

SRC TR 87-166

**Multiobjective Dynamic
Optimization of Semibatch Free
Radical Copolymerization Process
with Interactive CAD Tools**

by

D. Butala, K.Y. Choi, and M.K.H. Fan

Multiobjective Dynamic Optimization of Semibatch Free Radical Copolymerization Process with Interactive CAD Tools *

D. Butala, K.Y. Choi [†] and M.K.H. Fan [‡]

Department of Chemical and Nuclear Engineering
and Systems Research Center
University of Maryland
College Park, MD 20742

August 17, 1987

Keywords: *Polymerization, Optimal Control, Optimization, Open-loop Control*

Abstract

Optimal open loop control strategies are developed for batch and semibatch free radical copolymerization of styrene and acrylonitrile using the interactive computer aided design(CAD) tool CONSOLE, which was developed at the University of Maryland in 1987. CONSOLE emphasizes control engineer's intuition and man-machine interaction and includes a classification of various design specifications. Conflict resolution among the different objectives is made by scaling of specification space based on designer's knowledge of the polymerization process. A feasible direction algorithm is used to obtain optimal monomer addition and reactor temperature policies.

*This research was supported by the system Research Center at the University of Maryland, College Park.

[†]To whom correspondence should be addressed.

[‡]Electrical Engineering Department and Systems Research Center

Introduction

A precise control of polymer properties has become one of the major issues in optimizing industrial polymerization processes recently. Many polymerization processes involve batch or semi-batch reactors to produce small-to-medium volume engineering and specialty polymers. Although continuous processes, in general, produce polymers of more consistent quality in large volume through process automation than batch processes, the latter are still industrially very important and particularly well suited for the production of polymers of varying grades in a rapidly changing market environment.

In free radical copolymerization processes, controlling both copolymer composition and molecular weight or molecular weight distribution (MWD) is of primary importance. For instance, two styrene-acrylonitrile (SAN) copolymers differing more than 4% in acrylonitrile level are incompatible, resulting in poor physical and mechanical properties [1]. It is also well known that significant batch-to-batch variation in product polymer properties is quite common in industrial processes and resulting off-specification products are often wasted.

Many of the batch or semibatch polymerization reactor control problems stem from the lack of accurate on-line sensors for polymer property measurements. Although some promising progress has been made in recent years in developing on-line sensors for certain polymerization systems [2-6], on-line sensors for the measurement of many important polymer properties are not readily available at this time. Therefore, batch or semibatch copolymerization processes pose challenging open loop control problems (Task Level Control). Inevitably, accurate process models are required in order to synthesize open loop time varying control policies which minimize properly defined objective functions.

Semibatch free radical copolymerization process is a typical example of a multivariable open loop optimal control design problem. Here, one has to manipulate at least two control variables (e.g. monomer addition rate, reactor temperature) in order to obtain copolymers of desired composition and molecular weight or its MWD, in the shortest possible time under the operating constraints. If only one polymer quality parameter is controlled by manipulating one control variable, uncontrolled property parameters may deviate from their desired values as the reaction proceeds. In other words, performance objectives compete against each other and a compromise has to be considered. One simple technique used quite often for handling such problems is the weighted sum approach, in which the single cost is a weighted sum of various performance objectives. However,

this has the disadvantage of hiding the physical significance of these objectives when viewing the values of the course during an optimization. In other words, this technique gives a solution to the overall problem but does not provide insight into the conflicts among the competing objectives. Furthermore, it requires a priori knowledge of the weights to vary the emphasis given to each objective and adjusting them is usually a cumbersome process. In recent years several publications dealing with single cost function optimization in homopolymerization have appeared, [7–10]. Chen and Lee [11] used the single objective optimization for copolymerization reactor design. For such multiobjective optimization problem, as copolymerization process optimal solutions generally do not exist and one must be satisfied with obtaining a non-inferior solution or Pareto optimum. The non-inferior solution is one in which no decrease can be obtained in any of the objectives without causing a simultaneous increase in at least one of the other objectives. Tsoukas *et. al* [12]. were the first to apply the dynamic two-objective ϵ -constraint algorithm developed by Haimes *et. al.* [13] to a semibatch copolymerization process. Farber [14] reported the use of similar multiobjective optimization technique to determine the non-inferior sets for continuous copolymerization of styrene-acrylonitrile and methyl methacrylate-vinyl acetate systems.

With a rapid progress in computer technology, there is a growing interest in developing interactive optimization tools to solve a variety of engineering problems. In this paper, we apply a new methodology in solving an open loop optimal control problem for semibatch copolymerization processes. This methodology was developed by Nye and Tits [15] and it has been applied successfully to numerous design problems in various branches of engineering such as integrated circuits [16], control systems [17–22] or earthquake resistant structures [23]. The central idea in this computer aided design(CAD) methodology is to emphasize designer intuition and man-machine interaction in an optimization-based approach to engineering design in which the designer and the computer are complementary as they work together to optimize the performance of designs. Furthermore, it handles constrained multi-objective design problems where some of the objectives or the constraints could be ‘functional’. This means that the specification could also be a function of an independent variable and that the specification needs to be optimized or satisfied for all values of the independent variable in a given set. The delivery of designer intuition and knowledge pertaining to the design problem is through an application-oriented problem formulation. We summarize the procedure of the problem formulation below. For more details, see [15,24,25].

1. Partition of the various specifications into three categories:

- (a) **hard (functional) constraint** - a specification whose satisfaction is considered essential and hence achieving it should proceed with the utmost priority. For our design problem, good examples for hard constraints are the requirements of total reaction mass and operating temperature. It is clear that the resulting design has no engineering value if the total reaction mass exceeds the designed reactor volume.
- (b) **soft (functional) constraint** - a specification which involves a desired or target value, that the designer should try to approach and reach if possible, but such that no further gain would be obtained if the specification overachieved its target value. A soft constraint could be the product specifications. A slight violation of the constraint would probably not jeopardize the value of the design, even though a design satisfying the constraint would be preferable.
- (c) **(functional) objective** - a specification for which some quantity should be minimized or maximized. Minimization of deviation of product specification from their set values and minimization of reaction time will be our objectives.

Based on the above definition of constraints and objectives, the algorithm proceeds in three phases. In the phase I, only the hard constraints are considered, when all the hard constraints are satisfied, the second phase starts. In the phase II, objectives and soft constraints compete simultaneously, while hard constraints remain satisfied. The third phase starts only when all the soft constraints are satisfied, all objectives have reached at least their good values (see below) and hard constraints are still maintained satisfied. In the phase III effort is made to improve the objectives, while all hard and soft constraints are still kept satisfied.

2. Choose a good value (curve) and a bad value (curve) for each specification by uniform satisfaction/dissatisfaction rule: having all of the various (functional) objectives and soft (functional) constraints achieve their corresponding good values (curves) should provide the same level of satisfaction to the designer for each, while achieving the bad values (curves) should provide the same level of dissatisfaction. Having all of the various hard (functional) constraints achieve their corresponding good values (curves) should provide the same level of satisfaction to the designer for each, while achieving the bad values (curves) should provide the same level of dissatisfaction. The use of good and bad values in this way provides a very simple way to do tradeoff analysis; if the designer is dissatisfied with the performance level achieved by a particular objective or constraint, he simply changes what he considers to be satisfactory

(good value) or unsatisfactory (bad value).

With this problem formulation, comparison between various scaled specifications becomes meaningful. Namely, under the assumption that the levels of satisfaction are affine functions of the specifications, we can say that the i th specification is more satisfied than j th, if $f_s^i > f_s^j$ and vice versa. Hence the maximal scaled value of all specifications represents an index of the quality of the design. Therefore we consider the following nonlinear mathematical programming problem

$$\min_x \max_i f_s^i(x) \quad (1)$$

subject to

$$g_s^j(x) \leq 0, \quad j = 1, 2, \dots$$

where x is the design parameter vector, f_s^i and g_s^j are the i th ‘scaled’ (functional) objective and the j th (functional) constraint respectively. The ‘scaled’ (functional) objective is defined by

$$f_s^i = \frac{f^i - f_{good}^i}{f_{bad}^i - f_{good}^i} \quad (2)$$

where f^i is the i th (functional) objective and f_{good}^i, f_{bad}^i are its good value (curve) and bad value (curve) respectively. With this transformation, 0 and 1 correspond respectively to the specified good and bad values. A similar definition applies to the ‘scaled’ (functional) constraint. In case of functional objective, f_s^i stands for the maximal value of all possible values of the independent variable, and similarly, for the functional constraint, $g_s^j \leq 0$ means that the constraint must be satisfied for all possible value of the independent variable.

The methodology mentioned above has been implemented in the CAD package CONSOLE [24]. CONSOLE is an interactive optimization-based design tool for a very broad range of engineering systems provided that simulators are given. It was developed by Fan *et. al.* [24] at University of Maryland. CONSOLE meets many of the very specific requirements that design engineers demand of the packages, such as, (1)the description of design problem is closely related to the character of design, (2)can be linked with arbitrary simulators in an extremely easy way, (3)graphic capability, etc. CONSOLE also provides user interactive interface which allows the user to visualize various outputs related to the performance of the design at a specified iteration. Such outputs include displaying of design parameters, Performance Comb, active specifications and plots of functional objectives or functional constraints. See subsequent sections for more details.

Kinetics and Reactor Modeling

The polymerization reactor optimization problem was investigated with solution copolymerization of styrene and acrylonitrile. The solvent and initiator used were xylene and AIBN, respectively. The reasons for selecting this system were: SAN copolymer is commercially important and optimal control is necessary if copolymer composition has to be maintained at points other than the azeotropic point. The details of reaction kinetics and reactor modeling equations are described below and the numerical values of kinetic constants are listed in Table 1.

The following kinetic model is used to describe the homogeneous solution free radical copolymerization of styrene with acrylonitrile. At high solvent volume fraction, the effect of diffusion controlled termination (gel effect) is not significant. Penultimate effect is also assumed negligible (These assumptions do not restrict the applicability of the proposed controller design technique, however.).

