Integration of Scheduling and Control Operations

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Outline

Introduction

- Enterprise Wide Optimization (EWO) deals with the optimization of supply, manufacturing and distribution activities so to reduce costs and inventories
- At the manufacturing level EWO considers planning, scheduling and control operations
- EWO activities are at the interface between Chemical Engineering and Operations Research
- Nonlinear mathematical models are commonly used in manufacturing operations

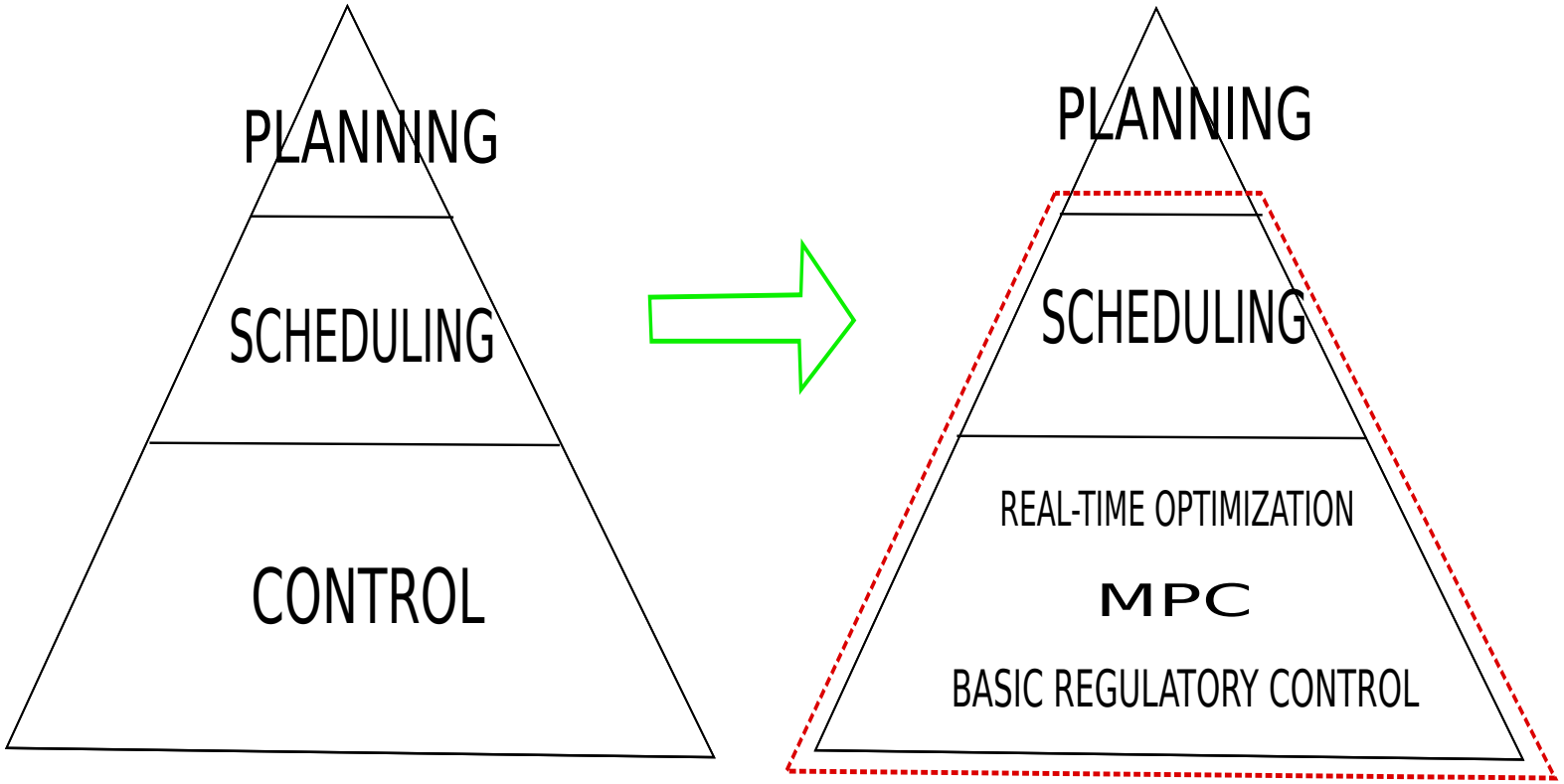
Introduction

Quoting Shobrys and White [1]:

- Planning: Defines desired changes to current business affecting access to raw material, production/distribution capacity, long term objectives
- Scheduling: Deals with the timing and volume of certain operations (i.e. start time, unit to be used,processing time, production level), medium term objectives
- Control: Rejection of upsets, tracking of signals to meet certain quality and production goals, short term objectives

[1] "Planning, scheduling and control systems: why cannot they work together", Donald E. Shobrys, Douglas C. White, Comput.Chem.Eng. 26 (2002) 149160

Introduction



Introduction

- Two main approaches have been used for dealing with Scheduling and Control problems
- The first one formulates the problem as a Mixed-Integer Dynamic Optimization (MIDO) problem
- MIDO problems can also incorporate logic decisions to switch among different conditions
- The second one uses agents (i.e. heuristics) to model optimal system behavior
- Published SC problems include polymerization reactors, water treatment plants, distillation columns and tubular reactors

Aims of this Talk

In this work, we propose a simultaneous approach to address scheduling and control problems for a set of continuous plants. We take advantage of the rich knowledge of scheduling and optimal control formulations, and we merge them so the final result is a formulation able to solve simultaneous scheduling and control problems.
We cast the problem as an optimization problem. In the proposed formulation:

- Integer variables are used to determine the best production sequence
- Continuous variables take into account production times, cycle time, and inventories

Because dynamic profiles of both manipulated and controlled variables are also decision variables, the resulting problem is cast as a mixed-integer dynamic optimization (MIDO) problem.

Problem Definition

Given are:

- A number of products to be manufactured in a single CSTR
- Lower bounds for the product demands
- Steady-state operating conditions for each desired product
- Cost of each product
- Inventory and raw materials costs

The problem consists in:

> *Simultaneous determination of a cyclic schedule (i.e. production wheel) and the control profile such that a given cost function is minimized*

Major decisions involve:

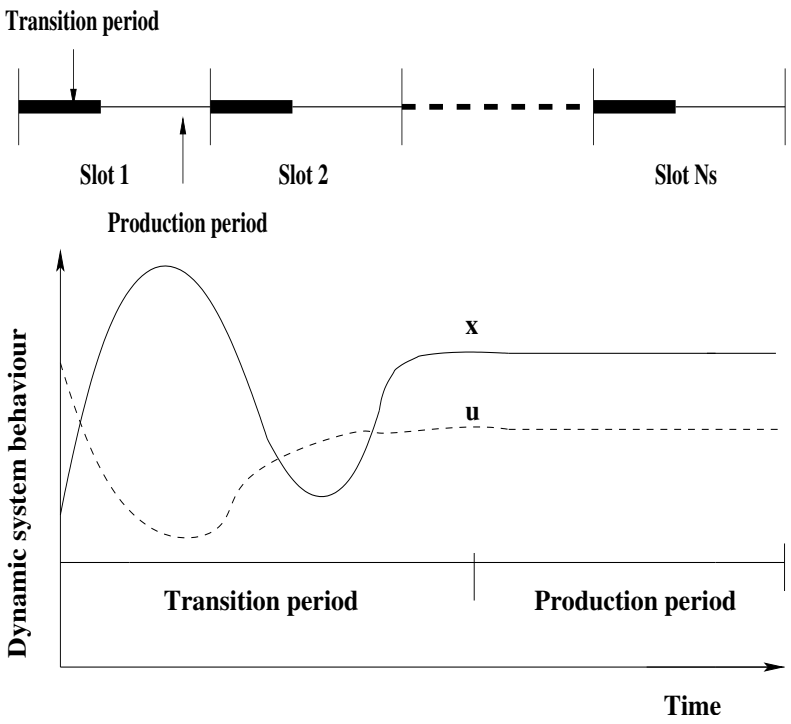
- Selecting the cyclic time and Sequence in which the products will be manufactured
- The transition times, Production rates, Length of processing times
- Amounts manufactured of each product
- Manipulated variables profiles for the transition

Problem Assumptions

- All products are manufactured in a single continuous reactor
- Products sequence follows a production wheel
- Cyclic time is divided into a series of slots

Two operations occur inside each slot:

