

# Simultaneous Scheduling and Control of Polymer Grade Transition Operations

Antonio Flores T., Sebastian Terrazas  
Universidad Iberoamericana  
Mexico DF, Mexico

and

Ignacio E. Grossmann  
Carnegie Mellon University  
Pittsburgh, PA USA

# Outline

- Introduction
- Objectives
- Problem formulation
- Scheduling formulation
- Optimal Control Formulation
- Case Studies
- Conclusions

# Introduction

- Polymer chemical plants can produce several different products (Grades)
  - Different grades are manufactured by changing processing conditions (i.e. flows, pressure, temperature, etc).
  - A common problem in the polymer industry deals with determining the best product sequence for manufacturing the grades (scheduling).
  - Grade transition operations generates off-specification material that should be minimized by optimal grade transition operations.

# Introduction

- Traditional **Scheduling and Control** problems have been addressed **sequentially**.
  - Scheduling deals with determining optimal assignments, production sequences, inventory levels, etc.
  - Optimal control may deal with determining minimum time optimal transition trajectories.
  - Commonly, in Scheduling formulations process dynamics is neglected.
  - Similarly, in Control formulation normally the production sequence is fixed.
- **Strong interactions between Scheduling and Control.**
- Part of an overall problem: **Planning, Scheduling and Control.**

# Objectives of this work

- To cast the **Simultaneous Scheduling and Control** problem as an optimization problem.
  - Integer variables used to determine the best production sequence.
  - Continuous variables used to determine production times, cycle times and inventory levels.
  - The dynamic profiles of both manipulated and controlled variables are also decision variables.
- The resulting optimization problem is a Mixed-Integer Dynamic Optimization (**MIDO**) problem.
- To solve the MIDO problem, we apply the simultaneous approach (based on collocation) to transform it into a **MINLP**.

# Problem Formulation

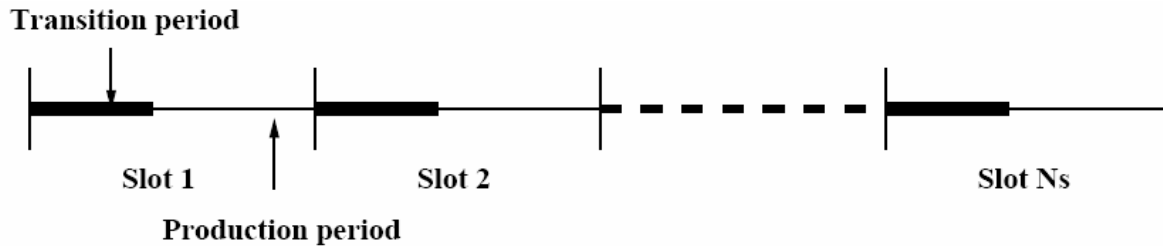
## Given

- A number of products to be manufactured.
- Lower bounds on the product demands.
- Steady-State operating conditions for each product.
- Cost of raw materials, inventory and products.

## Determine:

- **Cyclic scheduling** (i.e. production wheel):
  - Best production sequence, transition times, production times, lengths of processing times, amounts to be manufactured.
- **Control profile for manipulated and controlled variables.**

# Scheduling and Control Formulation



- Optimal cyclic sequence (production wheel PW).

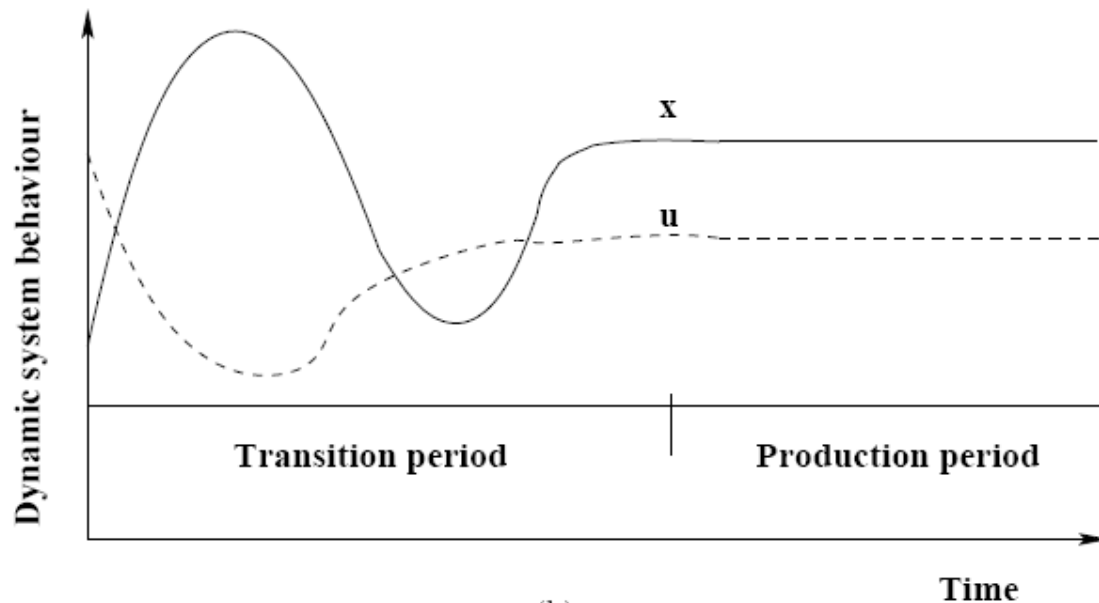
- Time is divided into slots.

- Inside each slot there is transition and production period.

- The number of slots and product transitions are equal.

- Each product is produced only once within each PW.

- When a PW is completed, a new identical cycle begins.



Total process profit: Amount and cost of manufactured product  
- Inventory cost - Transition Cost

- Objective function.

$$\max \left\{ \sum_{i=1}^{N_p} \frac{C_i^p W_i}{T_c} - \sum_{i=1}^{N_p} \frac{C_i^s (G_i - W_i/T_c)}{2\Theta_i} - \sum_{k=1}^{N_s} \sum_{f=1}^{N_{fe}} h_{fck} \sum_{c=1}^{N_{cp}} \frac{C^r t_{fck} \Omega_{c,N_{cp}}}{T_c} \left( (x_{fck}^1 - \bar{x}_k^1)^2 + \dots + (x_{fck}^n - \bar{x}_k^n)^2 + (u_{fck}^1 - \bar{u}_k^1)^2 + \dots + (u_{fck}^m - \bar{u}_k^m)^2 \right) \right\} \quad (1)$$

Transition Cost:  $\frac{1}{T_c} \int_0^{t_f} \left[ \sum_n (x^n - \bar{x}^n)^2 + \sum_m (u^m - \bar{u}^m)^2 \right] C^r dt$

Approximating in terms of Radau quadrature:

$$\sum_{k=1}^{N_s} \sum_{f=1}^{N_{fe}} h_{fck} \sum_{c=1}^{N_{cp}} \frac{C^r t_{fck} \Omega_{c,N_{cp}}}{T_c} \left( (x_{fck}^1 - \bar{x}_k^1)^2 + \dots + (x_{fck}^n - \bar{x}_k^n)^2 + (u_{fck}^1 - \bar{u}_k^1)^2 + \dots + (u_{fck}^m - \bar{u}_k^m)^2 \right)$$