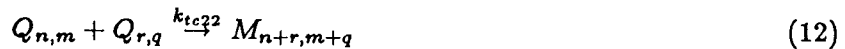
INITIATION



PROPAGATION



COMBINATION TERMINATION



DISPROPORTIONATION TERMINATION



Table 1: Numerical values of kinetic parameters and reaction conditions for Styrene-Acrylonitrile Copolymerization

	Parameter	Pre-exponential factor	Activation Energy (cal/gmol)	Ref
Initiator	k_d	$6.02 \times 10^{15} \text{sec}^{-1}$	31,730	(a)
AIBN	f	0.6	-	
Monomer		l/mol-sec		
Styrene	k_{p11}	1.06×10^7	7,067	
	k_{t11}	1.25×10^9	1,677	
	k_{f11}	2.31×10^6	12,670	
Acrylonitrile	k_{p22}	3.0×10^7	4,100	
	k_{t22}	3.3×10^{12}	5,400	
	k_{f22}	6.93×10^6	5,837	
	r_1	2.56(-)	1,190	
	r_2	$6.67 \times 10^{-5}(-)$	-4,340	
	k_{f12}	$30 \times k_{f11}$	12,670	
	k_{f21}	$5 \times k_{f22}$	5,837	
	ϕ_t	23(-)	-	
$\Delta H_r = 1.02[1 - (1.393F_1(1 - F_1))^{0.5}] + 16.03F_1 + 16.73(1 - F_1)$				(b)
Reactor Parameters:				
$f_s = 0.25, t_{max} = 5(\text{hrs}), V_{max} = 4.0(\text{l}), I_o = 0.05(\text{mol/l})$				
$h_c = 6.5 \times 10^{-4}(\text{kcl/sec} - \text{cm}^2 - ^\circ K), \rho C_p = 0.332(\text{kcl/l} - ^\circ K)$				

(a) Tsoukas, *et. al.* [12], (b) Miyama and Fujimoto [27]

$$P_{n,m} + Q_{r,q} \xrightarrow{k_{td12}} M_{n,m} + M_{r,q} \quad (14)$$

$$Q_{n,m} + Q_{r,q} \xrightarrow{k_{td22}} M_{n,m} + M_{r,q} \quad (15)$$

CHAIN TRANSFER

$$P_{n,m} + M_1 \xrightarrow{k_{f11}} M_{n,m} + P_{10} \quad (16)$$

$$P_{n,m} + M_2 \xrightarrow{k_{f12}} M_{n,m} + Q_{01} \quad (17)$$

$$Q_{n,m} + M_1 \xrightarrow{k_{f21}} M_{n,m} + P_{10} \quad (18)$$

$$Q_{n,m} + M_2 \xrightarrow{k_{f22}} M_{n,m} + Q_{01} \quad (19)$$

where $P_{n,m}$ represents a growing copolymer chain with n units of monomer 1 and m units of monomer 2, and monomer 1 on the end. Similarly, $Q_{n,m}$ represents growing copolymer chain with monomer 2 on the end. $M_{n,m}$ denotes inactive (or dead) polymer.

The copolymer molecular weight and MWD are computed by using three leading moments of the total number average copolymers. The instantaneous k -th moment is given by

$$\lambda_k^d = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} (nw_1 + mw_2)^k M_{n,m} \quad k = 0, 1, 2 \dots \quad (20)$$

where w_1 and w_2 are the molecular weights of monomer 1 (styrene) and monomer 2 (acrylonitrile), respectively. The total number average chain length (X_n), the total weight average chain length (X_w) and the polydispersity index (PD) which is a measure of molecular weight distribution broadening are expressed as:

$$X_n = \frac{\lambda_1^d}{\lambda_0^d} \quad (21)$$

$$X_w = \frac{\lambda_2^d}{\lambda_1^d} \quad (22)$$

$$PD = \frac{X_w}{X_n} \quad (23)$$

In order to maintain constant monomer mole ratio in the bulk phase, more reactive monomer or monomer mixture is injected with initiator to the reactor. Thus, the modeling equations of the semibatch copolymerization reactor of volume V take the following form:

Reactor Mass Balances:

$$\frac{dM_1}{dt} = \frac{u}{V}(M_{1f} - M_1) - [(k_{p11} + k_{f11})P + (k_{p21} + k_{f21})Q]M_1 \quad (24)$$

$$\frac{dM_2}{dt} = \frac{u}{V}(M_{2f} - M_2) - [(k_{p22} + k_{f22})Q + (k_{p12} + k_{f12})P]M_2 \quad (25)$$

$$\frac{dI}{dt} = \frac{u}{V}(I_f - I) - k_d I \quad (26)$$

$$\frac{dV}{dt} = u \quad (27)$$

Energy Balance

$$\rho C_p V \frac{dT}{dt} = V(\Delta H_r)(R_{cp}) - h_c A_c (T - T_c) + u \rho C_p (T_f - T) \quad (28)$$

where,

$$R_{cp} = [(k_{p11} + k_{f11})P + (k_{p21} + k_{f21})Q]M_1 + [(k_{p22} + k_{f22})Q + (k_{p12} + k_{f12})P]M_2 \quad (29)$$

Live Polymer Moments

$$P = \left(\frac{2fk_d I}{(k_{tc11} + k_{td11}) + 2\beta(k_{tc12} + k_{td12}) + \beta^2(k_{tc22} + k_{td22})} \right)^{1/2} \quad (30)$$

where,

$$\beta = \frac{k_{p12} + k_{f12}}{(k_{p21} + k_{f21})\phi} ; \phi = \frac{M_1}{M_2}$$

M_1 and M_2 are molar concentrations of monomer 1 (styrene) and monomer 2 (acrylonitrile), respectively, I is the initiator concentration, and u the volumetric monomer addition rate. Other parameters are defined in the Notation.

An application of pseudosteady state approximation to live polymers [26] leads to the following live polymer moment equations:

$$P_1 = \left(\frac{w_1 C_1 \alpha_1 + \frac{\alpha_1 \gamma}{r_1} Q_1 + w_1 (\alpha_1 P + \frac{\alpha_1 \gamma}{r_1} Q)}{(1 - \alpha_1)} \right) \quad (31)$$

$$Q_1 = \left(\frac{w_2 C_2 \alpha_2 + \frac{\alpha_2}{\gamma r_2} P_1 + w_2 (\alpha_2 Q + \frac{\alpha_2}{\gamma r_2} P)}{(1 - \alpha_2)} \right) \quad (32)$$

$$P_2 = \left(\frac{w_1^2 C_1 \alpha_1 + \frac{\alpha_1 \gamma}{r_1} Q_2 + 2w_1 \alpha_1 P_1 + \frac{2w_1 \alpha_1 \gamma}{r_1} Q_1 + w_1^2 (\alpha_1 P + \frac{\alpha_1 \gamma}{r_1} Q)}{(1 - \alpha_1)} \right) \quad (33)$$

$$Q_2 = \left(\frac{w_2^2 C_2 \alpha_2 + \frac{\alpha_2}{\gamma r_2} P_2 + \frac{2w_2 \alpha_2}{\gamma r_2} P_1 + 2w_2 \alpha_2 Q_1 + w_2^2 (\frac{\alpha_2}{\gamma r_2} P + \alpha_2 Q)}{(1 - \alpha_2)} \right) \quad (34)$$

where,

$$C_1 = \frac{(k_{f11}P + k_{f21}Q)M_1}{k_{p11}M_1}$$

$$C_2 = \frac{(k_{f22}Q + k_{f12}P)M_2}{k_{p22}M_2}$$

$$r_1 = \frac{k_{p11}}{k_{p12}} \quad ; \quad r_2 = \frac{k_{p22}}{k_{p21}}$$

$$\gamma = \frac{k_{p21}}{k_{p12}}$$

$$\alpha_1 = \left(\frac{k_{p11}M_1}{[(k_{p11} + k_{f11})M_1 + (k_{p12} + k_{f12})M_2 + (k_{tc11} + k_{td11})P + (k_{tc12} + k_{td12})Q]} \right)$$

$$\alpha_2 = \left(\frac{k_{p22}M_2}{[(k_{p22} + k_{f22})M_2 + (k_{p21} + k_{f21})M_1 + (k_{tc22} + k_{td22})Q + (k_{tc12} + k_{td12})P]} \right)$$

The moment equations for dead polymers are given by

$$\begin{aligned} \frac{d\lambda_0^d}{dt} = & \left(\frac{1}{2}k_{tc11} + k_{td11} \right) P^2 + \left(\frac{1}{2}k_{tc22} + k_{td22} \right) Q^2 + (k_{tc12} + 2k_{td12}) PQ \\ & + (k_{f11}M_1 + k_{f12}M_2)P + (k_{f22}M_2 + k_{f21}M_1)Q - \frac{\lambda_0^d}{V}u \end{aligned} \quad (35)$$

$$\begin{aligned} \frac{d\lambda_1^d}{dt} = & (k_{tc11}P + k_{td11}P + k_{tc12}Q + k_{td12}Q + k_{f11}M_1 + k_{f12}M_2)P_1 \\ & + (k_{tc22}Q + k_{td22}Q + k_{tc12}P + k_{td12}P + k_{f22}M_2 + k_{f21}M_1)Q_1 \\ & - \frac{\lambda_1^d}{V}u \end{aligned} \quad (36)$$

$$\begin{aligned} \frac{d\lambda_2^d}{dt} = & (k_{tc11}P + k_{td11}P + k_{tc12}Q + k_{td12}Q + k_{f11}M_1 + k_{f12}M_2)P_2 \\ & + (k_{tc22}Q + k_{td22}Q + k_{tc12}P + k_{td12}P + k_{f22}M_2 + k_{f21}M_1)Q_2 \\ & + k_{tc11}P_1^2 + k_{tc22}Q_1^2 + 2k_{tc12}P_1Q_1 - \frac{\lambda_2^d}{V}u \end{aligned} \quad (37)$$

The numerical values of kinetic parameters used in the simulations are listed in Table 1. The instantaneous copolymer composition (F_1) is determined by the relative reactivities of monomers (r_1 and r_2) and bulk phase monomer mole fractions (f_1 and f_2) as follows:

$$F_1 = \frac{r_1 f_1^2 + f_1 f_2}{r_1 f_1^2 + 2f_1 f_2 + r_2 f_2^2} \quad (38)$$

or in terms of monomer mole ratio, ϕ ,

$$F_1 = \frac{r_1 \phi^2 + \phi}{r_1 \phi^2 + 2\phi + r_2} \quad (39)$$

The conversion of monomer 1 is defined as follows:

$$x_1 = \frac{V_0 M_{10} + \int_0^t u(t) M_{1f} dt - V M_1(t)}{V_0 M_{10} + \int_0^t u(t) M_{1f} dt} \quad (40)$$

where V_0 is the initial reaction volume, M_{10} the initial monomer concentration in the reactor, M_{1f} the feed monomer concentration, and $u(t)$ the monomer feed rate.