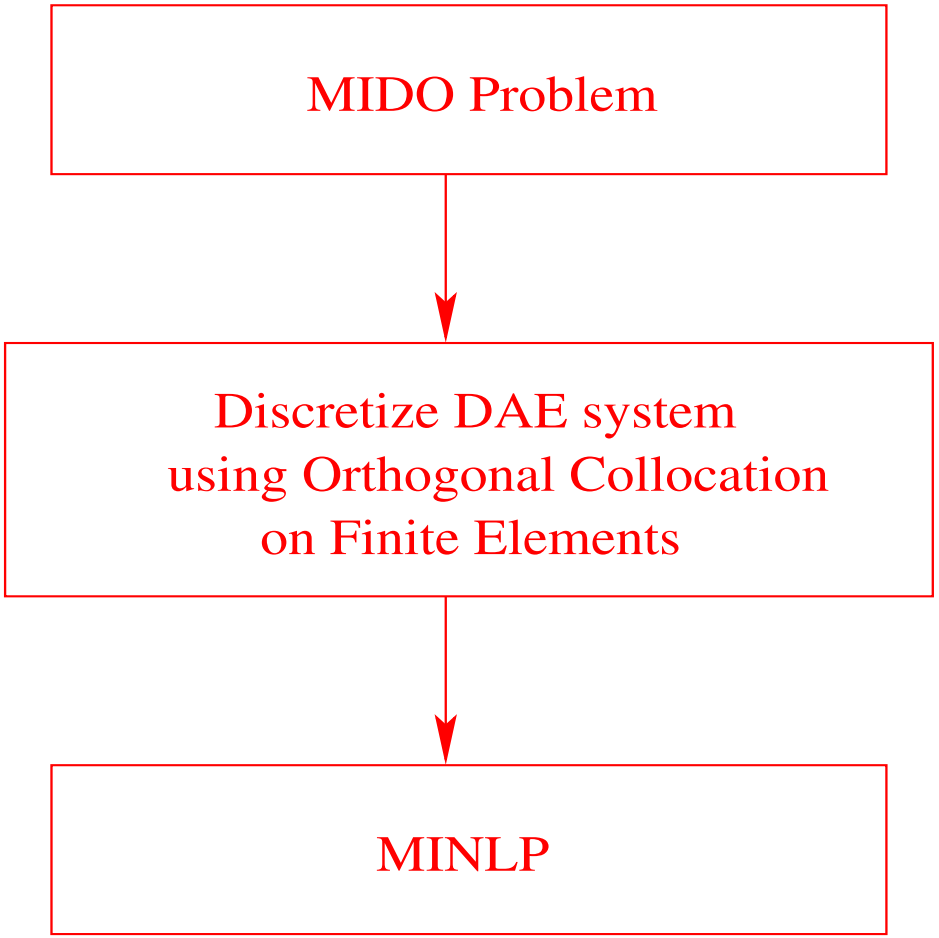
- Transition period: dynamic transitions between two products take place
- Production period: a given product is manufactured around steady-state conditions



Mixed-Integer Dynamic Optimization Approach

- Binary variables: Production sequence (i.e. slot product assignment)
- Continuous variables: Processing times, Transition times, Amounts manufactured
- Dynamic behaviour: During product transitions a dynamic model is used
- Mixed-Integer Dynamic Optimization is the natural algorithmic tool for SC problems
- Advantages: nonlinear behaviour, reliable MINLP solvers
- Disadvantages: MIDO problems are hard to solve, only medium size/small problems, off-line control policies, no uncertainties

Solving Mixed-Integer Dynamic Optimization Problems

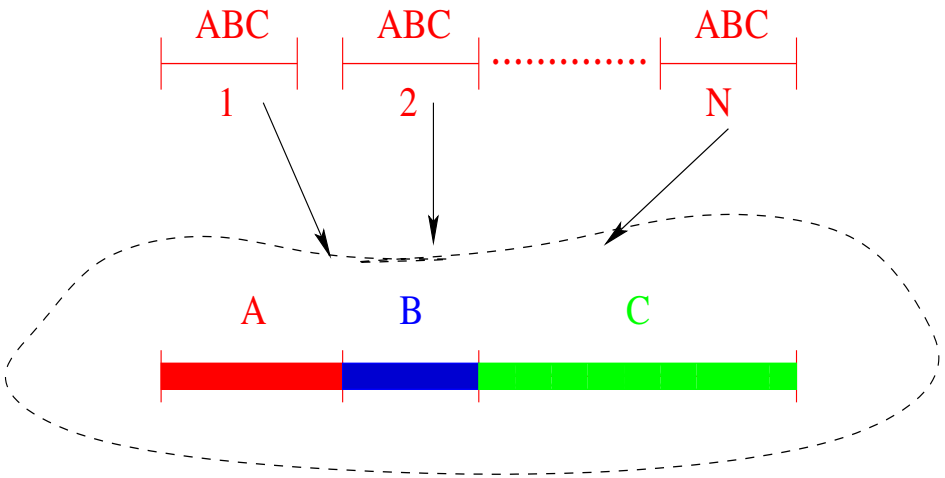


Solving Mixed-Integer Dynamic Optimization Problems

- For solving Scheduling and Control problems we will show first how to handle the solution of Scheduling problems and after the numerical solution of dynamic optimization problems will be addressed
- Scheduling: single stage and multiple stages
- Control: lumped and distributed parameters system
- Other MIDO solution approaches proposed

Single Stage Cycle Scheduling Formulation

In this section we will describe a scheduling formulation for continuous plants as proposed by Pinto and Grossmann. The formulation assumes a cyclic production sequence. Let us assume that a given plant manufactures the products A,B,C in the sequence A $\rightarrow$ B $\rightarrow$ C:



- Objective function

$$\phi = \sum_{i=1}^{N_p} \frac{C_i^p W_i}{T_c} - \sum_{i}^{N_p} \sum_{i'}^{N_p} \sum_{k}^{N_s} \frac{C_{i'i}^t Z_{ii'k}}{T_c} - \sum_{i=1}^{N_p} C_i^s \frac{(G_i - W_i/T_c)}{T_c} \frac{t_i}{2} \qquad (1)$$

where C_i^p is the product cost, $C_{i'i}^t$ is the transition cost from product i to product i', C_i^s is the inventory cost, T_c is the total cycle time, N_p is the number of products, N_s is the number of slots.

- Product assignment

$$\sum_{k=1}^{N_s} y_{ik} = 1, \ \forall i \tag{2a}$$

$$\sum_{i=1}^{N_p} y_{ik} = 1, \ \forall k \tag{2b}$$

$$y'_{ik} = y_{i,k-1}, \ \forall i, k \neq 1 \tag{2c}$$

$$y'_{i,1} = y_{i,N_s}, \ \forall i \tag{2d}$$

Equation 2a states that, within each production wheel, any product can only be manufactured once, while constraint 2b implies that only one product is manufactured at each time slot. Due to this constraint, the number of products and slots turns out to be the same. Equation 2c defines backward binary variable (y'_{ik}) meaning that such variable for product i in slot k takes the value assigned to the same binary variable but one slot backwards $k-1$. At the first slot, Equation 2d defines the backward binary variable as the value of the same variable at the last slot. This type of assignment reflects our assumption of cyclic production wheel. The variable y'_{ik} will be used later to determine the sequence of product transitions.

- Amounts manufactured

$$W_i \geq D_i T_c, \ \forall i \tag{3a}$$
$$W_i = G_i \Theta_i, \ \forall i \tag{3b}$$
$$G_i = F^o(1 - X_i), \ \forall i \tag{3c}$$

Equation 3a states that the total amount manufactured of each product i (W_i) must be equal or greater than the desired demand rate (D_i) times the duration of the production wheel, while Equation 3b indicates that the amount manufactured of product i is computed as the product of the production rate (G_i) times the time used (Θ_i) for manufacturing such product. The production rate is computed from Equation 3c as a simple relationship between the feed stream flowrate (F^o) and the conversion (X_i).

- Processing times

$$\theta_{ik} \leq \theta^{max} y_{ik}, \ \forall i, k \tag{4a}$$
$$\Theta_i = \sum_{k=1}^{N_s} \theta_{ik}, \ \forall i \tag{4b}$$
$$p_k = \sum_{i=1}^{N_p} \theta_{ik}, \ \forall k \tag{4c}$$

The constraint given by Equation 4a sets an upper bound on the time used for manufacturing product i at slot k (θ_{ik}). Equation 4b is the time used for manufacturing product i, while Equation 4c defines the duration time at slot k (p_k).

- Transitions between products

$$z_{ipk} \geq y'_{pk} + y_{ik} - 1, \ \forall i, p, k \tag{5}$$

The constraint given in Equation 5 is used for defining the binary production transition variable z_{ipk}. If such variable is equal to 1 then a dynamic transition will occur from product i to product p within slot k, z_{ipk} will be zero otherwise.

- Timing relations

$$\theta_k^t = \sum_{i=1}^{N_p} \sum_{p=1}^{N_p} t_{pi}^t z_{ipk}, \ \forall k \tag{6a}$$

$$t_1^s = 0 \tag{6b}$$

$$t_k^e = t_k^s + p_k + \sum_{i=1}^{N_p} \sum_{p=1}^{N_p} t_{pi}^t z_{ipk}, \ \forall k \tag{6c}$$

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

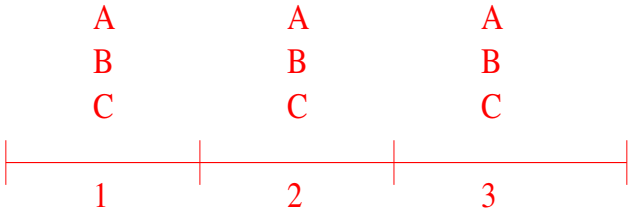
$$t_k^e \leq T_c, \ \forall k \tag{6e}$$

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

Equation 6a defines the transition time from product i to product p at slot k. It should be remarked that the term t_{pi}^t stands only for an estimate of the expected transition times. Equation 6b sets to zero the time at the beginning of the production wheel cycle corresponding to the first slot. Equation 6c is used for computing the time at the end of each slot as the sum of the slot start time plus the processing time and the transition time. Equation 6d states that the start time at all the slots, different than the first one, is just the end time of the previous slot. Equation 6e is used to force that the end time at each slot be less than the production wheel cyclic time. Finally, Equation 6f is used to obtain the time value inside each finite element and for each internal collocation point.