## a) Product assignment

$$\sum_{k=1}^{N_s} y_{ik} = 1, \forall i$$

Any product can only be manufactured once.

$$\sum_{i=1}^{N_p} y_{ik} = 1, \forall k$$

One product at each slot

$$y'_{ik} = y_{i,k-1}, \forall i, k \neq 1$$

Backward binary variable

$$y'_{i,1} = y_{i,N_s}, \forall i$$

Backward binary variable in the first slot

## b) Amounts manufactured

$$W_i \geq D_i T_c, \forall i$$

Total amount manufactured  $\geq$  (Demand)(Production wheel time)

$$W_i = G_i \Theta_i, \forall i$$

Total amount manufactured = (Production rate)(Production time)

$$G_i = F^o(1 - X_i), \forall i$$

Production rate = F(Operating conditions)

## c) Processing times

$$\theta_{ik} \leq \theta^{max} y_{ik}, \forall i, k$$

Upper bound on the time used for manufacturing product  $i$  at slot  $k$

$$\theta_i = \sum_{k=1}^{N_s} \theta_{ik}, \forall i$$

Time for manufacturing product  $i$

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

Duration time of slot  $k$

## d) Transitions between products

$$z_{ipk} \geq y'_{pk} + y_{ik} - 1, \forall i, p, k$$

Binary transition variable:

= 1 -> Transition from product  $i$  to product  $p$

= 0 -> Otherwise

## e) Timing relations

$$\theta_k^t = \sum_{i=1}^{N_p} \sum_{p=1}^{N_p} t_{pi}^t z_{ipk}, \quad \forall k$$

Transition time from product  $i$  to product  $p$  at slot  $k$

$$t_1^s = 0$$

Time at the beginning of the production wheel (first slot)

$$t_k^e = t_k^s + p_k + \sum_{i=1}^{N_p} \sum_{p=1}^{N_p} t_{pi}^t z_{ipk}, \quad \forall k$$

Time at the end of each slot (Processing+Transition times)

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

Starting time for each slot  $k$

$$t_k^e \leq T_c, \quad \forall k$$

End time at each slot  $\leq$  production wheel cyclic time

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

Time values inside each element  $f$  and each collocation point  $c$

## Indices

Products	$i, p = 1, \dots, N_p$
Slots	$k = 1, \dots, N_s$
Finite elements	$f = 1, \dots, N_{fe}$
Collocation points	$c, l = 1, \dots, N_{cp}$
System states	$n = 1, \dots, N_x$
Manipulated variables	$m = 1, \dots, N_u$

## 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
$D_i$	Demand rate [kg/h]
$C_i^p$	Price of products [\$/kg]
$C_i^s$	Cost of inventory [\\$]
$C^r$	Cost of raw material [\\$]
$h_{fk}$	Length of finite element $f$ in slot $k$
$\Omega_{N_{cp}, N_{cp}}$	Matrix of Radau quadrature weights
$\theta^{max}$	Upper bound on processing time
$t_{ip}^t$	Estimated value of the transition time between product $i$ and $p$
$x_{ss,i}^n$	$n$ -th state steady value of product $i$
$u_{ss,i}^m$	$m$ -th manipulated variable value of product $i$
$F^o$	Feed stream volumetric flow rate
$X_i$	Conversion degree
$x_{min}^n, x_{max}^n$	Minimum and maximum value of the state $x^n$
$u_{min}^m, u_{max}^m$	Minimum and maximum value of the manipulated variable $u^m$
$\gamma_{N_{cp}}$	Roots of the Lagrange orthogonal polynomial

## Decision variables

$y_{ik}$	Binary variable to denote if product $i$ is assigned to slot $k$
$y'_{ik}$	Binary auxiliary variable
$z_{ipk}$	Binary variable to denote if product $i$ is followed by product $p$ in 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 value inside each finite element $k$ and for each internal collocation point $c$
$G_i$	Production rate
$T_c$	Total production wheel time [h]
$x_{fck}^n$	$N$ -th system state in finite element $f$ and collocation point $c$ of slot $k$
$u_{fck}^m$	$M$ -th manipulated variable in finite element $f$ and collocation point $c$ of slot $k$
$W_i$	Amount produced of each product [kg]
$\theta_{ik}$	Processing time of product $i$ in slot $k$
$\theta_k^t$	Transition time at slot $k$
$\Theta_i$	Total processing time of product $i$
$x_{o,fk}^n$	$n$ -th 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 slot $k$
$\bar{u}_k^m$	Desired value of the $m$ -th manipulated variable at the end of slot $k$
$x_{in,k}^n$	$n$ -th state value at the beginning of slot $k$
$u_{in,k}^m$	$m$ -th manipulated variable value at the beginning of slot $k$
$X_i$	Conversion

# Simultaneous Approach for solving Carnegie Mellon Dynamic Optimization Problems Problem

$$\min \int_0^{\Theta} \|z(t) - \hat{z}\|^2 dt$$

$$\text{s.t.} \quad \frac{dz(t)}{dt} = F(z(t), u(t), t) \quad z(0) = z^0$$

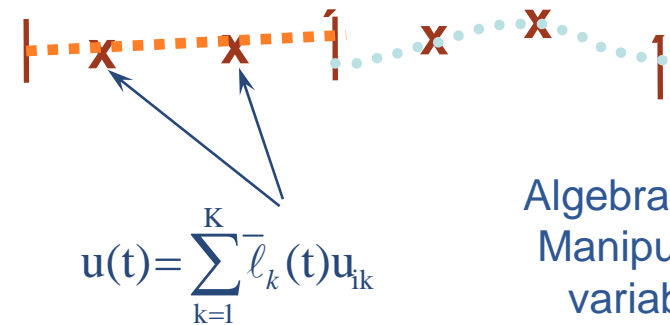
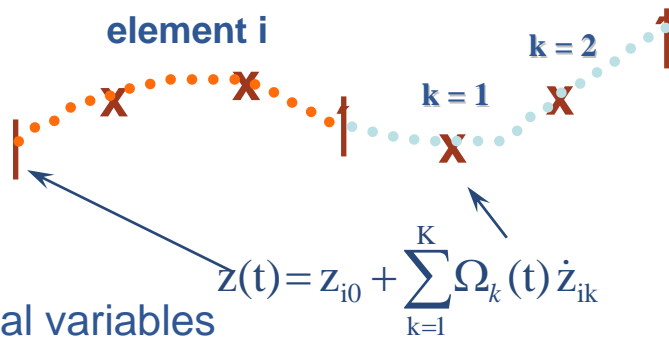
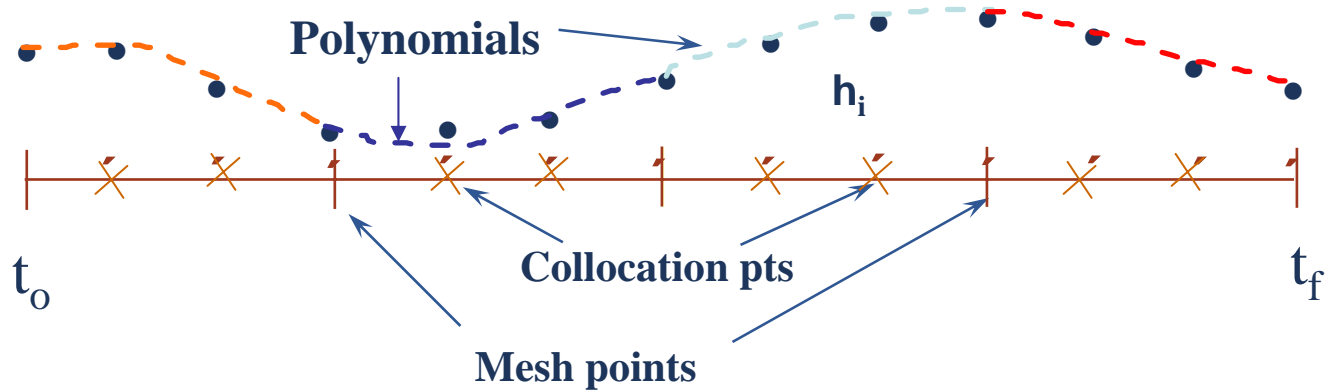
$$z(t) = z_{i-1} + h_i \sum_{q=1}^{ncol} \Omega_q \left( \frac{t - t_{i-1}}{h_i} \right) \frac{dz}{dt}_{i,q}$$