Problem Definition

The first step in the design of the optimal control policy is to specify the objectives, hard constraints and soft constraints. For our problem the objective is to minimize the deviation of copolymer composition and MW from their respective desired values. In other words the objective is to minimize the squared errors for desired copolymer composition and MW during the entire span of reaction time. For this purpose the reactor temperature and the monomer feed rate containing the mixture of monomers, solvent and initiator are selected as control variables. Instead of an actual optimal control which is obtainable by the application of Pontryagin's principle, third order polynomials in time are assumed for both monomer feedrate and reactor temperature profiles. This will result in a suboptimal solution. However, it is our experience that if the order of the polynomials is sufficient, then the obtained performance will be very close to the true optimal. The open loop optimal control profiles will be obtained by control vector parameterization, therefore the design parameters are the coefficients of the polynomials as shown below;

$$u_1(\text{Feedrate}) = a_0 + a_i \sum_{i=1}^3 t^i \quad (41)$$

$$u_2(\text{Temperature}) = b_0 + b_i \sum_{i=1}^3 t^i \quad (42)$$

The batch reactor optimal control problem is considered as a dynamic optimization problem and thus it becomes an infinite dimensional problem. For our purpose this infinite dimensional problem was approximated by a finite dimensional problem, where the entire span of reaction time is divided into mesh type structure with a desired number of mesh points. As the number of mesh points increases, the problem approaches the actual dynamic optimization problem. In our case 20 mesh points have been found satisfactory and used for this purpose. According to this convention, time dependent quantities like MW, copolymer composition, reactor temperature, feedrate, etc. are considered as functional quantities and time dependent objectives and constraints will be defined as functional objective and functional constraints, respectively. Now their values will be considered only at finite number of time instants(mesh points). This allows us to specify the good and bad values of functional objectives and functional constraints at each mesh point corresponding to the desired value of the independent variable(i.e. time). The algorithm will try to satisfy the functional objectives and the functional constraints at each individual mesh point.

In our problem it is desired to maintain specified molecular weight and copolymer composition during the entire span of the reaction. Therefore, they are considered as functional objectives. Also reactor temperature and feedrate are time dependent quantities and so the constraints associated with them were defined as functional constraints. Constraints on operating variables are necessary for safe and reasonable operation of the reactor. Based on the requirements for reaction rate, heat transfer limitations and reactor safety, upper and lower bounds on reactor temperature are defined as constraints. Similarly upper and lower bounds on feed rate are defined as constraints, this is necessary to avoid negative flowrate and to limit the maximum flowrate which can be handled by the reactor system. The type of constraints defined for upper and lower bounds are hard constraints, because if they are violated the design will not have any engineering value. Another hard constraint is defined for the volume of total reactor mass and obviously it should not exceed the designed reactor volume. This quantity is considered only at the final time (at the last mesh point) and so it is not a functional constraint.

In mathematical notations, we can formulate the problem as follows:

Objectives:

$$\min\{f_{1i} = (\phi(i) - \phi_s)^2\}; \quad i = 1, \dots, N \quad (43.a)$$

$$\min\{f_{2i} = (M_N(i) - M_{Ns})^2\}; \quad i = 1, \dots, N \quad (43.b)$$

Hard constraints:

$$0.0 \leq u_{1i} \text{ (feed rate)} \leq 0.07(l/min.) \quad (44.a)$$

$$323 \leq u_{2i} \text{ (temperature)} \leq 368(K) \quad (44.b)$$

$$V_{i=N} \leq 4.0(l) \quad (44.c)$$

where N is the number of mesh points, the subscript i represents the i th mesh point, f_{ki} represents the k th objective at the i th mesh point and ϕ_s and M_{N_s} are the desired monomer mole ratio and the number average molecular weight. The desired value for ϕ_s was selected as 1.0 and the same for M_{N_s} was chosen as 30,000. Where as, u_{ik} represents the k th control at the i th mesh point.

In the case of molecular weight control, the initial deviation from the desired specification is very high. This is because of the fact that at the initial stage of the reaction, MW suddenly rises to the peak value and then tends to decrease with time. Thus the objectives at the initial mesh points will be always the worst. This is not desirable for our problem as the final properties are of more importance than the initial values. To avoid this drawback, two modifications are made in defining the objective for the molecular weight control; (1) a first few initial mesh points are not considered and, (2) different weights are used for the different mesh points.

Finally, the objective function definition is modified to achieve the desired properties in minimum possible time. For this case, objectives for the properties were transformed to soft constraints and the soft constraints for the final conversion and for the volume of final reaction mass are defined as shown below.

Soft constraints:

$$(\phi(i) - \phi_s)^2 = 0.0; \quad i = 1, \dots, N \quad (45.a)$$

$$(M_N(i) - M_{N_s})^2 = 0.0; \quad i = 1, \dots, N \quad (45.b)$$

$$X_{i=N} = 0.75 \quad (45.c)$$

$$3.0(l) \leq V_{i=N} \leq 4.0(l) \quad (45.d)$$

One more design parameter (i.e., final reaction time) is included in the problem definition and all the other hard constraints are kept as before. Here, optimization ends when the point is reached where the scaled value of time can not be improved any further without deteriorating the scaled values of the properties by the same amount.

Synthesis of Optimal Control Policies

The algorithm used in CONSOLE is a method of feasible direction. The basic operation of such method can be described in the following procedure.

Step 1: Initialization.

Step 2: Stop if a certain criterion for the current design parameters is satisfied.

Step 3: Find a search direction such that it is a descent direction for all ϵ -active specifications. A specification is said to be ϵ -active if the sum of its scaled value and ϵ is larger than the scaled values of all specifications. If the search direction is large enough in magnitude, proceed to the next step. Otherwise, reduce ϵ and go to Step 2.

Step 4: Along the search direction, perform a line search such that the maximum of the scaled values of all specifications is sufficiently decreased.

Step 5: Update the design parameters and go to Step 2.

A detailed description of the actual optimization algorithm used is given in [15,25]. Following description in the rest of this section explains how the Pcomb performance chart and other graphical representation of CONSOLE can be used to obtain the desired optimal control policies for semibatch copolymerization process. The complex information that needs to be conveyed to designer requires graphical feedback showing algorithm and problem performance. Figure 1(a) illustrates the displays of initial parameter values in polynomials and the initial performance for the optimization problem of maintaining desired polymer properties (molecular weight and copolymer composition) during the entire span of reaction, when the final time is fixed.

The performance of CONSOLE is displayed as a chart in the lower half of Figure 1(a) and it is called the Pcomb performance comb. This allows a designer using the multiple objective formulation quickly to grasp the performance tradeoffs of a design. Figure 1(a) clearly shows that our initial choice of parameters is unsatisfactory. The interpretation of the Pcomb diagram is as follows:

On the Pcomb display, the first row displays the current iteration number, phase number(I ~ III), the value of ϵ and the worst (largest) scaled value. Second row is the heading. Following that, there is a row associated with each specification and it is identified by both a symbol and its name. For instance, in the third row of the Pcomb display in Figure 1(a), 'FO1' identifies

Design Parameters:

Name	Value	Variation wrt 0	Prev	Iter=0
a1	3.33000e+02	5.0e+00		
a2	1.00000e+01	1.0e+00		
a3	1.00000e-01	1.0e-02		
a4	1.00000e-01	1.0e-02		
b1	2.00000e+01	1.0e+00		
b2	-1.00000e+00	1.0e-01		
b3	-1.00000e-01	1.0e-02		
b4	-1.00000e-02	1.0e-03		

Pcomb (Iter= 0) (Phase 1) (eps= 1.000) (MAX_HARD= 35)

SPECIFICATION	PRESENT	GOOD		G	B		BAD
FO1 (MN-MNs)^2	1.57e+08	0.00e+00	=====			>	2.50e+07
FO2 ($\phi - \phi_s$)^2	4.75e-02	0.00e+00	=====				5.08e-02
C1 final vol	5.91e+00	4.00e+00	-----			>	4.10e+00
FC1 upper flow	2.00e-02	7.00e-02	<--				7.50e-02
FC2 lower flow	1.12e-02	0.00e+00	<-----				-5.00e-03
FC3 upper flow	3.98e+02	3.63e+02	-----			>	3.64e+02
FC4 lower flow	3.33e+02	3.28e+02	*-----				3.23e+02

Figure 1(a) Open loop control of SAN copolymerization reactor, initial design parameters and their performance comb, as displayed by CONSOLE(semibatch nonisothermal reaction with fixed final time, Case:3).

the first functional objective $(M_N - M_{N_s})^2$ (minimization of squared error for desired MW). The number under PRESENT is its current (unscaled) value. Its good and bad values are indicated under GOOD and BAD respectively. When displaying a functional specification, its current, good and bad values are displayed at the independent variable where the specification has the maximal 'scaled' value. The scaled value of the specification is graphically displayed between good value column and bad value column. The position of the tip of each line represents the scaled value. If the scaled value is between -1 and 2, the corresponding tip position is shown in the display window and it is marked by a '*'. Therefore, the tip position lying under the heading G represents the scaled value 0, and similarly, under the heading B stands for the scaled value 1. If the scaled value is less than -1, it is displayed by an arrow towards the left. If the scaled value is more than 2, it is then displayed by an arrow towards the right. For example, in Figure 1(a), the scaled value of 'FO2' is 0.75 and its tip position is about three quarters away from 'G' to 'B'. As 'FC1' and 'FC2' have scaled values less than -1, they are indicated by left-towardsing arrows on the left. Where as, 'C1' and 'FC3' have scaled values more than 2 and are indicated by right-towardsing arrows on the right. Notice that some lines in Figure 1(a) are drawn from the left, where as, some are drawn from right. Lines drawn from the left stand for specifications which are to be minimized or constrained for upper bounds and similar arguments applies to the lines drawn from the right. Notice also that, the line corresponding to 'FO1' and 'FO2' are drawn by characters '=' while others are drawn by '-'. Lines drawn by '=' represent either objectives or soft constraints, and lines drawn by '-' represent hard constraints.