Simple Single Line Scheduling Example

Let us assume that a given plant facility manufactures three products: A,B,C. We would like to compute the optimal cyclic production sequence that maximizes the process profit while meeting the demand rate of each product.



Process data

Product	Demand rate	Price Products	Process rates	Inventory cost
A	2.1	320	8	1.5
B	3	430	9	1
C	4	450	12	2

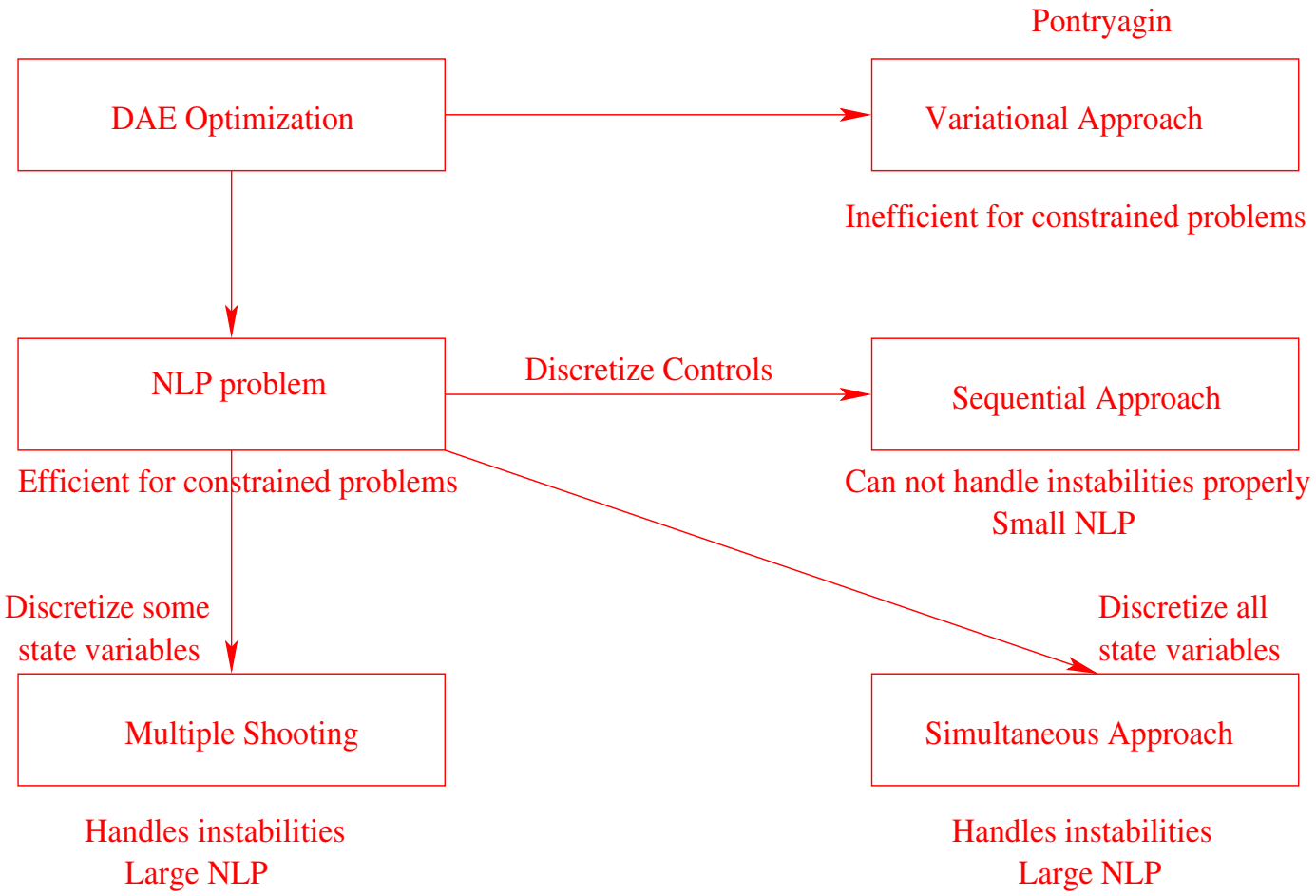
Transition times
(Transition cost)

	A	B	C
A		10 (4000)	20 (8000)
B	15 (3500)		30 (6000)
C	10 (7000)	25 (5500)	

Optimal Cyclic Scheduling Results: Profit=329

Slot	Product	Process time	Amount Manufactured	Start time	End time
1	B	235.3	2117.7	0	265.3
2	A	185.3	1482.4	265.3	460.6
3	C	235.3	2823.5	460.6	705.9

Full Discretization Optimal Control Formulation



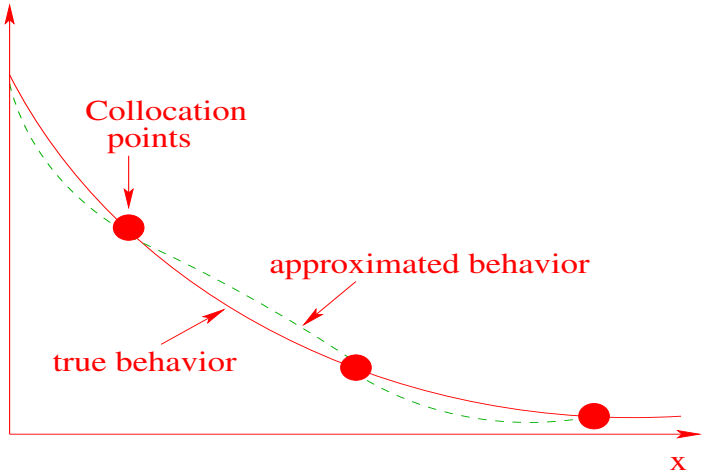
Discretizing ODEs using Orthogonal Collocation

Given an ODE system:

$$\frac{dx}{dt} = f(x, u, p), \quad x(0) = x_{init}$$

where $x(t)$ are the system states, $u(t)$ is the manipulated variable and p are the system parameters.
The aim is to approximate the behaviour of x and u by Lagrange interpolation polynomials (of orders $\mathcal{K}+1$ and $\mathcal{K}$, respectively) at collocation or discretization points t_k:

$$\begin{aligned}
x_{k+1}(t) &= \sum_{k=0}^{\mathcal{K}} x_k \ell_k^x(t), \quad \ell_k^x(t) = \prod_{\substack{j=0 \\ j\neq k}}^{\mathcal{K}} \frac{t - t_j}{t_k - t_j} \\
u_k(t) &= \sum_{k=1}^{\mathcal{K}} u_k \ell_k^u(t), \quad \ell_k^u(t) = \prod_{\substack{j=1 \\ j\neq k}}^{\mathcal{K}} \frac{t - t_j}{t_k - t_j} \\
x_{N+1}(t_k) &= x_k, \quad u_N(t_k) = u_k
\end{aligned}$$



Therefore replacing into the original ODE system, we get the system residual $\mathcal{R}(t_k)$:

$$\mathcal{R}(t_k) = \sum_{j=0}^{\mathcal{K}} x_j \frac{d\ell_j(t_k)}{dt} - f(x_k, u_k, p) = 0, \quad k = 1, .., \mathcal{K}$$

Transformation of a Dynamic Optimization problem into a NLP

Original dynamic optimization problem

$$\min_{x,u} \phi(x,u)$$

s.t.

$$\frac{dx(t)}{dt} = F\left(x(t), u(t), t, p\right)$$
$$x(0) = x^0$$
$$g(x(t), u(t), p) \leq 0$$
$$h(x(t), u(t), p) = 0$$
$$x^l \leq x \leq x^u$$
$$u^l \leq u \leq u^u$$

Discretized NLP

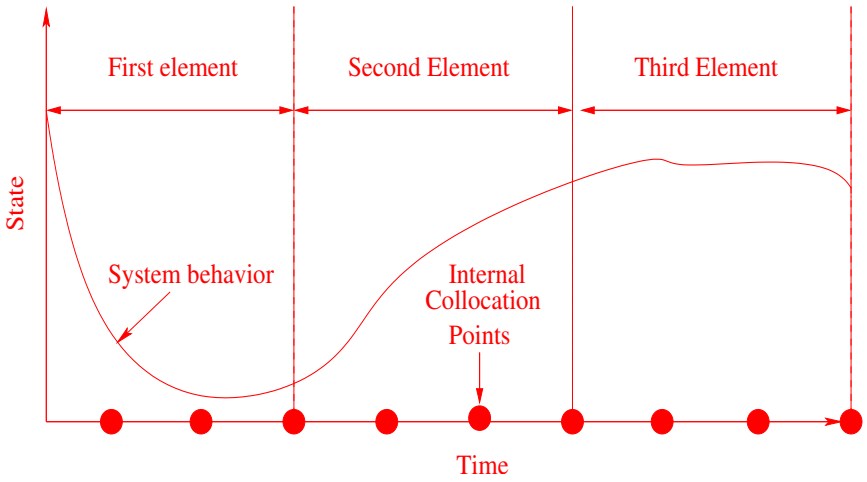
$$\min_{x_k, u_k} \phi(x_k, u_k)$$

s.t.

$$\sum_{j=0}^{\mathcal{K}} x_j \dot{\ell}_j(t_k) - F\left(x_k, u_k\right) = 0, \;\; k = 1, ..., \mathcal{K}$$
$$x_0 = x(0)$$
$$g(x_k, u_k, p) \leq 0, \;\; k = 1, ..., \mathcal{K}$$
$$h(x_k, u_k, p) = 0, \;\; k = 1, ..., \mathcal{K}$$
$$x^l \leq x \leq x^u$$
$$u^l \leq u \leq u^u$$

Approximation of a Dynamic Optimization Problem using Orthogonal Collocation of Finite Elements

Sometimes it is convenient to use Orthogonal Collocation on Finite Elements to approximate the behavior of systems exhibiting fast dynamics.



$$\min_{x_k, u_k} \phi(x, u)$$

s.t.

$$\sum_{j=0}^{\mathcal{K}} x_{ij} \dot{\ell}_j(\tau_k) - h_i F(x_{ik}, u_{ik}) = 0, \ \ k = 1, \ldots, NC \quad i=1,\ldots,NE$$

$$x_{10} = x(0)$$

$$g(x_{ik}, u_{ik}, p) = 0, \ \ i = 1, \ldots, NE; k = 1, .., NC$$

$$x^l_{ij} \leq x_{ij} \leq x^u_{ij}, \ \ i = 1, \ldots, NE; k = 1, .., NC$$

$$u^l_{ij} \leq u_{ij} \leq u^u_{ij}, \ \ i = 1, \ldots, NE; k = 1, .., NC$$

where NE is the number of finite elements, NC is the number of internal collocation points, h_i is the length of each element.