$$z_i = z_{i-1} + h_i \sum_{q=1}^{ncol} \Omega_q \left( \frac{t - t_{i-1}}{h_i} \right) \frac{dz}{dt}_{i,q}$$

$$u(t) = \sum_{q=1}^{ncol} \psi_q \left( \frac{t - t_{i-1}}{h_i} \right) u_{i,q}$$

- Few discrete decisions
- Can exhibit instability due to:
  - Open loop models
  - Choice of control laws
  - Can add stability constraints
- Requires simultaneous approach
  - Large, nonlinear NLP sub-problem
  - NLP expense >> MILP expense

# Simultaneous Formulation Collocation on Finite Elements



Algebraic and  
Manipulated  
variables  
Discontinuous

Differential variables  
Continuous

# Control Formulation

a) Dynamic mathematical model discretization

$$x_{fck}^n = x_{o,fk}^n + \theta_k^t h_{fk} \sum_{l=1}^{N_{cp}} \Omega_{lc} \dot{x}_{flk}^n, \quad \forall n, f, c, k$$

b) Continuity constraint between finite elements

$$x_{o,fk}^n = x_{o,f-1,k}^n + \theta_k^t h_{f-1,k} \sum_{l=1}^{N_{cp}} \Omega_{l,N_{cp}} \dot{x}_{f-1,l,k}^n, \quad \forall n, f \geq 2, k$$

c) Model behavior at each collocation point

$$\dot{x}_{fck}^n = f^n(x_{fck}^1, \dots, x_{fck}^n, u_{fck}^1, \dots, u_{fck}^m), \quad \forall n, f, c, k$$

e) Lower and upper bounds on the decision variables

$$x_{min}^n \leq x_{fck}^n \leq x_{max}^n, \quad \forall n, f, c, k$$

$$u_{min}^m \leq u_{fck}^m \leq u_{max}^m, \quad \forall m, f, c, k$$

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

$$x_{in,1}^n = \sum_{i=1}^{N_p} x_{ss,i}^n y_{i,N_s}, \quad \forall n$$

$$x_{in,k}^n = \sum_{i=1}^{N_p} x_{ss,i}^n y_{i,k-1}, \quad \forall n, k \neq 1$$

$$\bar{x}_k^n = \sum_{i=1}^{N_p} x_{ss,i}^n y_{i,k}, \quad \forall n, k$$

$$u_{in,1}^m = \sum_{i=1}^{N_p} u_{ss,i}^m y_{i,N_s}, \quad \forall m$$

$$u_{in,k}^m = \sum_{i=1}^{N_p} u_{ss,i}^m y_{i,k-1}, \quad \forall m, k \neq 1$$

$$\bar{u}_k^m = \sum_{i=1}^{N_p} u_{ss,i}^m y_{i,k}, \quad \forall m, k$$

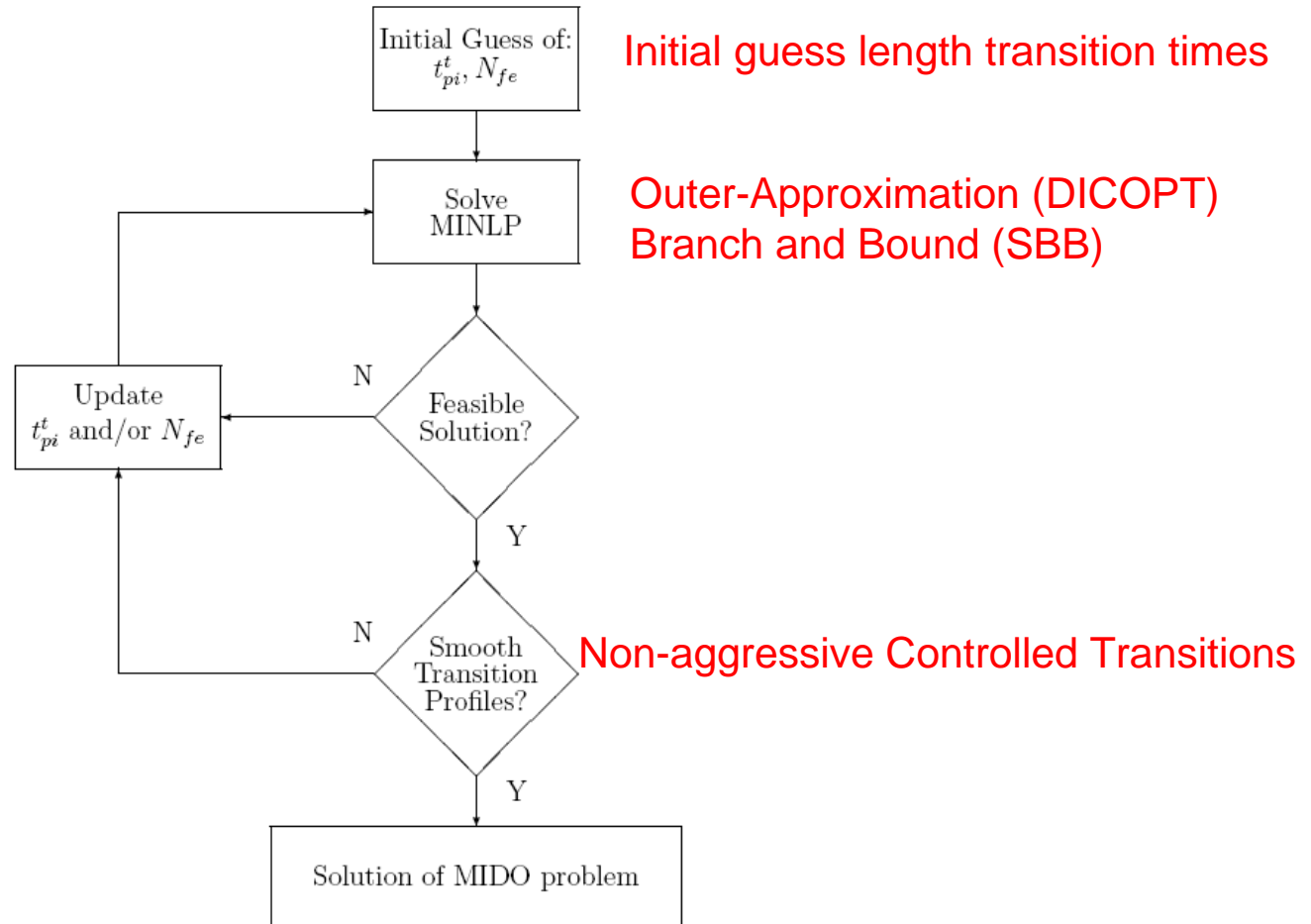
$$u_{1,1,k}^m = u_{in,k}^m, \quad \forall m, k$$