The Pcomb may be output automatically during each optimization iteration or manually after, say, adjusting the good or bad values for a particular objective or constraint. Tradeoffs between competing objectives or constraints are explored by adjusting good and bad values after best or near best performance of the system being designed has been achieved following several iterations of optimization. Basically, after several optimization algorithms have been carried out with a set of good and bad values, the designer displays a performance comb and decides whether the present values of objectives and constraints are satisfying. A designer who is not happy with the present performance can adjust good and/or bad values to reflect these feelings and then resume optimization.

In the example Pcomb shown, it is clear that many of the specifications are definitely not satisfying. The final volume is almost two liters above the target value, the product molecular weight specification is not met, and the temperature limit is not observed.

Plots of the functional specifications are given in Figure 1(b). Figure 1(b) illustrates the graphical representation of two functional objectives and their current values at each mesh point. The plots also represent the *good curve*(desired level) as curve:2 and, the *bad curve* as curve:3. The aim is to keep the constraint curve:1 below curve:2 and curve:3 (in the case of minimizing). It can be observed that for the case of molecular weight the initial eight mesh points are neglected, whereas, for the case of copolymer composition the initial four mesh points are neglected. In both cases one can observe that curve:1 is going away from the *good curve* and for molecular weight it is even going out of the bounds. Not only is the final product far too low and the molecular weight far off-spec, but the control is not even feasible.

After running COSOLVE for 22 iterations, the results obtained are shown in Figures 2(a)-(b). Figure 2(a) shows the Pcomb display for this set of parameters. It can be observed that the performance has been improved significantly for both the objectives and for all the constraints. As shown in Figure 2(b) the property objectives are well within the bound and very close to the *good curves*. This could be taken as a feasible solution or it could be improved further depending upon the requirements of the user.

Results and Discussion

Optimal control policies for several cases were developed using this methodology, the results of optimal control are shown in Figures 3-7. The desired value for copolymer composition (F_1) was selected such that the weight% acrylonitrile in the copolymer is in the range of 25% to 35%, and the desired value of number average molecular weight was chosen as 30,000. Initial reactor volume was 1.0 liter and other initial design parameters were, $f_s = 0.25$ (*mole fraction*), $I_0 = 0.05$ (*mol/lit*), $\phi_s = \phi_0 = 1.0$. Solvent mole fraction and initiator concentration in the feed were the same as their initial values and the monomer mole ratio in the feed, M_1/M_2 , was 1.5.

The first plot in Figure 3 shows the optimal control profile for the reactor temperature when only molecular weight is controlled. Response of MW after the use of the optimal temperature profile is also shown in the same plot. Initial deviation in MW from the desired value is very low and at the end of the reaction the desired value is achieved accurately. It can be observed from the polydispersity plot that control of MW is sufficient to obtain the narrowed molecular weight distribution. However, the second plot showing the copolymer composition proves that when only MW is controlled, the copolymer composition deviates considerably from its desired

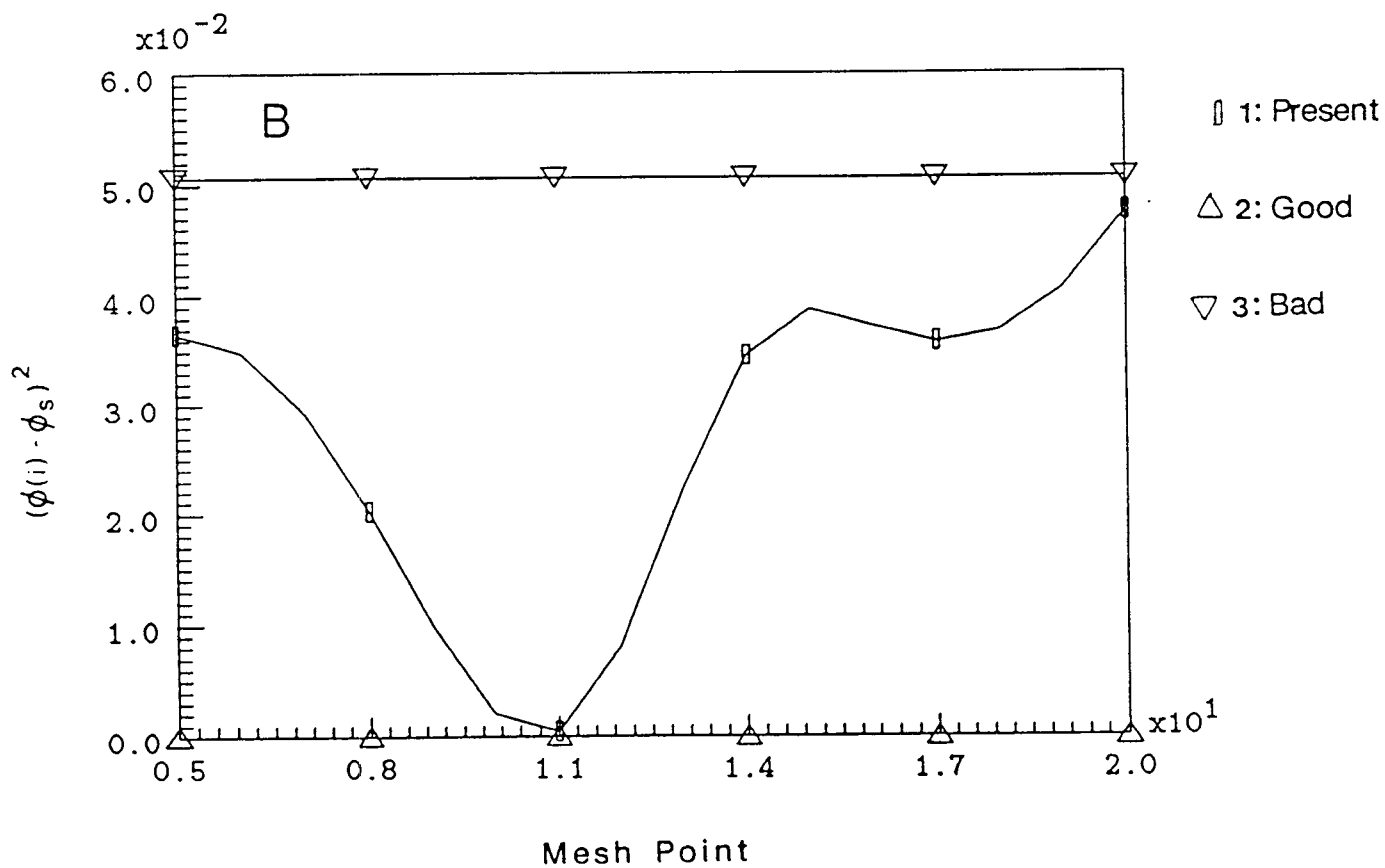
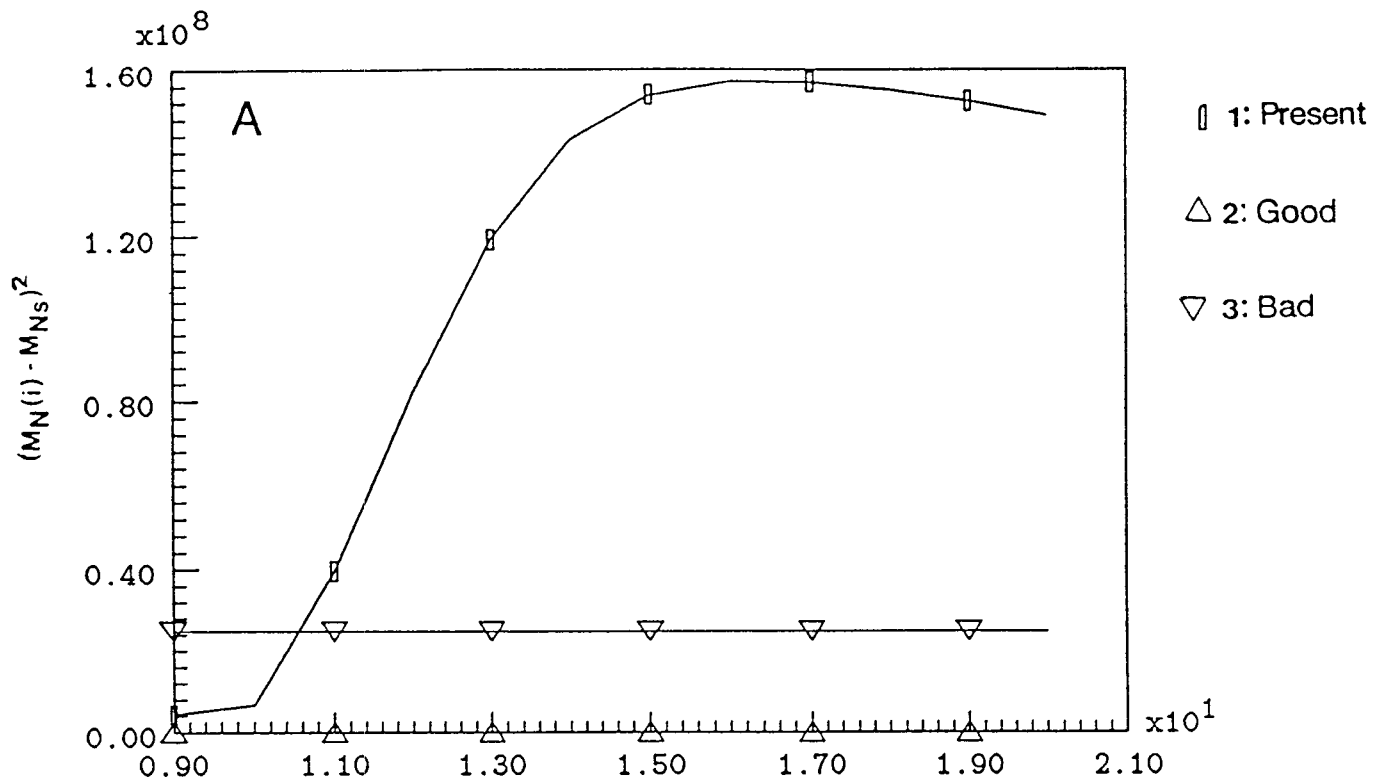