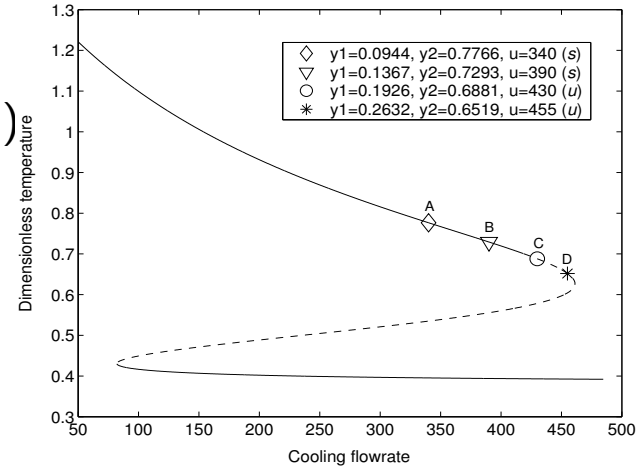
Dynamic optimal transition between two steady-states: Hicks CSTR

Let us consider the dimensionless mathematical model of a non-isothermal CSTR as proposed by Hicks and Ray modified for displaying nonlinearities:

$$\frac{dC}{dt} = \frac{1-C}{\theta} - k_{10}e^{-N/T}C$$

$$\frac{dT}{dt} = \frac{y_f - T}{\theta} + k_{10}e^{-N/T}C - \alpha U(T - y_c)$$

Desired Transition B → A



Parameter values

θ	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
α	1.95×10^{-4}	Heat transfer area
N	5	$E_1/(RJc_f)$

Desired dynamic transition

	C	T	U
Initial (B)	0.1367	0.7293	390
Final (A)	0.0944	0.7766	340

C = Concentration (c/c_f), T = temperature (T_r/Jc_f), y_c = Coolant temperature (T_c/Jc_f), y_f = feed temperature (T_f/Jc_f), U = Cooling flowrate. c and T_r are nondimensionless concentration and reactor temperature.

- Objective function
  As objective function the requirement of minimum transition time between the initial and final steady-states will be imposed:

$$\text{Min} \int_0^{t_f} \left\{ \alpha_1 (C(t) - C_{des})^2 + \alpha_2 (T(t) - T_{des})^2 + \alpha_3 (U(t) - U_{des})^2 \right\} dt$$

the subscript "des" stands for the final desired values. α_i, $i = 1, 2, 3$ are weighting factors. The above integral is approximated using a Radau quadrature procedure:

$$\text{Min } \Phi = \sum_{i=1}^{N_e} h_i \sum_{j=1}^{N_c} W_j \left[\alpha_1 (C_{ij} - C_{des})^2 + \alpha_2 (T_{ij} - T_{des})^2 + \alpha_3 (U_{ij} - U_{des})^2 \right]$$

N_e is the number of finite elements (N_e=3), N_c is the number of collocation points including the right boundary in each element (so in this case $N_c = 3$), C_{ij} and T_{ij} are the dimensionless concentration and temperature values at each discretized ij point, h_i is the finite element length of the i−th element, W_j are the Radau quadrature weights.

- Mass balance constraints
  The value of the dimensionless concentration at each one of the discretized points (C_{ij}) is approximated using the following monomial basis representation:

$$C_{ij} = C_i^o + h_i \theta \sum_{k=1}^{N_c} A_{kj} \frac{dC_{ik}}{dt}, \quad i = 1, ..., N_e; \quad j = 1, ..., N_c$$

  C_i^o is the concentration at the beginning of each element, A_{kj} is the collocation matrix. Note that C_1^o stands for the initial concentration. The length of each finite element (h_i)can be computed as:

$$h_i = \frac{1}{N_e}$$

- Energy balance

$$T_{ij} = T_i^o + h_i \theta \sum_{k=1}^{N_c} A_{kj} \frac{dT_{ik}}{dt}, \quad i = 1, ..., N_e; \quad j = 1, ..., N_c$$

  similarly, T_i^o is the temperature at the beginning of each element. Again, note that T_1^o stands for the initial reactor temperature.

- Mass balance continuity constrains between finite elements
  Only the system states must be continuous when crossing from one finite element to the next one. Algebraic and manipulated variables are allowed to exhibit discontinuous behaviour between finite elements. To force continuous concentration profiles all the elements at the beginning of each element ($C_i,\ i = 2, ..., N_e^o$) are computed in terms of the same monomial basis used before:

$$C_i^o = C_{i-1}^o + h_{i-1}\theta \sum_{k=1}^{N_c} A_{k,N_c} \frac{dC_{i-1,k}}{dt},\ \ i = 2, ..., N_e$$

- Energy balance continuity constrains between finite elements

$$T_i^o = T_{i-1}^o + h_{i-1}\theta \sum_{k=1}^{N_c} A_{k,N_c} \frac{dT_{i-1,k}}{dt},\ \ i = 2, ..., N_e$$

- Approximation of the dynamic behaviour of the mass balance at each collocation point
  The first order derivatives of the concentration at each collocation point (ij) are obtained from the corresponding continuous mathematical model:

$$\frac{dC_{i,j}}{dt} = \frac{1 - C_{ij}}{\theta} - k_{10}e^{-N/T_{ij}}C_{ij}, \quad i = 1, ..., N_e; \quad j = 1, ..., N_c$$

- Approximation of the dynamic behaviour of the energy balance at each collocation point

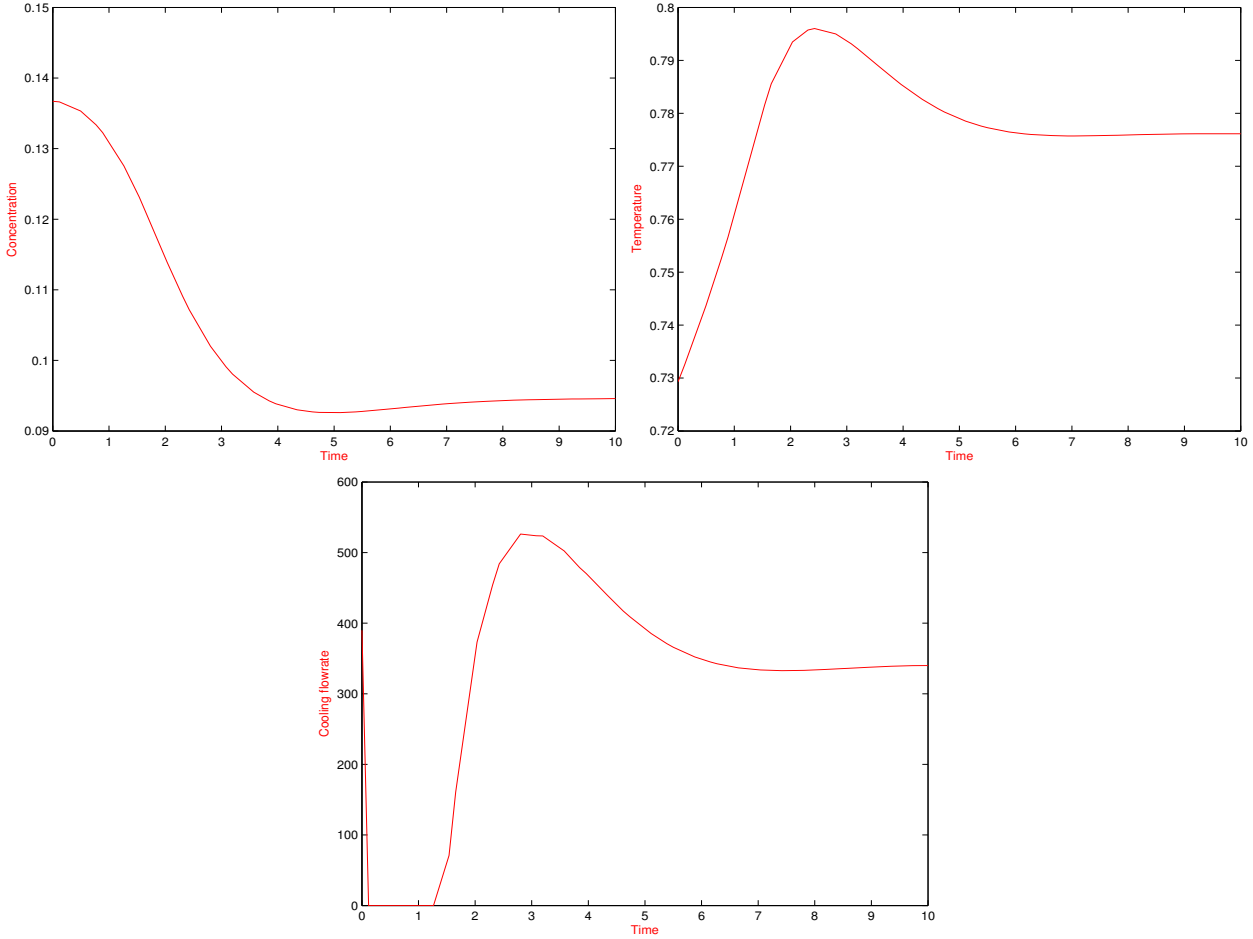
$$\frac{dT_{i,j}}{dt} = \frac{y_f - T_{ij}}{\theta} + k_{10}e^{-N/T_{ij}}C_{ij} - \alpha U_{ij}(T_{ij} - y_c), \quad i = 1, ..., N_e; \quad j = 1, ..., N_c$$