$$u_{N_{fe},N_{cp},k}^m = \bar{u}_{in,k}^m, \quad \forall m, k$$

$$x_{o,1,k}^n = x_{in,k}^n, \quad \forall n, k$$

# Solution Algorithms

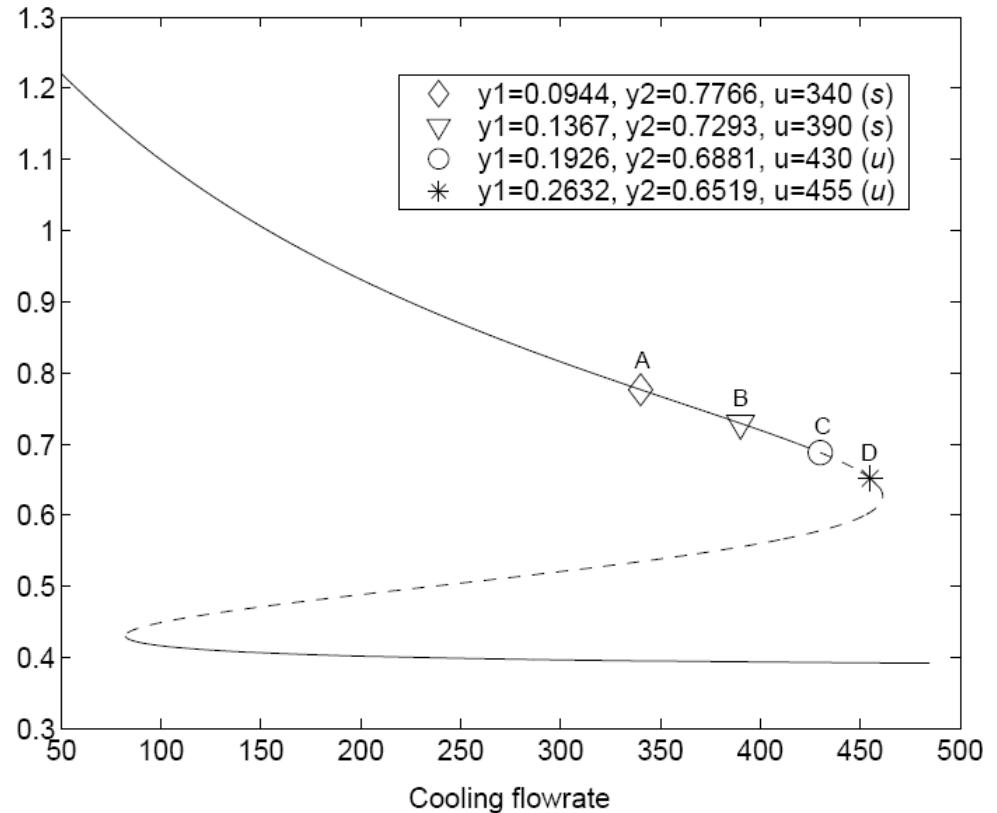
- (1) Direct Method: Transition time is a decision variable.
- (2) Iterative Method: Transition time determined using an iterative approach.



$$\frac{dy_1}{dt} = \frac{1 - y_1}{\theta} - k_{10}e^{-N/y_2}y_1$$

$$\frac{dy_2}{dt} = \frac{y_f - y_2}{\theta} + k_{10}e^{-N/y_2}y_1 - \alpha u(y_2 - y_c)$$

Dimensionless temperature



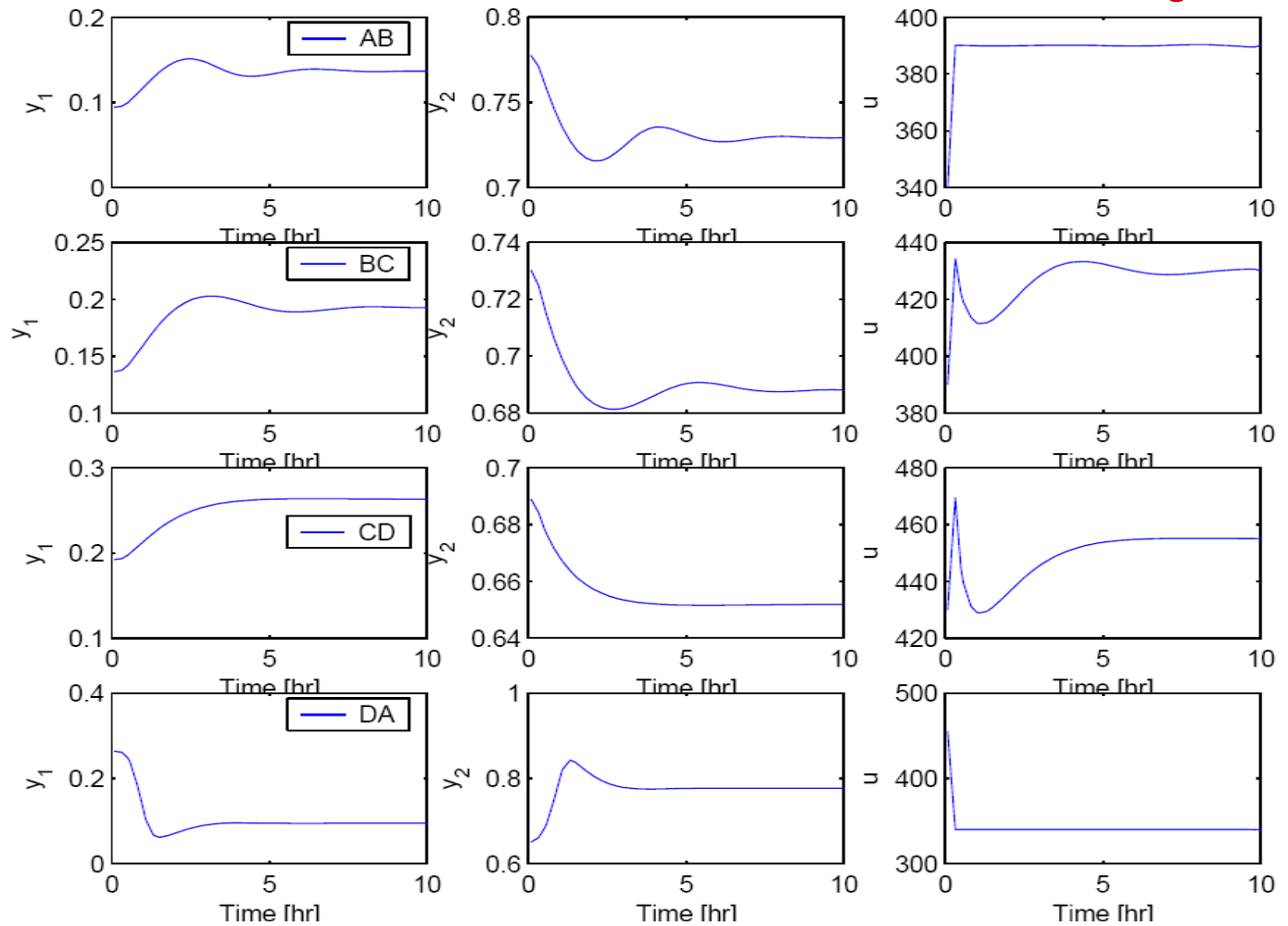
Product	Demand [Kg/h]	Product cost [\$/kg]	Inventory cost [\$]
A	100	100	1
B	200	50	1.3
C	400	30	1.4
D	500	80	1.1