Figure 1(b) Open loop control of SAN copolymerization reactor, performance plots of functional objectives with initial design parameters, as displayed by CONSOLE (Case:3): [A] Molecular Weight; [B] Bulk Phase Composition

Design Parameters:

Name	Value	Variation	wrt 0	Prev	Iter=22
a1	3.53188e+02	5.0e+00	6%	0%	
a2	-3.19240e+00	1.0e+00	-68%	0%	
a3	9.13515e-02	1.0e-02	9%	0%	
a4	5.31340e-02	1.0e-02	47%	0%	
b1	9.69793e+00	1.0e+00	52%	0%	
b2	-3.74885e-01	1.0e-01	63%	0%	
b3	-4.07314e-02	1.0e-02	59%	0%	
b4	-6.40500e-03	1.0e-03	36%	0%	

(Note: 0% change indicates change less than 1% or no change at all)

Pcomb (Iter= 22) (Phase 2) (eps= 6.104E-5) (MAX_COST_SOFT= 0.0766327)

SPECIFICATION	PRESENT	GOOD		G	B	BAD
FO1 (MN-MNs)^2	1.92e+06	0.00e+00	*****			2.50e+07
FO2 ($\phi - \phi_s$)^2	3.88e-03	0.00e+00	*****			5.06e-02
C1 final vol	3.47e+00	4.00e+00	<--			4.10e+00
FC1 upper flow	9.70e-03	7.00e-02	<--			7.50e-02
FC2 lower flow	6.00e-03	0.00e+00	<-----			-5.00e-03
FC3 upper temp	3.53e+02	3.63e+02	<--			3.64e+02
FC4 lower temp	3.45e+02	3.28e+02	<-----			3.23e+02

Figure 2(a) Open loop control of SAN copolymerization reactor, performance plots of functional objectives with initial design parameters, as displayed by CONSOLE, (Case:3)

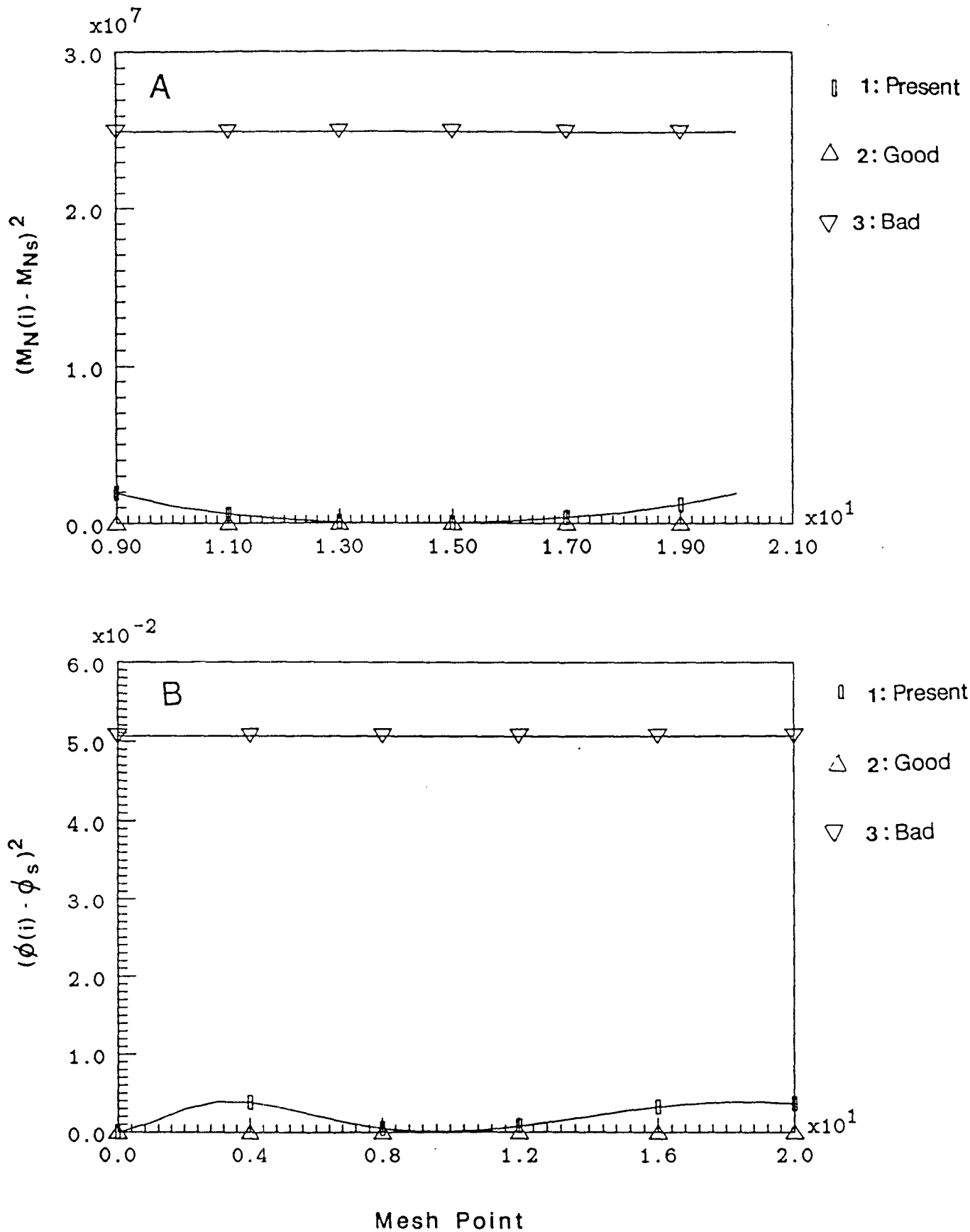


Figure 2(b) Open loop control of SAN copolymerization reactor, performance plots of functional objectives with final design parameters, as displayed by CONSOLE (Case:3): [A] Molecular Weight; [B] Bulk Phase Composition

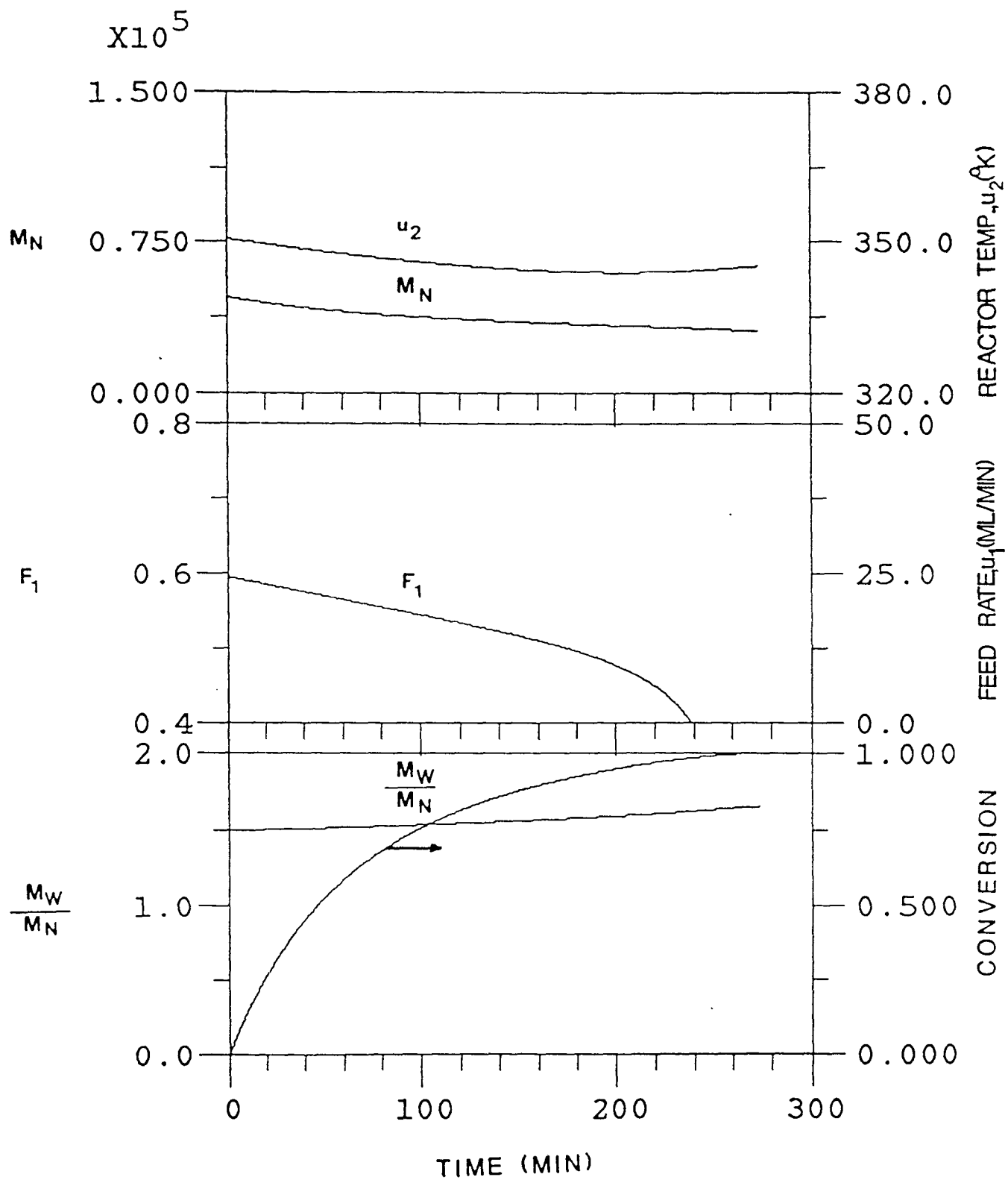


Figure 3 Open loop copolymer molecular weight control in a batch reactor with control profile obtained by the use of CONSOLE (batch nonisothermal reaction with fixed final time, Case:1).

value. Figure 4, illustrates the results of optimal control when only the copolymer composition is controlled. For this case reactor temperature was kept constant at $333.0^{\circ}K$. As shown by the figure, copolymer composition is maintained well at its desired level. Though polydispersity is maintained well, the MW is far away from its desired value and it shows the continuously decreasing trend. Because of low temperature the final monomer conversion achieved is below 50%. The third case, where a combination of two controls was used is shown in Figure 5. Here, MW and copolymer composition were controlled simultaneously. Very good results were achieved for both MW control and copolymer composition control. Copolymer composition is maintained at its desired level through out the reaction, where as, for MW the initial deviation from the desired value is reduced and eventually the desired value is obtained with very little error. Polydispersity remains at a good level and monomer conversion of 80% is achieved. For all the three cases MW and copolymer composition were controlled at several mesh points.