- Initial values constraints

$$\begin{aligned} C_1^o &= C_{init} \\ T_1^o &= T_{init} \end{aligned}$$

the subscript "init" stands for the initial steady-state values from which the optimal dynamic transition will be computed.

Dynamic Transitions profiles for the Hicks CSTR example



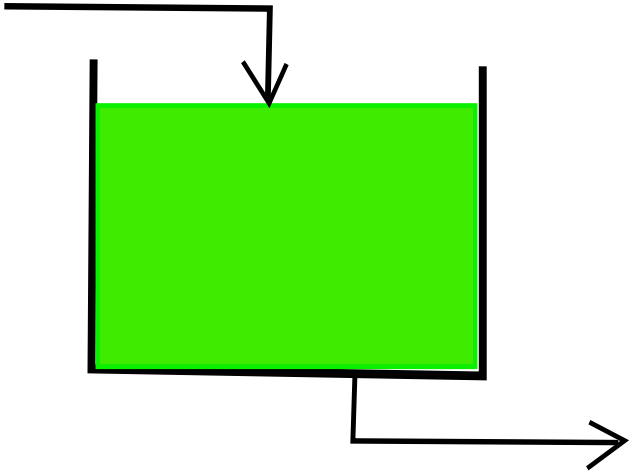
Simultaneous Scheduling and Control problems

- We have shown how to handle the solution of Scheduling and Optimal Control problems
- Because of strong interactions between Scheduling and Control Problems better optimal solutions can be found by the simultaneous solution of these problems
- No need to neglect process dynamics (Scheduling)
- No need to fix production sequence (Control)
- Merge both formulations and solve MIDO problem

Simultaneous Scheduling and Control problems

- Full discretization approaches lead to large size MINLP problems
- Reliable MINLP solvers are needed
- Problem solution is highly-dependent on MINLP initialization scheme
- Use Scheduling and Control MINLP solutions for providing acceptable initial guesses of the decision variables
- Develop your Scheduling and Control formulation step by step

Case Study 1: Single line Multiproduct CSTR



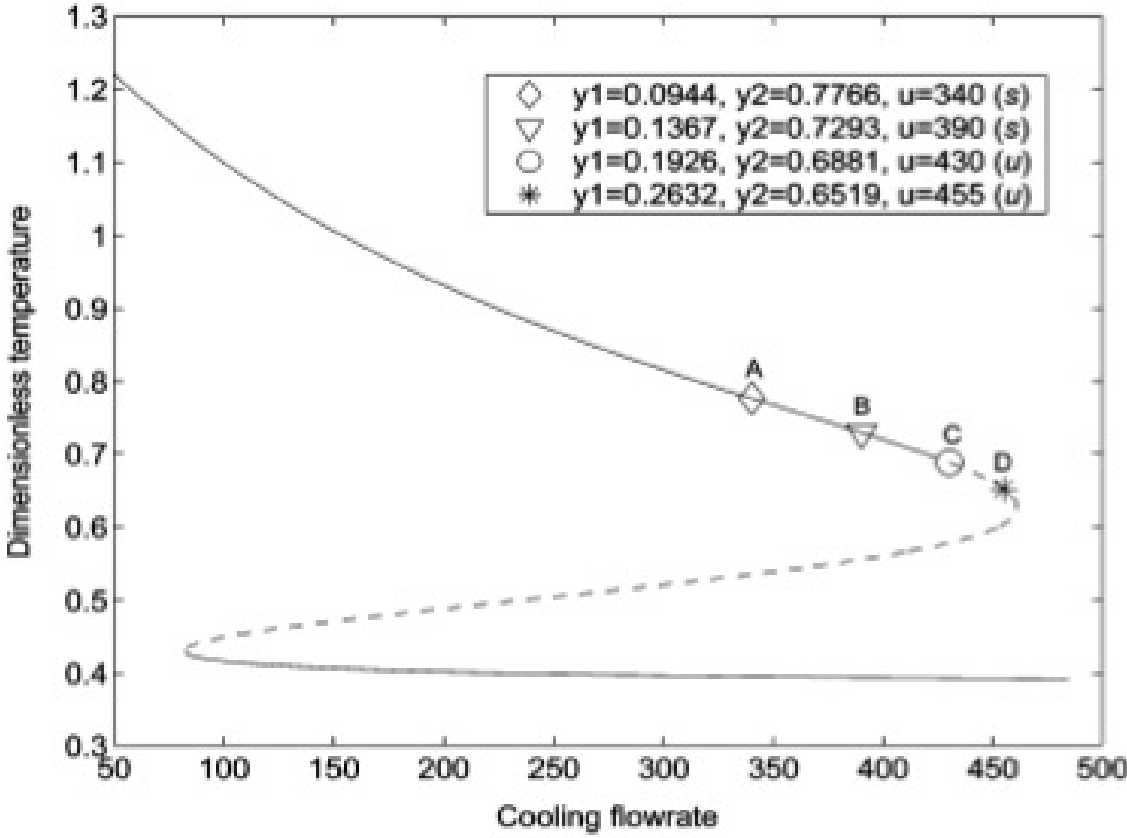


Figure 11. Multiplicity map (— stable solution, – – unstable solution).

Case Study 1: Single line Multiproduct CSTR

Table 10. Process Data for the Third Case Study[a]

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

[a] A, B, C, and D stand for the four products to be manufactured. Information about the steady-state design for each one of the products is shown in Figure 11. The cost of the raw material (C^r) Is $10.

Table 11. Simultaneous Scheduling and Control Results for the Third Case Study[a]

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	15 831.7	10	0	38.3
2	B	13.1	613.6	8 044.9	10	38.3	61.4
3	C	13.4	656.1	8 748.9	10	61.4	84.8
4	D	5.8	688.3	4 022.5	10	84.8	100.6

[a] The objective function value is $7657 and 100.6 h of total cycle time.

CPU time: 254 s, Sbb

Case Study 1: Single line Multiproduct CSTR

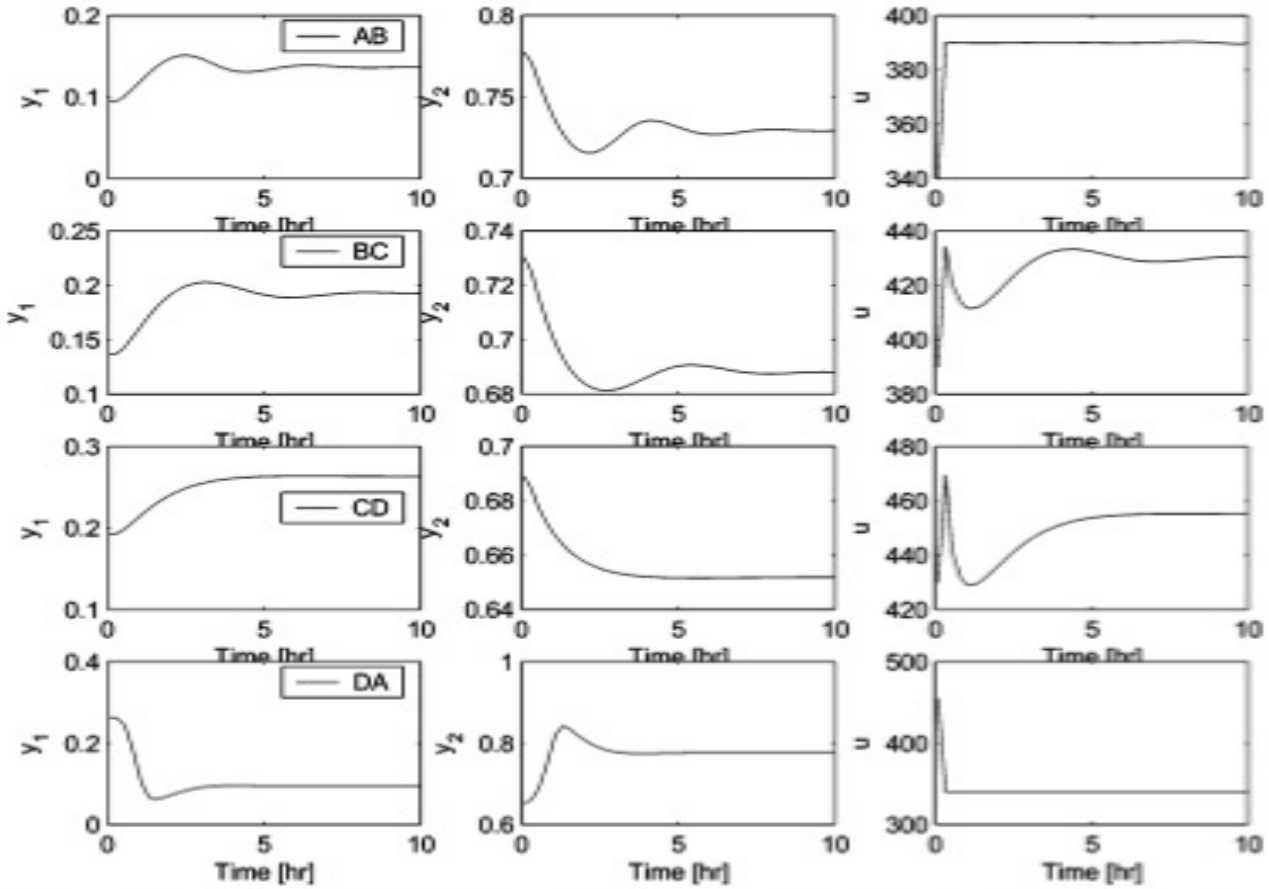


Figure 12. Optimal schedule and dynamic profiles for the third case study.