$\theta$	20	Residence time	$T_f$	300	Feed temperature
$J$	100	$(-\Delta H)/(\rho C_p)$	$k_{10}$	300	Preexponential factor
$c_f$	7.6	Feed concentration	$T_c$	290	Coolant temperature
$\alpha$	$1.95 \times 10^{-4}$	Dimensionless heat transfer area	$N$	5	$E_1/(R J c_f)$

Sequence:  
A->B->C->D->

Cost: \$6070

Cycle time: 100.6 hrs



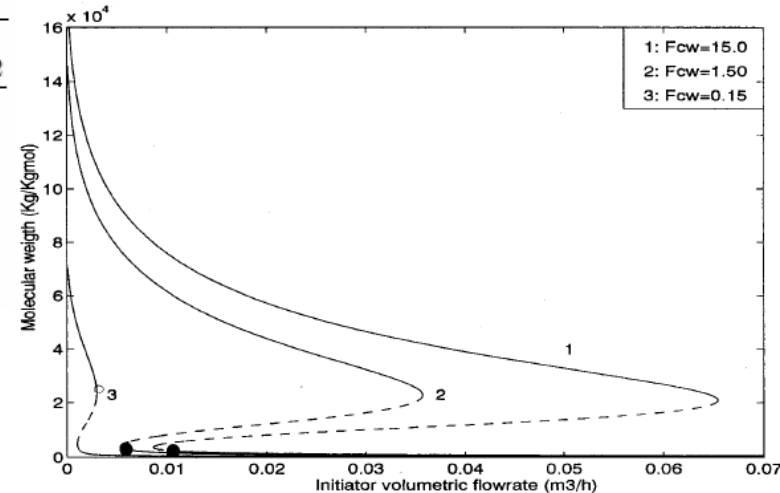
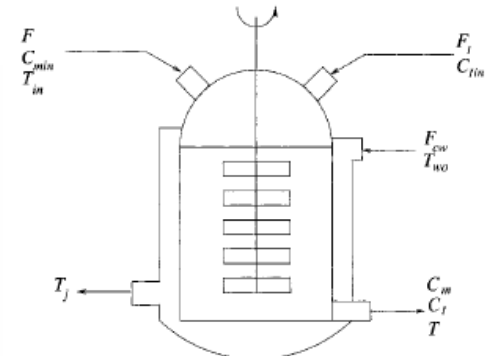
Slot	Product	Process time [h]	Production rate [Kg/h]	$w$ [Kg]	Transition Time [h]	T start [h]	T end [h]
1	A	28.3	559.9	15831.7	10	0	38.3
2	B	13.1	613.6	8044.9	10	38.3	61.4
3	C	13.4	656.1	8748.9	10	61.4	84.8
4	D	5.8	688.3	4022.5	10	84.8	100.6

$$\frac{dx_1}{dt} = -\frac{V}{\hat{Q}_m} (k_p + k_{fm}) x_1 \sqrt{\frac{2f^* k_i \hat{C}_i x_2}{k_{td} + k_{tc}}} + \bar{Q}_m (x_{1in} - x_1)$$

$$\frac{dx_2}{dt} = -\frac{V k_i}{\hat{Q}_m} x_2 + \frac{1}{\hat{Q}_m \hat{C}_i} (\hat{Q}_i \hat{C}_i x_{2in} \bar{Q}_i - \bar{Q}_m \hat{Q}_m \hat{C}_i x_2)$$

$$\frac{dx_3}{dt} = \frac{V(0.5k_{tc} + k_{td})}{\hat{Q}_m \hat{D}_0} \left[ \frac{2f^* k_i \hat{C}_i x_2}{k_{td} + k_{tc}} \right] + \frac{V k_{fm} \hat{C}_m}{\hat{Q}_m \hat{D}_0} x_1 \sqrt{\frac{2f^* k_i \hat{C}_i x_2}{k_{td} + k_{tc}}}$$

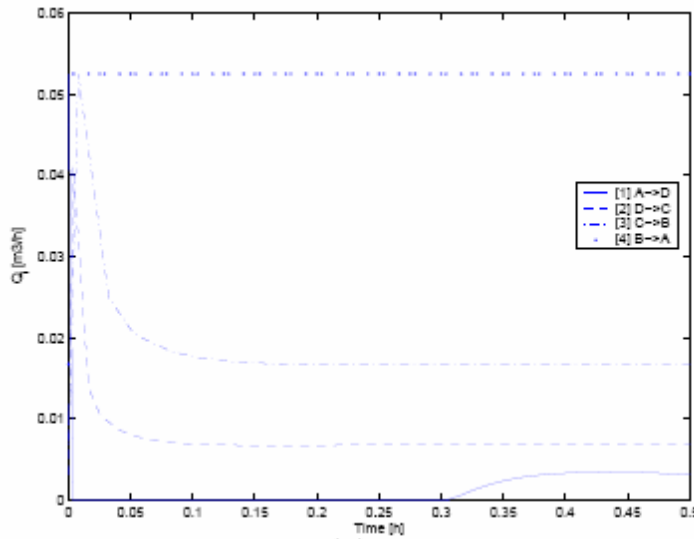
$$\frac{dx_4}{dt} = \frac{V M_m (k_p + k_{fm}) \hat{C}_m}{\hat{Q}_m \hat{D}_1} x_1 \sqrt{\frac{2f^* k_i \hat{C}_i x_2}{k_{td} + k_{tc}}} - \bar{Q}_m x_4;$$



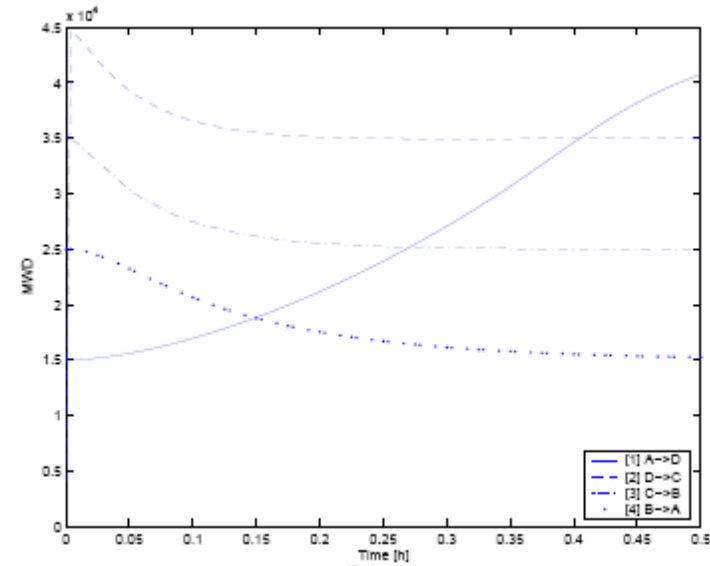
Grade design information. The demand rate is in [kg/h] and the price in [\$/kg].