In the next case the aim was set to achieve desired MW and copolymer composition only at the final time, keeping all the other variables same as before. The results obtained are shown in Figure 6. Because of the fact that MW is controlled only at the final time, a very high initial deviation from the desired value is obvious, however, the desired value at the final time is reached very accurately. It can also be observed that though copolymer composition is controlled only at the final time the desired value is maintained throughout the reaction span. This leads to a conclusion that it is important to control MW at an early stage, whereas copolymer composition should be controlled at the final stage of the reaction. Note that very desirable polydispersity and conversion values are obtained.

Finally the commercially important case of minimization of batch polymerization time was studied. Desired MW, copolymer composition, monomer conversion and desired minimum and maximum limit of reaction mass at final time were set as soft constraints and constraints on temperature and flowrate were kept as before. The final time is an additional design parameter and was included in the problem definition and optimization was performed again with the design parameters obtained in Case 4(c.f. Figure 6). The objective was to minimize the reaction time while still maintaining the desired specifications at the final time. The results obtained are illustrated in Figure 7. It can be observed that the path followed by the optimal control profiles is almost same as that followed by the profiles for the Case 4. Note, that the same desired properties are obtained in the shorter reaction span. In the other word, there is no need to continue the reaction for 5 hours, instead the same level of satisfaction for all the objectives and the constraints can be

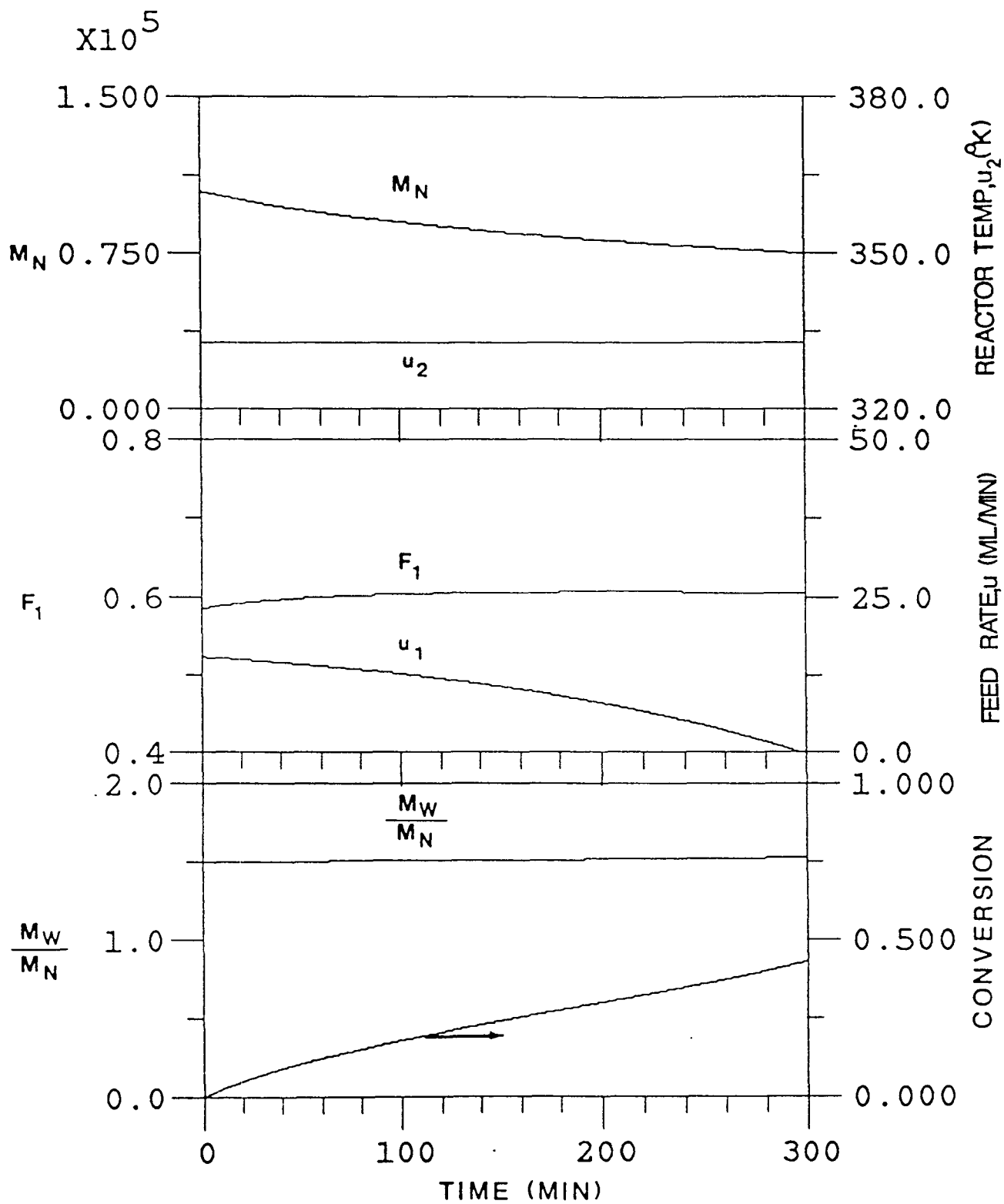


Figure 4 Open loop copolymer composition control in a semibatch reactor with control profile obtained by the use of CONSOLE (semibatch isothermal reaction with fixed final time, Case:2).

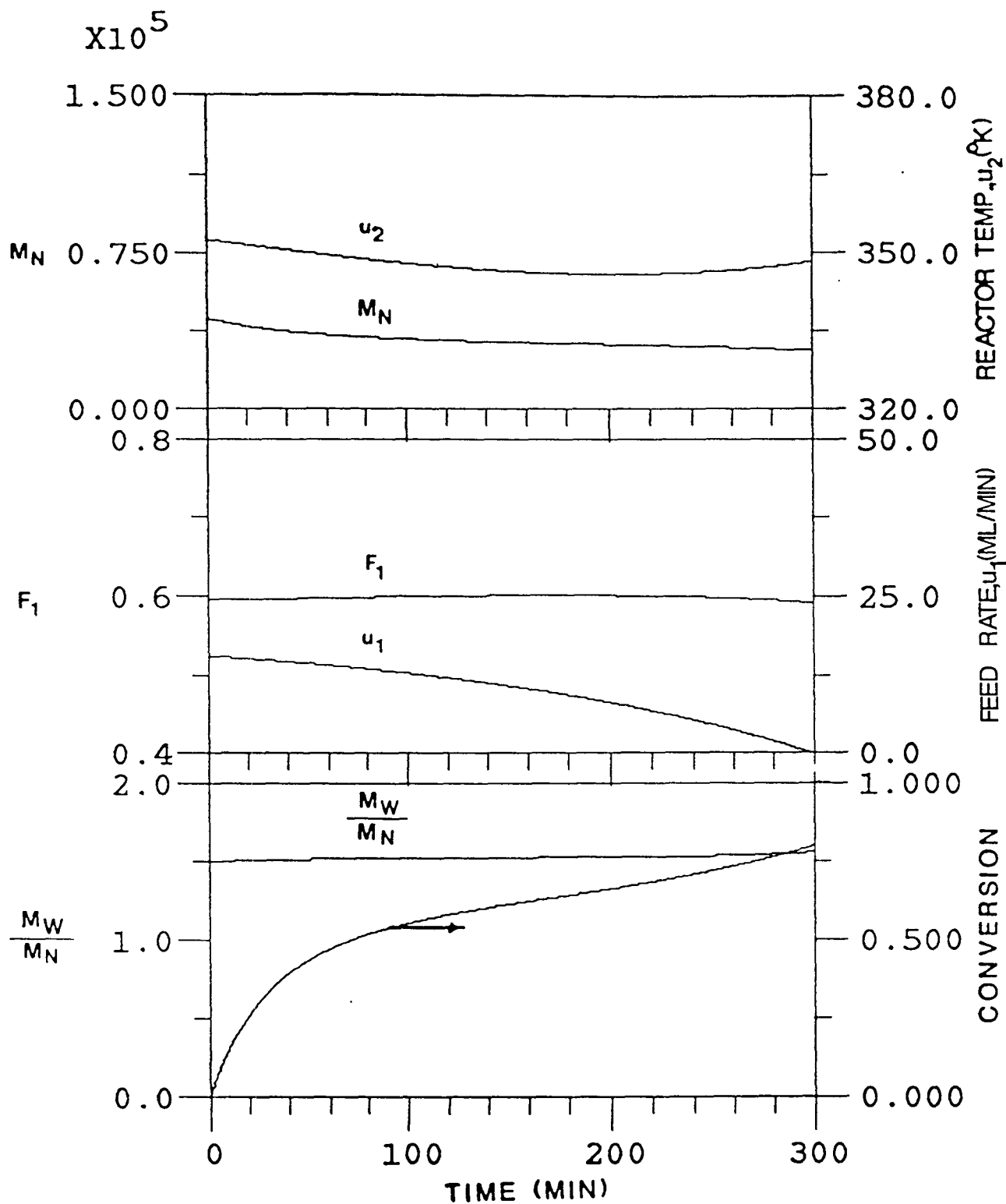


Figure 5 Open loop copolymer composition and molecular weight control in a semi-batch reactor with control profiles obtained by the use of CONSOLE (Case:3).