Case Study 2: Single line HIPS Polymerization CSTR

- Initiator concentration

$$\frac{dC_i}{dt} = \frac{Q_i C_i^f - QC_i}{V} - K_d C_i$$

- Monomer concentration

$$\frac{dC_m}{dt} = \frac{Q}{V}(C_m^f - C_m) - K_p C_m(\mu_r^o + \mu_b^o)$$

- Butadiene concentration

$$\frac{dC_b}{dt} = \frac{Q}{V}(C_b^f - C_b) - C_b(K_{i2}C_r + K_{fs}\mu_r^o + K_{fb}\mu_b^o)$$

- Radicals concentration

$$\frac{dC_r}{dt} = -\frac{Q}{V}C_r + 2f^* K_d C_i - C_r(K_{i1}C_m + K_{i2}C_b)$$

- Branched radicals concentration

$$\frac{dC_{br}}{dt} = -\frac{Q}{V}C_{br} + C_b(K_{i2}C_r + K_{fb}(\mu_r^o + \mu_b^o)) - C_{br}(K_{i3}C_m + K_t(\mu_r^o + \mu_b^o + C_{br}))$$

- Reactor temperature

$$\frac{dT}{dt} = \frac{Q}{V}(T^f - T) + \frac{\Delta H_r K_p C_m(\mu_r^o + \mu_b^o)}{\rho_s C_{ps}} - \frac{UA(T - T_j)}{\rho_s C_{ps} V}$$

- Cooling jacket temperature

$$\frac{dT_j}{dt} = \frac{Q_w}{V_c}(T_j^f - T_j) + \frac{UA(T - T_j)}{\rho_w C_{pw} V_c}$$

- Zeroth moment live polymer

$$\frac{d\lambda_p^o}{dt} = -\frac{Q}{V}\lambda_p^o + \frac{K_t}{2}(\mu_r^o)^2 + (K_{fs}C_m + K_{fb}C_b)\mu_r^o \quad (4$$

- First moment live polymer

$$\frac{d\lambda_p^1}{dt} = -\frac{Q}{V}\lambda_p^1 + K_t\mu_r^1\mu_r^o + (K_{fs}C_m + K_{fb}C_b)\mu_r^1 \quad (4$$

- Zeroth moment dead polymer

$$\frac{d\mu_r^o}{dt} = -\frac{Q}{V}\mu_r^o + 2K_{io}C_m^3 + K_{i1}C_rC_m + C_mK_{fs}(\mu_r^o + \mu_b^o) - (K_pC_m + K_t(\mu_r^o + \mu_b^o + C_{br}) + K_{fs}C_m + K_{fb}C_b)\ \mu_r^o + K_pC_m\mu_r^o \quad (4$$

- First moment dead polymer

$$\frac{d\mu_r^1}{dt} = -\frac{Q}{V}\mu_r^1 - (K_pC_m + K_t(\mu_r^o + \mu_b^o + C_{br}) + K_{fs}C_m + K_{fb}C_b)\mu_r^1 + K_pC_m(\mu_r^1 + \mu_r^o) \quad (5$$

- Zeroth moment butadiene

$$\frac{d\mu_b^o}{dt} = -\frac{Q}{V}\mu_b^o + K_{i3}C_{br}C_m - (K_pC_m + K_t(\mu_r^o + \mu_b^o + C_{br}) + K_{fs}C_m + K_{fb}C_b)\mu_b^o + K_pC_m\mu_b^o \quad (5$$

- Number molecular weight distribution

$$M_n = \frac{\lambda_p^1 + \mu_r^1}{\lambda_p^o + \mu_r^o} \quad (5$$

Case Study 2: Single line HIPS Polymerization CSTR

Table 2. HIPS Grade Design Information

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

Demand rate is in [kg/hr], inventory cost is in [$/kg-hr], monomer and initiator costs are in [$/lt of feed stream] and prices are in [$/kg].

Table 3. Simultaneous Scheduling and Control Results for Grade Transition in a HIPS Polymerization CSTR

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

The optimal cyclic sequence is $E \rightarrow A \rightarrow B \rightarrow C \rightarrow D$. The objective function value is $ 1,456/hr and 32.3 h of total cycle time.

Statistics: 6666 Constraints, 6267 continuous variables, 25 binaries, 7640 s CPU time (IBM 1.6 Ghz), Dicopt

Case Study 2: Single line HIPS Polymerization CSTR

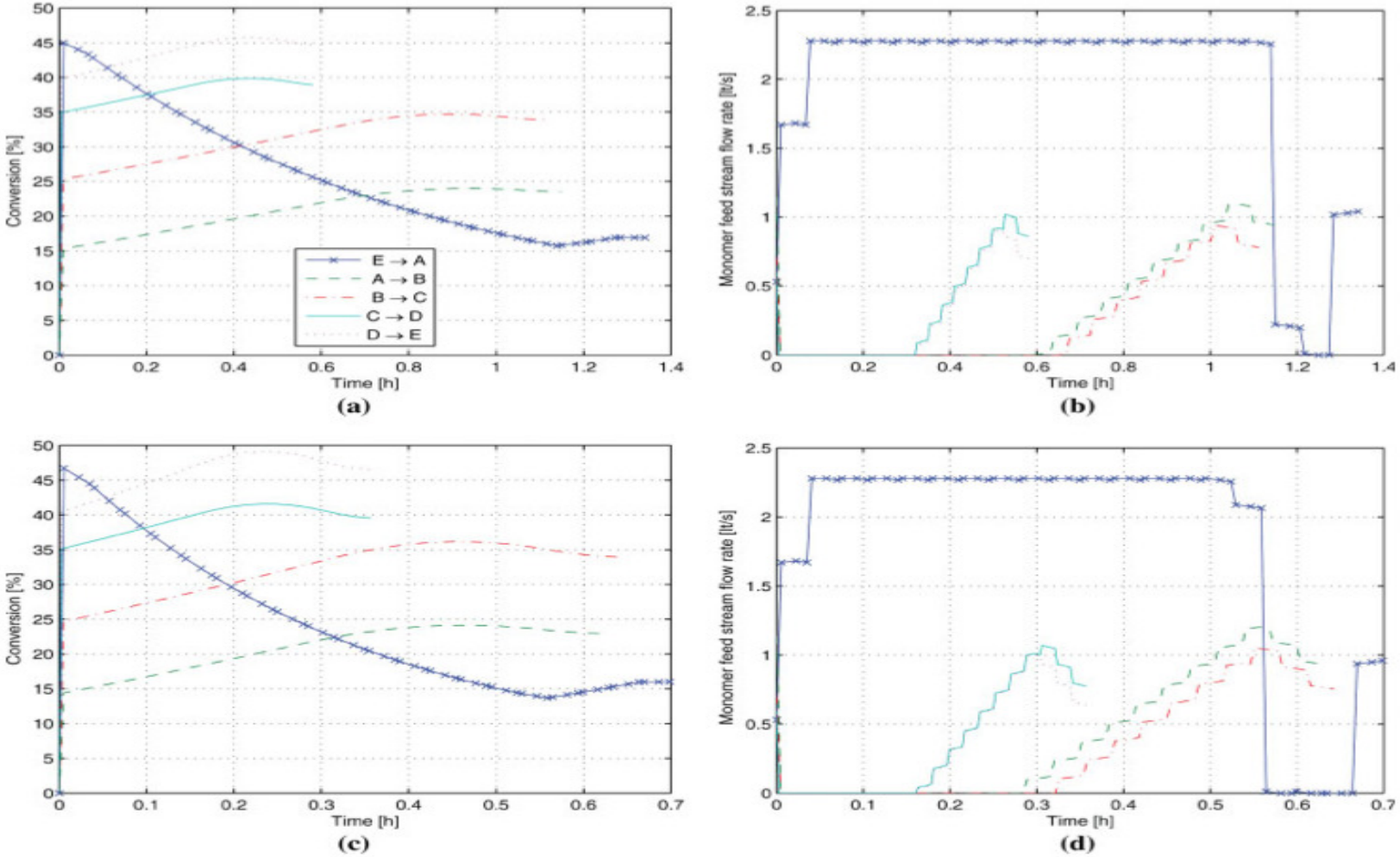


Figure 5. Conversion (a), and monomer feed stream flow rate (b), profiles of chosen grade transition in original (reactor volume = 6,000 lts); conversion (c), and monomer feed stream flow rate (d), profiles of chosen grade transition in modified systems (reactor volume = 2500 lts).