Grade	$Q_i$	$C_m$	$C_i$	$D_0$	$D_1$	$MWD$	Demand rate	Price
A	0.05245	5.1788	0.4153	0.0055	82.2185	15000	0.8	10
B	0.01673	5.5068	0.1325	0.0020	49.3761	25000	0.7	12
C	0.006863	5.6745	0.0543	0.0009	32.5877	35000	1	13
D	0.003114	5.7768	0.0247	0.0005	22.3467	45000	0.8	15

## Dynamic Transitions Profiles



(a)



(b)

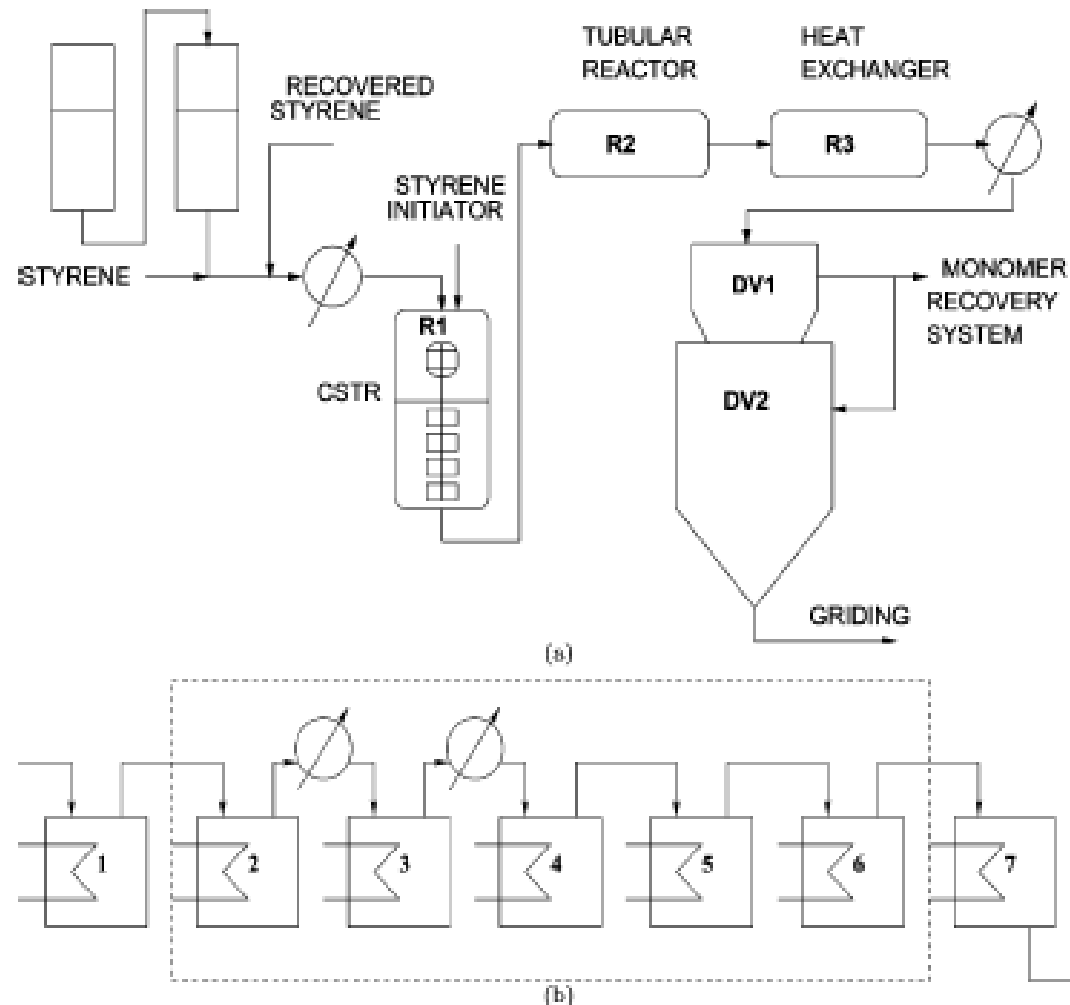
Sequence: A->D->C->B->

Cycle time: 400 hrs

Simultaneous scheduling and control results for grade transition in a MMA polymerization CSTR. The objective function value is \$ 54 and 400 h of total cycle time.

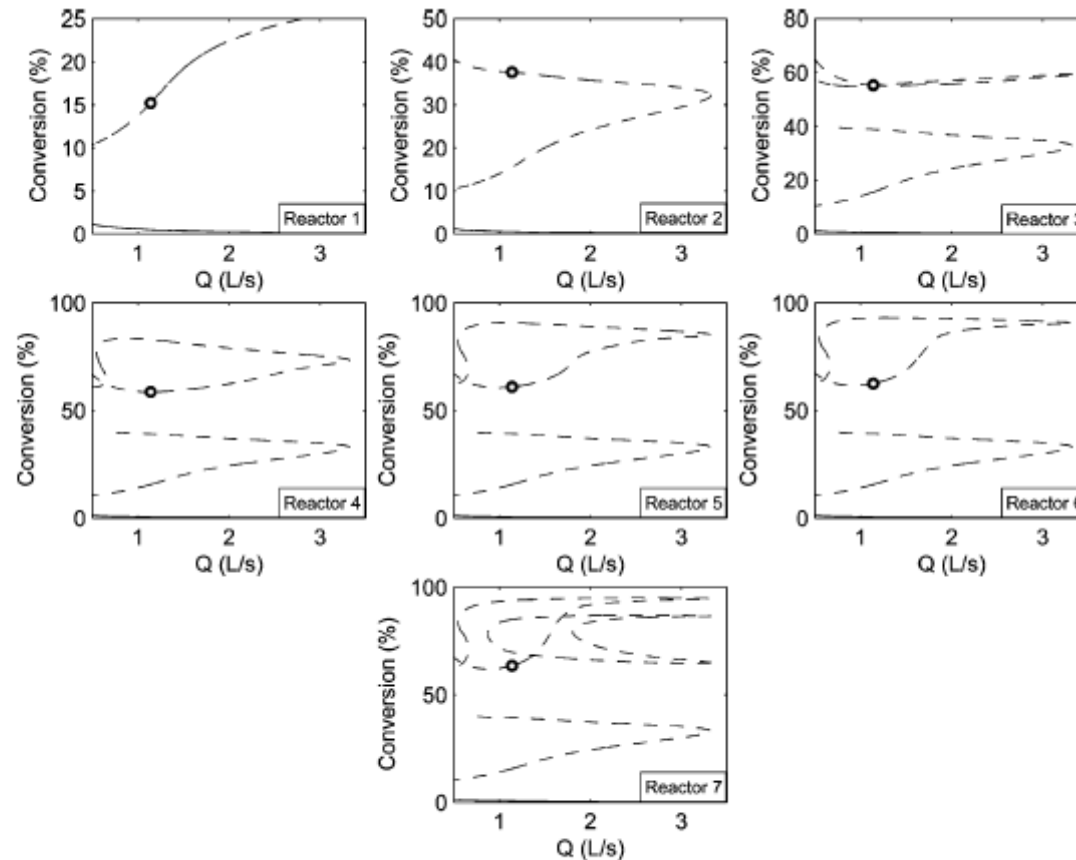
Slot	Product	Process time [h]	Production rate [Kg/h]	$w$ [Kg]	Transition Time [h]	T start [h]	T end [h]
1	A	80	4	320	5	0	85
2	D	100	5	500	5	85	190
3	C	100	4	400	10	190	300
4	B	95	5	475	5	300	400

