\$/kg)
h_{fk} = length of finite element f in slot k
Ω_{cc} = matrix of Radau quadrature weights
$\bar{x}_k^n$ = desired value of the nth system state at slot k
θ^{max} = upper bound on processing time
ω_q = probability associated with scenario q
$MWD_{ss,i}$ = desired molecular weight distribution of grade i
x_{min}^n, x_{max}^n = minimum and maximum value of the state x^n
u_{min}^m, u_{max}^m = minimum and maximum value of the manipulated variable u^m
$\dot{x}_{tol}^n$ = maximum absolute value for state derivatives at the end of dynamic transition
x_{tol}^n = maximum absolute deviation from desired final value, allowable for state variable x^n at the end of dynamic transition
u_{cont}^f = maximum absolute change for u^m between finite elements
u_{cont}^c = maximum absolute change for u^m between collocation points
γ_c = roots of the Lagrange orthogonal polynomial
Q_{max}^m = maximum monomer flow rate (lt/hr)
Q_{max}^I = maximum initiator flow rate (lt/hr)
T_j^* = an expected jacket temperature used to calculate average heat required in order to cool down water after process
T_{amb} = room temperature (K)
λ_{hv} = water latent heat of vaporization (kJ/kg)
P_cw = percent of water lost during cooling operations (%)
ρ = monomer feed stream density (kg/m^3)
C_p = monomer feed stream heat capacity (kJ/kg K)
ρ_w = cooling water density (kg/m^3)
C_{pw} = cooling water heat capacity (kJ/kg K)
MW_{mon} = monomer molecular weight (kmol/kg)
MW_{ini} = initiator molecular weight (kmol/kg)
d_{min}, d_{max} = lower and upper bounds on design variables
U^p = upper bound on production

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