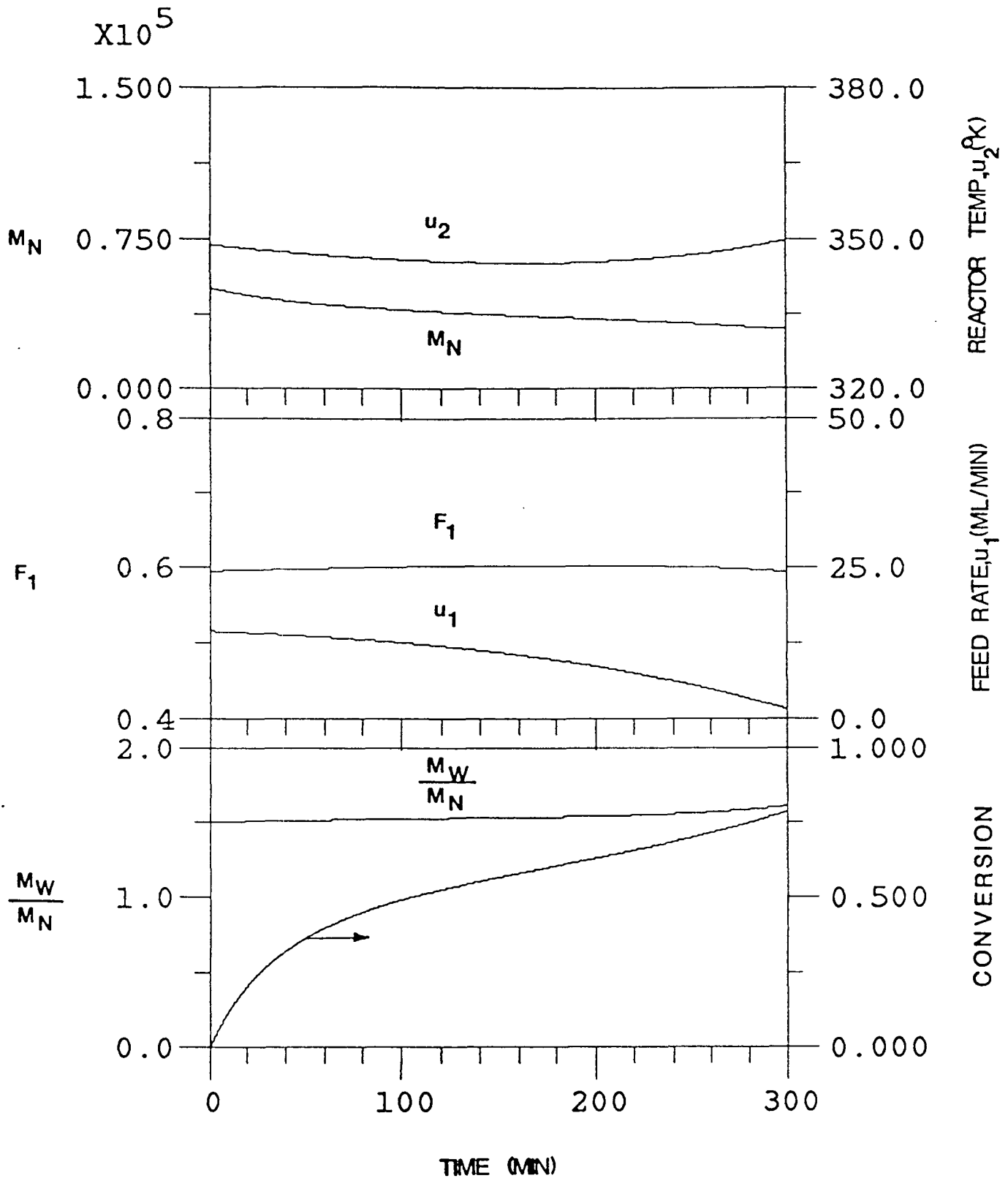


Figure 6 Open loop copolymer composition and molecular weight control at final time in a semibatch reactor with control profiles obtained by the use of CONSOLE (semibatch isothermal reaction with fixed final time and properties control only at the final time, Case:4).

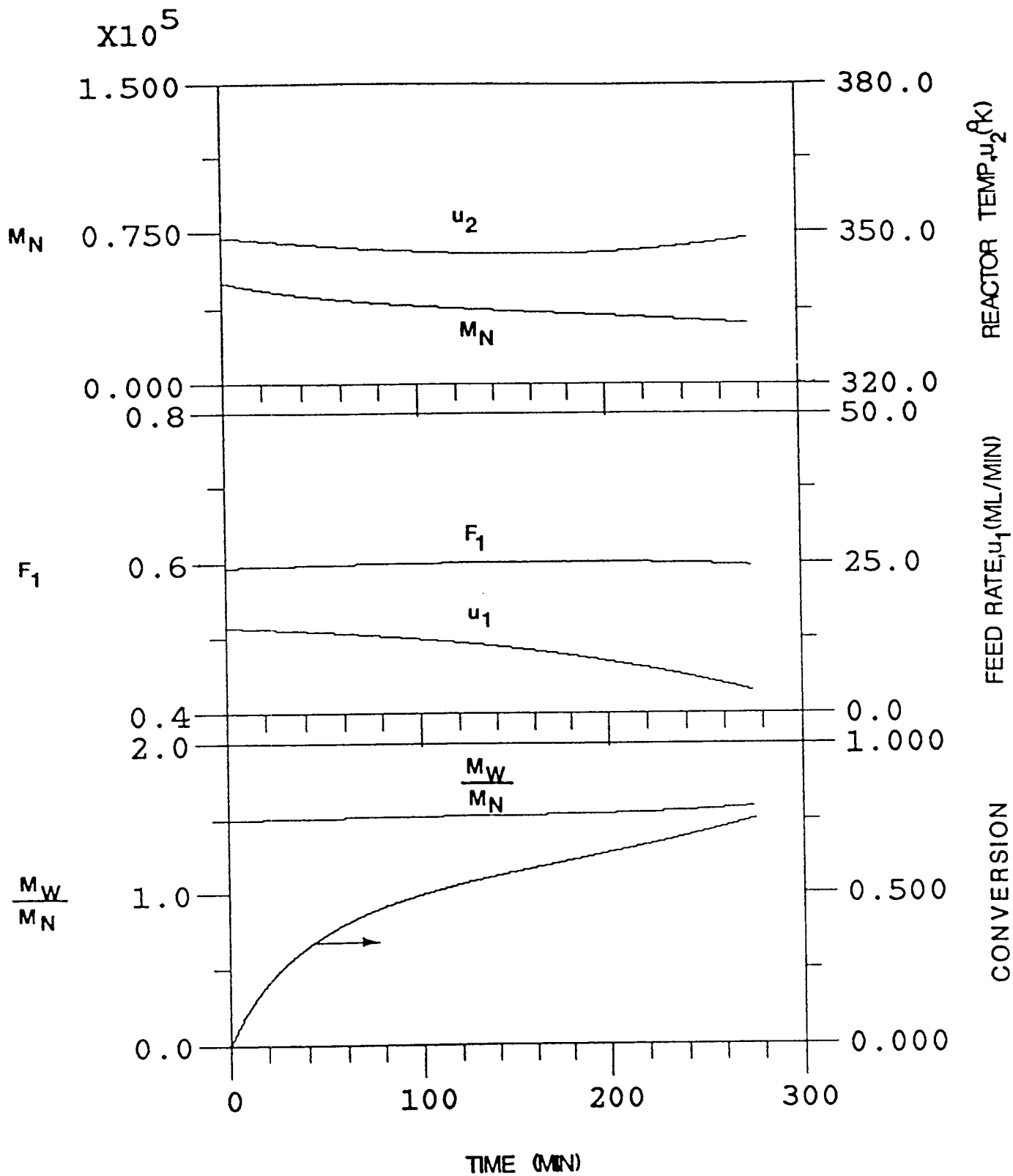


Figure 7 Minimum end time problem for open loop copolymer composition and molecular weight control in a semibatch reactor (semibatch nonisothermal reaction with final time minimization, Case:5).

obtained within 4.58 hours. This indicates that there is no other optimal path which gives the same level of satisfaction for the desired properties and simultaneously minimize the reaction time.

Conclusions

In this paper, we have introduced a user interactive CAD package for optimization, 'CONSOLE', developed at the University of Maryland, to solve the optimal control problem of controlling copolymer composition and molecular weight for semibatch copolymerization reactor. The multivariable dynamic optimization approach is used for this problem, where the control variables are parameterized as third order polynomials in time. The coefficients of these polynomials are considered as the design parameters of the multivariable optimization problem. For our study reactor temperature and feed rate are used as the control variables. The dynamic optimization problem associated with the batch or the semibatch processes is approximated by the use of mesh type structure, where the infinite dimension is reduced to the finite dimension equivalent to the number of mesh points. The time dependent objectives and constraints are defined as functional quantities and their specifications are observed only at the definite number of time instants corresponding to the mesh points. Constraints on the time varying variables and the static variables are also included in the problem definition.

It has been shown that CONSOLE provides a very good approach for resolving the tradeoffs between the competing objectives by introducing the concept of good values and bad values. The criterias of selecting the good values and the bad values are related with the designer's intuition and his knowledge of the problem. The whole concept of objectives, soft constraints, hard constraints and their related good and bad values is easy to understand and provides the platform for design engineers' intuition. One definite advantage gained over the single cost function approach is the elimination of cumbersome process of selecting the weights for the individual objective. Five different cases based on the different objectives are studied. For all the cases, numerical simulations show excellent open loop controls of copolymer composition and molecular weight. The control profiles obtained are easy to implement in any computer control systems. The successful use of this approach for the multivariable dynamic optimization problem such as copolymerization reactor optimization studied in this work opens the door for many other dynamic chemical reactor systems.