# High-Impact Polystyrene Process Flowsheet



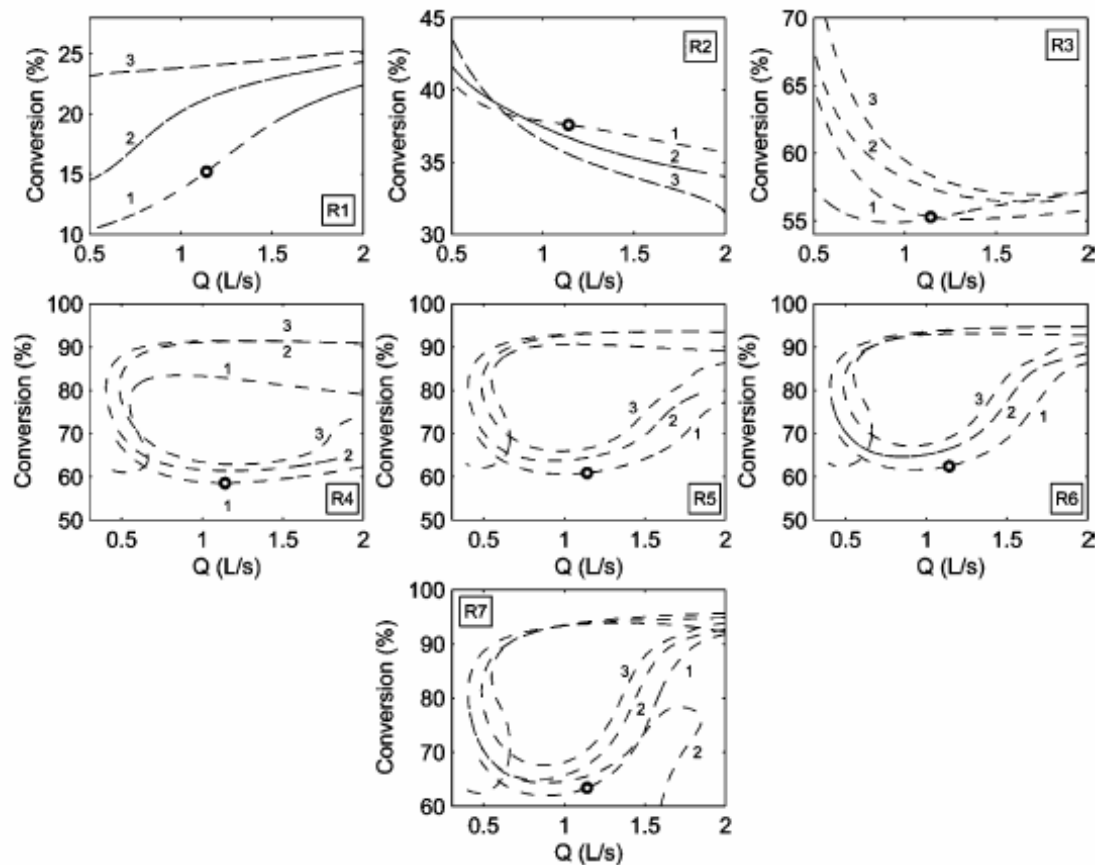
**Figure 1.** (a) Flowsheet of the HIPS plant and (b) approximation of the HIPS plant by a set of seven series-connected CSTRs. The dashed box stands for the five CSTRs employed for approximating the steady-state behavior of the R2 tubular reactor.

# Nonlinear Bifurcation Behaviour-1



**Figure 2.** Monomer conversion bifurcation diagram using the monomer flow rate ( $Q$ ) as the main continuation parameter. The “O” symbol stands for the nominal steady state. The continuous and dashed lines represent open-loop stable and unstable steady states, respectively.

# Nonlinear Bifurcation Behaviour-2



**Figure 3.** Monomer conversion bifurcation diagram using the monomer flow rate ( $Q$ ) as the main continuation parameter and the initiator flow rate ( $Q_i$ ) as the secondary continuation parameter. 1,  $Q_i = 15 \times 10^{-4}$  L/s; 2,  $Q_i = 7.5 \times 10^{-4}$  L/s; and 3,  $Q_i = 3 \times 10^{-4}$  L/s.

# Isothermal HIPS Polymerization in a CSTR

$$\frac{dx_1}{dt} = \frac{Q_{imax}x_{1o}u_i - Q_{max}x_1u_f}{V} - k_d x_1$$

$$\frac{dx_2}{dt} = Q_{max}u_f \frac{x_{2o} - x_2}{V} - k_p x_2 (\mu_{rmax}^r x_6 + \mu_{bmax}^0 x_7)$$

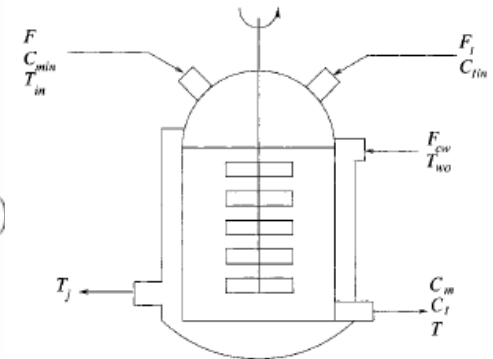
$$\frac{dx_3}{dt} = Q_{max}u_f \frac{x_{3o} - x_3}{V} - x_3 (k_{I2} C_{rmax} x_4 + k_{fs} \mu_{rmax}^0 x_6 + k_{fb} \mu_{bmax}^0 x_7)$$

$$\frac{dx_4}{dt} = 2f_a \frac{k_d C_{imax} x_1}{C_{rmax}} - x_4 (k_{I1} C_{mmax} x_2 + k_{I2} C_{bmax} x_3)$$

$$\frac{dx_5}{dt} = \frac{C_{bmax} x_3}{C_{brmax}} (k_{I2} C_{rmax} x_4 + k_{fb} (\mu_{rmax}^0 x_6 + \mu_{bmax}^0 x_7)) - x_5 (k_{I3} C_{mmax} x_2 + k_t (\mu_{rmax}^0 x_6 + \mu_{bmax}^0 x_7 + C_{bmax} x_5))$$

$$\frac{dx_6}{dt} = \frac{2k_{I0} (C_{mmax} x_2)^2 + k_{I1} C_{rmax} x_4 C_{mmax} x_2 + C_{mmax} x_2 k_{fs} \mu_{rmax}^0 x_6 \mu_{bmax}^0 x_7}{\mu_{rmax}^0} - (k_p C_{mmax} x_2 + k_t (\mu_{rmax}^0 x_6 + \mu_{bmax}^0 x_7 + C_{brmax} x_5) + k_{fs} C_{mmax} x_2 + k_{fb} C_{bmax} x_3) x_6 + k_p C_{mmax} x_2 x_6$$