Case Study 3: Single line HIPS Polymerization Plant

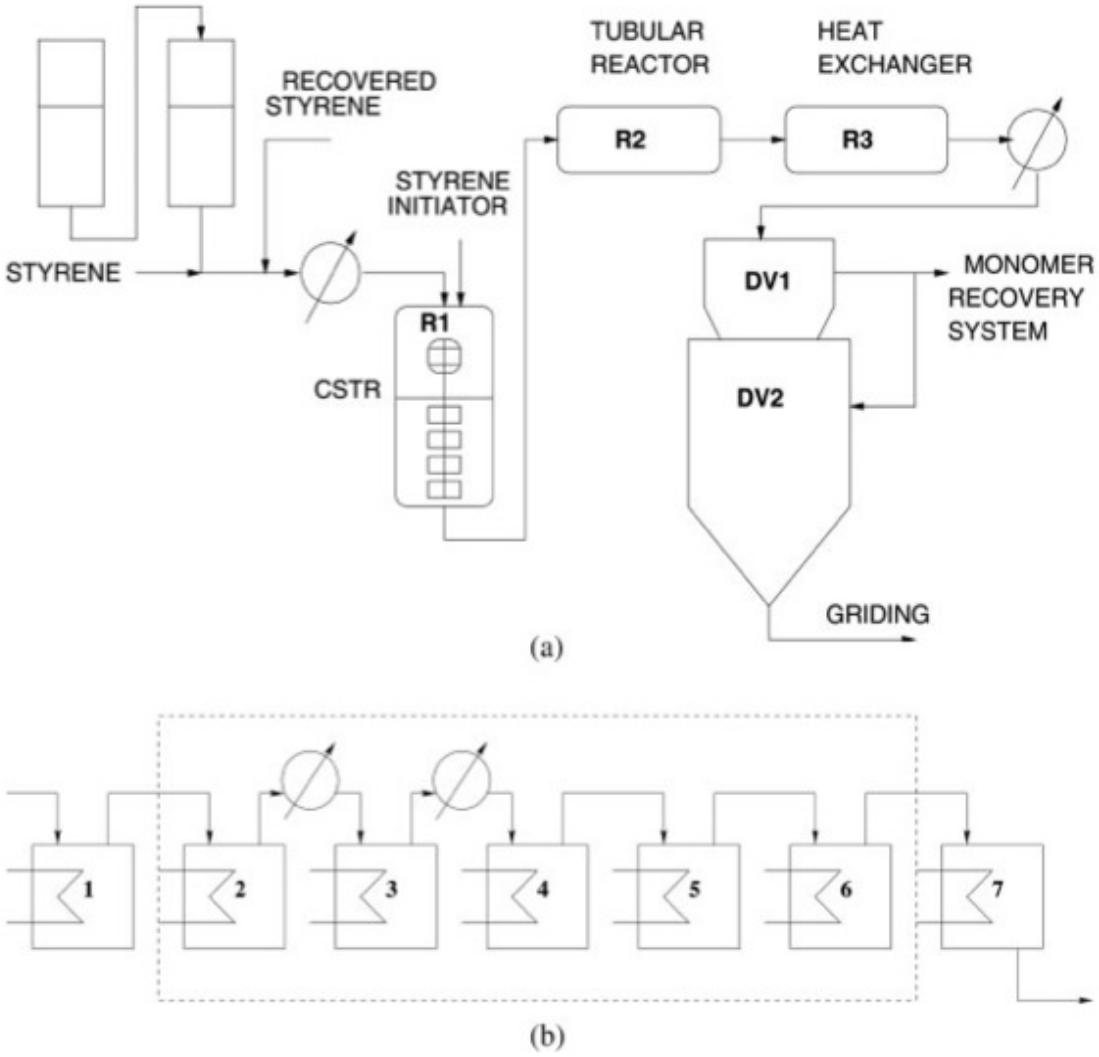


Figure 8. (a) Flow sheet of the HIPS plant. (b) approximation of the HIPS plant by a set of 7 series-connected

Case Study 3: Single line HIPS Polymerization Plant

Table 14. Steady States and Grade Information of the HIPS Polymerization Reaction Train

	State N	State A	State B	State C
C_m [mol/L]	3.1344	2.3018	1.4534	0.7519
$T_{reactor}$ [K]	395	440	476	517
$X\%$	64	73	83	91
Q_w [L/s]	1.14	1.48	1.64	2.10
Demand [kg/hr]	350	325	300	250
Price [$/kg]	3.2	4.3	4.5	5.0
Inv. Cost [$/hr-kg]	0.16	0.21	0.22	0.25
Mono. Cost [$/lt$_{feed}$]	1	1	1	1
Init. Cost [$/lt$_{feed}$]	100	100	100	100

State values and conversion correspond the last CSTR of the reaction train.

Table 16. Simultaneous Scheduling and Control Results Using Decomposition Heuristic, for Grade Transition in a HIPS Polymerization Train

Product	Process T [h]	Production [kg]	Trans T [h]	T start[h]	T end [h]
A	3.72	12742.20	5.96	0	8.62
N	2.66	13722.37	3.37	8.62	15.72
C	18.40	1.2501e5	1.43	15.72	35.54
B	2.22	11762.03	1.45	35.54	39.21

The objective function value is $ 6,245/h and 39.2 h of total cycle time.

Case Study 3: Single line HIPS Polymerization Plant

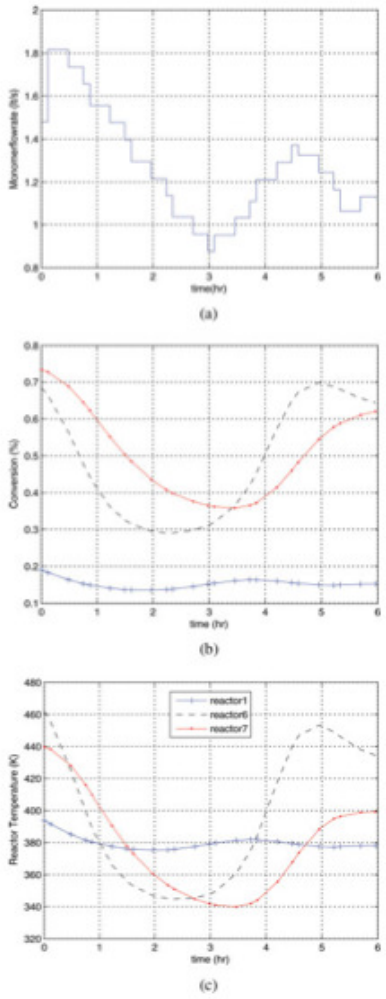


Figure 10. Monomer feed stream (a), conversion (b), and temperature profiles (c) of reactors 1,6 and 7 in slot 1.

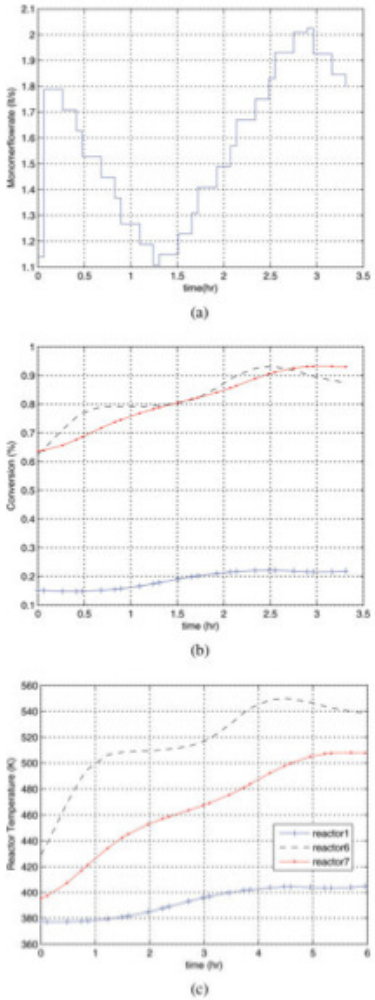


Figure 11. Monomer feed stream (a), conversion (b), and temperature profiles (c) of reactors 1,6 and 7 in slot 2.

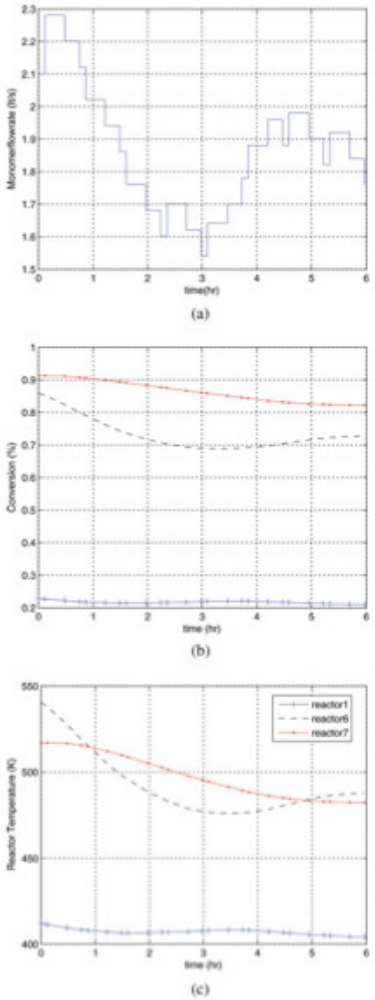


Figure 12. Monomer feed stream (a), conversion (b), and temperature profiles (c) of reactors 1,6 and 7 in slot 3.