Notation

A_c	Heat transfer area per reactor volume ($cm^2/liter$)
C_p	Specific Heat of reaction mixture ($cal/g^\circ K$)
F_i	Mole fraction of i th monomer in copolymer, $i = 1, 2$
f	Initiator efficiency
f_i	Mole fraction of i th monomer in reaction mixture; $i = 1, 2$
h_c	Overall heat transfer coefficient ($cal/cm^2 - sec - ^\circ K$)
I	Initiator concentration in reaction mixture ($mol/liter$)
I_f	Initiator concentration in feed ($mole/liter$)
k_d	Initiator decomposition rate constant (sec^{-1})
k_{fij}	Chain transfer rate constant; $i, j = 1, 2$ ($liter/mole - sec$)
k_{pij}	Propagation rate constant; $i, j = 1, 2$ ($liter/mole - sec$)
k_{tcij}	Combination termination rate constant; $i, j = 1, 2$ ($liter/mole/ - sec$)
k_{tdij}	Disproportionation termination rate constant; $i, j = 1, 2$ ($liter/mole - sec$)
M_i	i th monomer concentration in reaction mixture; $i = 1, 2$ ($mole/liter$)
$M_{i,f}$	i th monomer concentration in feed; $i = 1, 2$ ($mole/liter$)
M_N	Total number average molecular weight
M_{NS}	Desired value of total number average molecular weight
M_W	Total weight average molecular weight
P	Total growing polymer concentration of type-1 ($mole/liter$)
P_i	i th moment of the total number MWD of radicals of type-1
$P_{n,m}$	Concentration of growing polymer containing n units of monomer-1 and m units of monomer-2 ($mole/liter$)
PD	Polydispersity
Q	Total growing polymer concentration of type-2 ($mole/liter$)
Q_i	i th moment of the total number MWD of radicals of type-2
$Q_{n,m}$	Concentration of growing polymer containing n units of monomer-1 and m units of monomer-2 and ending in monomer-2 ($mole/liter$)
R_p	Copolymerization reaction rate ($mole/liter - sec$)
r_{ij}	Monomer reactivity ratio
T	Reactor Temperature ($^\circ K$)
T_c	Jacket media temperature ($^\circ K$)
T_f	Monomer feed temperature ($^\circ K$)

- t Reaction time (*min*)
- u Monomer feed rate (*liter/min*)
- u_i i th manipulated variable; $i = 1$, Feed rate; $i = 2$, Reactor temperature
- V Reactor volume (*liter*)
- w_i Molecular weight of i th monomer; $i = 1, 2$ (*g/mol*)

Greek Letters

- ΔH_r Heat of copolymerization (*cal/mol*)
- λ_k^d k th moment of the dead copolymer total number MWD; $k = 0, 1, 2$
- ρ Density of reaction mixture (*g/liter*)
- ϕ Molar ratio of monomers in reaction mixture
- ϕ_f Monomer mole ration in feed stream
- ϕ_s Desired value of molar ratio of monomers in reaction mixture
- ϕ_t Cross termination factor

References

- [1] G. E. Molau, "Heterogeneous Polymer Systems III. Phase Separation in Styrene- Acrylonitrile Copolymers," *Polymers Letters* 3 (1965), 1007–1015.
- [2] M. J. Pollock, "Modeling and control of Sustained Oscillations in the Continuous Polymerization of Vinyl Acetate," in *Ph.D. Thesis*, McMaster University, .
- [3] A. Guyot, J. Guillot, C. Pichot & L. R. Guerrero, "New Design for Producing Constant Composition Copolymers in Emulsion Polymerization," *ACS Symp. Ser.* (1981).
- [4] M. Alonso, F. Resasens & L. Puigjaner, "Estimation of Copolymer Composition from On-line Headspace Analysis in Batch Emulsion Polymerization," *Chem. Eng. Sci.* 41 (1986), 1039–1044.
- [5] F. J. Shork & W. H. Ray, "On-line measurements of Surface Tension and Density with Applications to Emulsion Polymerization," *J. Appl. Poly. Sci.* 28 (1983), 407.
- [6] J. H. Jo, "Digital Monitoring and Estimation of Polymerization Reactors," in *Ph.D. Thesis*, Northwestern University, Evanston, Ill., 1975.
- [7] J. N. Farber & R. L. Laurence, "The Minimum Time Problem in Batch Radical Polymerization: A Comparison of Two Policies," *Chem. Eng. Commun.* 46 (1986), 347–364.
- [8] G. Z. A. Wu, L. A. Denton & R. L. Laurence, "Batch Polymerization of Styrene - Optimal Temperature Histories," *Poly. Eng. Sci.* 22 (1982), 1–8.
- [9] I. M. Thomas & C. Kiparissides, "Computation of the Near Optimal Temperature and Initiator Policies for a Batch Polymerization Reactors," *Cand. J. Chem. Eng.* 62 (1984), 284–291.
- [10] S. R. Ponnuswamy, "On-line Measurements and Control of a Batch Polymerization Reactor," in *Ph.D. Thesis*, University of Alberta, Edmonton, Alberta, 1984.
- [11] S. Chen & S. Lee, "Minimum End Time Policies for Batchwise Radical Chain Polymerization. Part VI: The Initiator Addition Policies for Copolymerization with Constant Copolymer Composition," *Poly. Eng. Sci.* 27 (1987), 573–581.
- [12] A. Tsoukas, M. Tirrell & G. Stephanopoulos, "Multiobjective Dynamic Optimization of Semi-batch Copolymerization Reactors," *Chem. Eng. Sci.* 37 (1982), 1785–1795.
- [13] Y. Y. Haines, W. A. Hall & H. T. Freedman, *Multiobjective Optimization in Water Resources System*, Elsevier, New York, 1975.
- [14] J. N. Farber, "Steady state Multiobjective Optimization of Continuous Copolymerization Reactors," *Poly. Eng. Sci.* 26 (1986).

- [15] W. T. Nye & A. L. Tits, "An Application-Oriented, Optimization-based Methodology for Interactive Design of Engineering System," *Int. J. Control* 00 (1985), 1-29.
- [16] W. T. Nye, A. Sangiovanni-Vincentelli, J. P. Spoto & A. L. Tits, "DELIGHT.SPICE: An Optimization-Based System for the Design of Integrated Circuits," *Proceedings of the 1983 Custom Integrated Circuits Conference*, Rochester, N.Y. (May 1983).
- [17] J. S. Baras, M. K. H. Fan, W. T. Nye & A. L. Tits, "DELIGHT.LQG: A CAD System for Control System Design Using LQG Controller Structure," *18th Annual Conference on Information Science and Systems*, Princeton, New Jersey (March 1984).
- [18] M. K. H. Fan, W. T. Nye & A. L. Tits, "DELIGHT.MaryLin Users's Guide," in *Technical Report TR-85-9*, Systems Research Center, University of Maryland, College Park, Maryland, 1985.
- [19] M. K. H. Fan, C. D. Walrath, A. L. Tits, W. T. Nye, M. Rimer, R. T. Grant & W. S. Levine, "Two Case studies in Optimization-Based Computer-Aided Design of Control Systems," *Proceedings of the IEEE Control Systems Society 2nd Symposium on Computer-Aided Control System Design (CACSD)*, Santa Barbara, California (March 1985).
- [20] M. K. H. Fan, C. D. Walrath, C. Lee, A. L. Tits, M. Rimer, R. Grant & W. S. Levine, "Design of a Flight Controller for an F14 Aircraft Using the DELIGHT.MaryLin Optimization-Based CACSD System," in *Technical Report TR-85-16*, Systems Research Center, University of Maryland, College Park, Maryland, 1985.
- [21] X. Chen, "Object-Oriented Manipulator Design Exerciser (OOMANEX)," in *Master Thesis, Electrical Engineering Department*, University of Maryland, College Park, Maryland, August 1987.
- [22] L. S. Wang, "Control System Design of a Flexible Arm," in *Master Thesis, Electrical Engineering Department*, University of Maryland, College Park, Maryland, August 1987.
- [23] M. A. Austin, "A Methodology for Incorporating Uncertainties and Multiple Objectives into the Computer-Aided Design of Seismic-Resistant Steel Structures," in *Ph.D. Thesis, Department of Structural Engineering*, University of California, Berkeley, California, 1985.
- [24] M.K.H Fan, L.S. Wang, J. Koninckx & A.L. Tits, "CONSOLE: An CAD Tandem for Optimization-Based Design Interacting with Arbitrary Simulators," University of Maryland, College Park, MD, March, 1987.

- [25] W. T. Nye, "DELIGHT: An Interactive System for Optimization-Based Engineering Design," in *Ph.D. Thesis*, University of California, Berkeley, C.A., June, 1983.
- [26] W. H. Ray & R. L. Laurence, "Polymerization Reaction Engineering," in *Chemical Reactor Theory - Review*, L. Lapidus & N. R. Amundson, eds., Prentice Hall, New York, 1977.
- [27] H. Miyama & S. Fujimoto, "Heat of Copolymerization of Acrylonitrile with Methyl Methacrylate, Styrene and Vinyl acetate," *J. Poly. Sci.* 54 (1961), 532–534.

Figure Captions

- Figure 1(a) Open loop control of SAN copolymerization reactor, initial design parameters and their performance comb, as displayed by CONSOLE (semibatch nonisothermal reaction with fixed final time, Case:3).
- Figure 1(b) Open loop control of SAN copolymerization reactor, performance plots of functional objectives with initial design parameters, as displayed by CONSOLE (Case:3): [A] Molecular Weight; [B] Bulk Phase Composition
- Figure 2(a) Open loop control of SAN copolymerization reactor, final design parameters and their performance comb as displayed by CONSOLE (Case:3).
- Figure 2(b) Open loop control of SAN copolymerization reactor, performance plots of functional objectives with final design parameters, as displayed by CONSOLE (Case:3): [A] Molecular Weight; [B] Bulk Phase Composition
- Figure 3 Open loop copolymer molecular weight control in a batch reactor with control profile obtained by the use of CONSOLE (batch nonisothermal reaction with fixed final time, Case:1).
- Figure 4 Open loop copolymer composition control in a semibatch reactor with control profile obtained by the use of CONSOLE (semibatch isothermal reaction with fixed final time, Case:2).
- Figure 5 Open loop copolymer composition and molecular weight control in a semibatch reactor with control profiles obtained by the use of CONSOLE (Case:3).
- Figure 6 Open loop copolymer composition and molecular weight control at final time in a semibatch reactor with control profiles obtained by the use of CONSOLE (semibatch isothermal reaction with fixed final time and properties control only at the final time, Case:4).
- Figure 7 Minimum end time problem for open loop copolymer composition and molecular weight control in a semibatch reactor (semibatch nonisothermal reaction with final time minimization, Case:5).