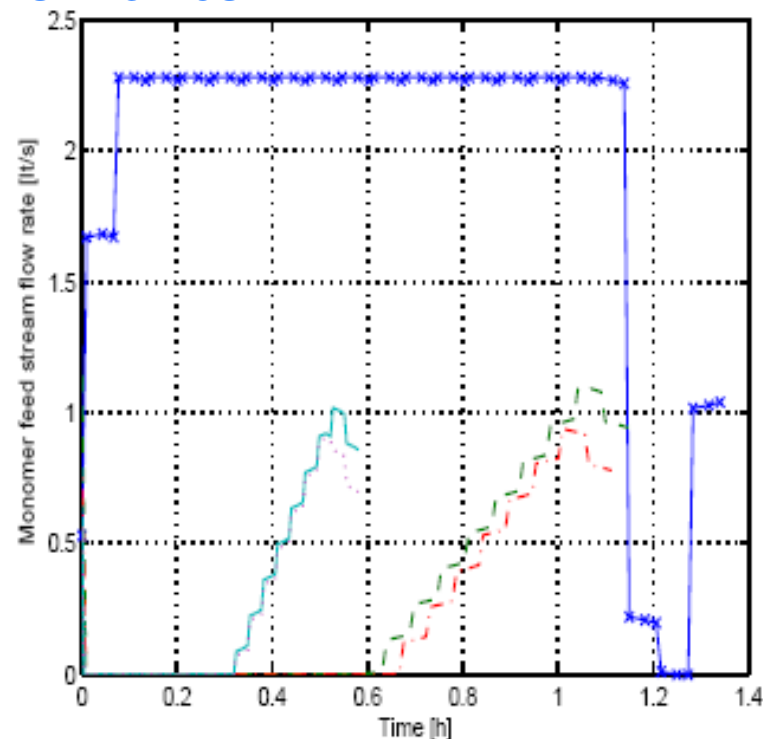
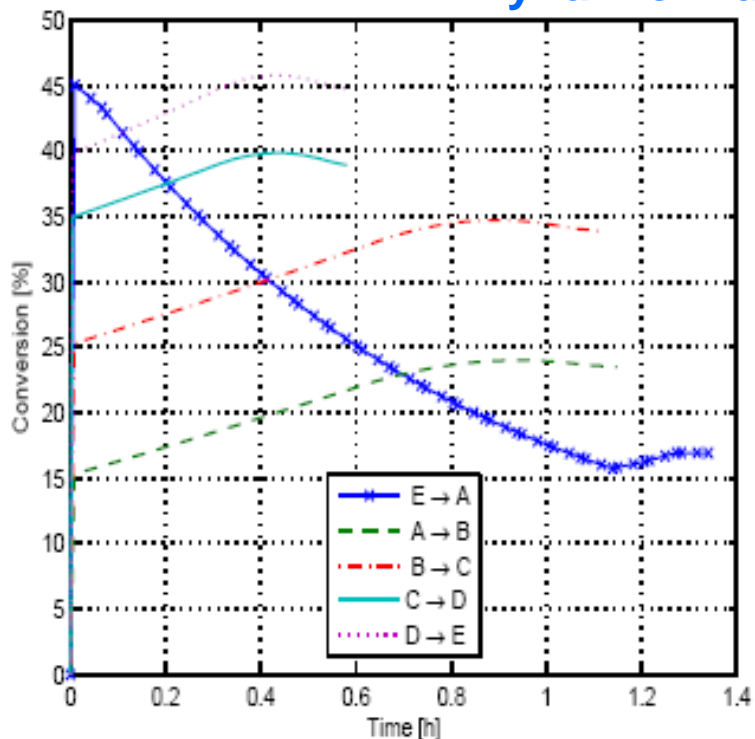
$$\frac{dx_7}{dt} = \frac{k_{I3} C_{brmax} C_{mmax} x_5 x_2}{\mu_{bmax}^0} - (k_p C_{mmax} x_2 + k_t (\mu_{rmax}^0 x_6 + \mu_{bmax}^0 x_7 + C_{brmax} x_5) + k_{fs} C_{mmax} x_2 k_{fb} C_{bmax} x_3) x_7 + k_p C_{mmax} x_2 x_7$$



Grade	Q[l/s]	Conv.	Demand (kg/hr)	Inv. Cost	Monomer Cost	Initiator Cost	Price
A	1.14	15	50	0.15	1	10	3.2
B	0.75	25	60	0.20	1	10	4.3
C	0.56	35	65	0.15	1	10	4.5
D	0.60	40	70	0.10	1	10	5.0
E	0.53	45	60	0.25	1	10	5.5

# Simultaneous Scheduling and Control Results

## Dynamic Transitions Profiles



Sequence: E → A → B → C → D

Profit: \$1456/h, Cycle time: 32.3 hrs

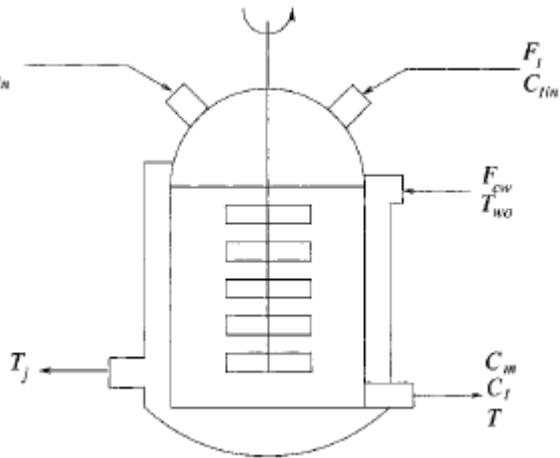
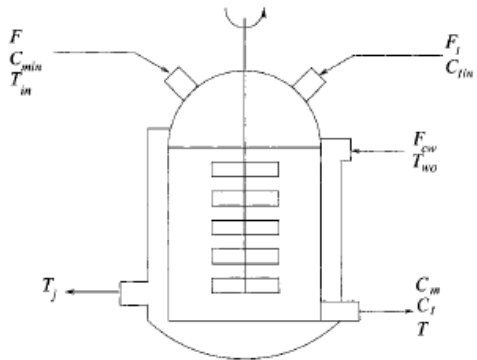
Product	Process T [h]	production [kg]	Trans T [h]	T start[h]	T end [h]
<i>E</i>	2.48	1937	1.34	0	3.83
<i>A</i>	2.87	1614	1.15	3.83	7.85
<i>B</i>	3.17	1937	1.11	7.85	12.14
<i>C</i>	3.10	2099	0.58	12.14	15.82
<i>D</i>	15.81	11370	0.67	15.82	32.29

# Conclusions

- Solving the Scheduling and Control problem sequentially, rather than simultaneously, can lead to **suboptimal solutions**.
- We have proposed a **simultaneous scheduling and control optimization formulation**.
  - A dynamic process model was used to remove the constant transition time assumption
  - The solution of the underlying MIDO problem turned out to be computationally intensive as process nonlinearities increased.
- Future work is aimed at using **MINLP decomposition techniques** for addressing larger scale and complex dynamic systems.

# Additional Future Work

## Parallel Plants



- Scheduling, Control, Grade Design
- Batch Processes
- Handling Uncertainty
- Real Time Formulation
- Planning, Scheduling, Control