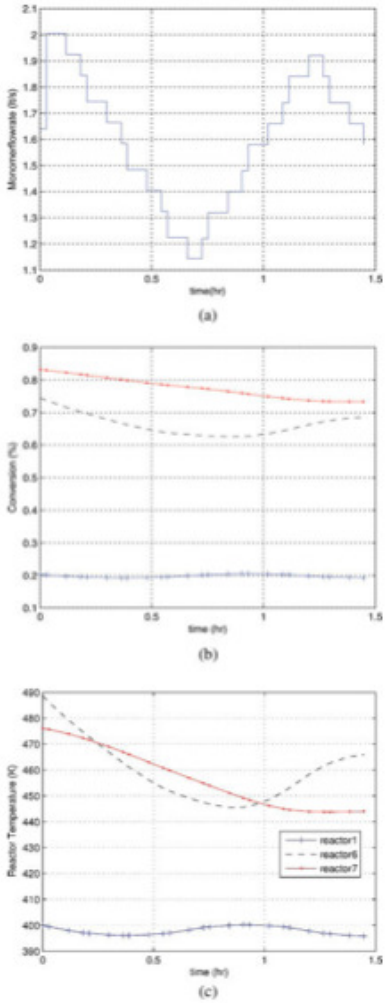


Figure 13. Monomer feed stream (a), conversion (b), and temperature profiles (c) of reactors 1,6 and 7 in slot 4.

Case Study 4: Single line Multiproduct Tubular Catalytic Reactor

$$\frac{\partial C_A}{\partial t} = -\frac{v}{\varepsilon}\frac{\partial C_A}{\partial x} + \frac{\mu(1-\varepsilon)}{\varepsilon}[-k_1 e^{-E_1/RT} C_A - k_3 e^{-E_3/RT} C_A] \quad (46)$$

$$\frac{\partial C_B}{\partial t} = -\frac{v}{\varepsilon}\frac{\partial C_B}{\partial x} + \frac{\mu(1-\varepsilon)}{\varepsilon}[k_1 e^{-E_1/RT} C_A - k_2 e^{-E_2/RT} C_B] \quad (47)$$

$$\frac{\partial T}{\partial t} = -\frac{v}{\mathrm{Le}}\frac{\partial T}{\partial x} + \frac{\mu(1-\varepsilon)}{\mathrm{Le}\rho_f C_{pf}}[-\Delta H_{r1} k_1 e^{-E_1/RT} C_A - \Delta H_{r2} k_2 e^{-E_2/RT} C_B - \Delta H_{r3} k_3 e^{-E_3/RT} C_A] + \frac{2UL}{\mathrm{Le} r' \rho_f C_{pf}}(T_w - T) \quad (48)$$

$$C_A\Big|_{x=0,t} = C_A^f + \frac{D_m}{v}\frac{\partial C_A}{\partial x}$$

$$C_B\Big|_{x=0,t} = C_B^f + \frac{D_m}{v}\frac{\partial C_B}{\partial x}$$

$$T\Big|_{x=0,t} = T^f + \frac{D_t}{v}\frac{\partial T}{\partial x}$$

$$\frac{\partial C_A}{\partial x}\Big|_{x=L,t} = 0$$

$$\frac{\partial C_B}{\partial x}\Big|_{x=L,t} = 0$$

$$\frac{\partial T}{\partial x}\Big|_{x=L,t} = 0$$

$$\hat{C}_A\Big|_{\hat{x},\theta=0} = \frac{C_A^s}{C_A^f} \qquad \hat{C}_B\Big|_{\hat{x},\theta=0} = \frac{C_B^s}{C_B^f} \qquad \hat{T}\Big|_{\hat{x},\theta=0} = \frac{T^s}{T^f}$$

Table 7. Process Data for the Nonisothermal Catalytic Fixed-Bed Tubular Reactor Case Study[a]

product	conversion fraction	demand rate [kg/s]	process cost [$/kg]	inventory cost [$/kg]	transition cost [$]					
					A	B	C	D	E	F
A	0.5	1	270	1.5	0	5	6	7	8	9
B	0.6	2	280	1	10	0	5	8	6	10
C	0.7	1.2	350	2	7	10	0	8	7	11
D	0.8	3	380	3	6	10	10	0	12	8
E	0.9	1.5	430	2.5	8	9	10	10	0	10
F	0.99	2	380	1.2	11	8	7	9	11	0

[a] A, B, C, D, E, and F stand for the five products to be manufactured.

Table 8. Simultaneous Scheduling and Control Results for the Nonisothermal Catalytic Fixed-Bed Tubular Reactor Case Study[a]

slot	prod.	$\hat{C}_A$	$\hat{C}_B$	$\hat{T}_r$	v [m/s]	θ [h]	amount produced [kg]	production rate [kg/m]	process time [h]	T start [h]	T end [h]
1	A	0.5	0.442	1.007	4.879	1.6	1479.119	3745.322	0.395	0	10.39
2	B	0.4	0.529	1.006	3.655	1.6	2958.238	3367.079	0.879	10.39	21.27
3	E	0.1	0.768	1.004	1.393	1.5	2218.679	1924.178	1.153	21.27	32.42
4	F	0.01	0.791	1.004	0.664	1.7	2958.238	1008.935	2.932	32.42	45.36
5	D	0.2	0.694	1.005	2.03	1.6	4437.358	2493.723	1.779	45.36	57.14
6	C	0.3	0.613	1.005	2.751	1.5	4174527.473	2956.504	1411.981	57.14	1479.12

[a] The best production sequence is A → B → E → F → D → C featuring 1479.119 h as total cyclic time and objective function value of $787 919.947. The optimal solution was computed in 12.08 h CPU time. θ stands for transition times.

Statistics: 40537 equations, 40952 cont. vars, 72 discrete vars, 12 h CPU time, Sbb

Case Study 4: Single line Tubular Catalytic Reactor

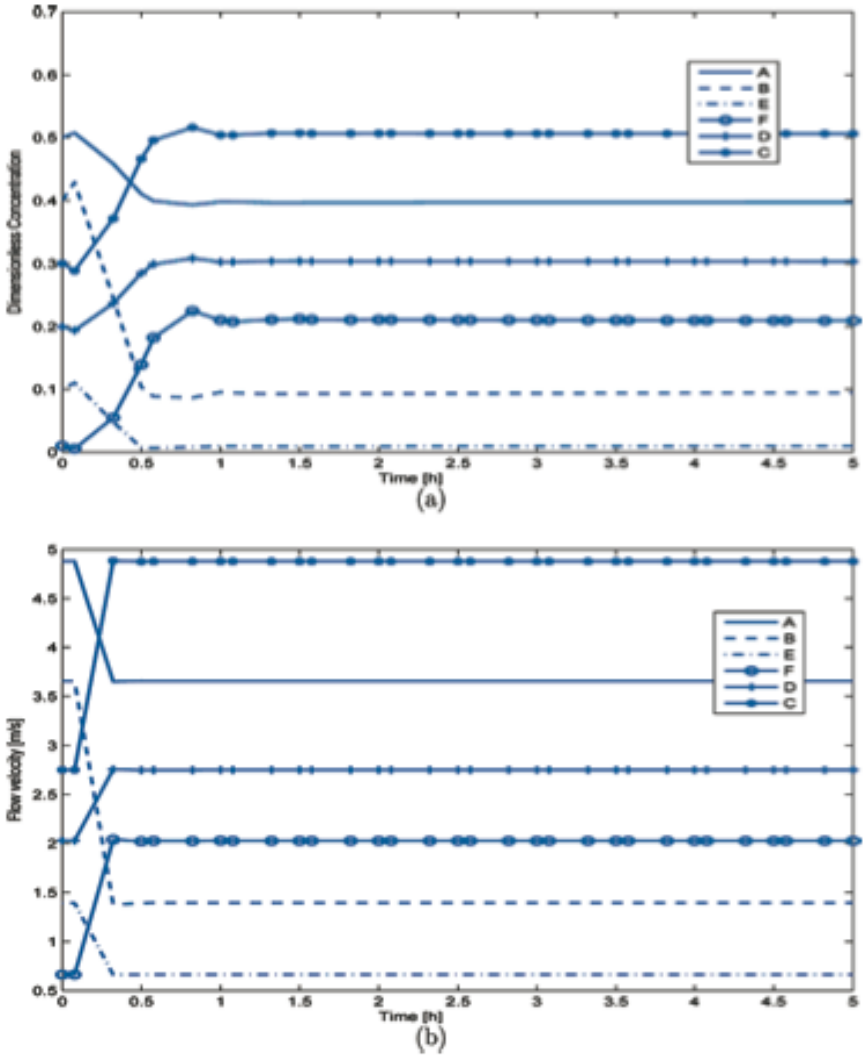


Figure 5. Optimal dynamic transition profiles for the nonisothermal catalytic fixed-bed tubular reactor. The optimal production sequence is: A → B → E → F → D → C.

Parallel Lines Continuous Scheduling Problems

We used Sahinidis and Grossmann scheduling formulation for parallel lines continuous systems

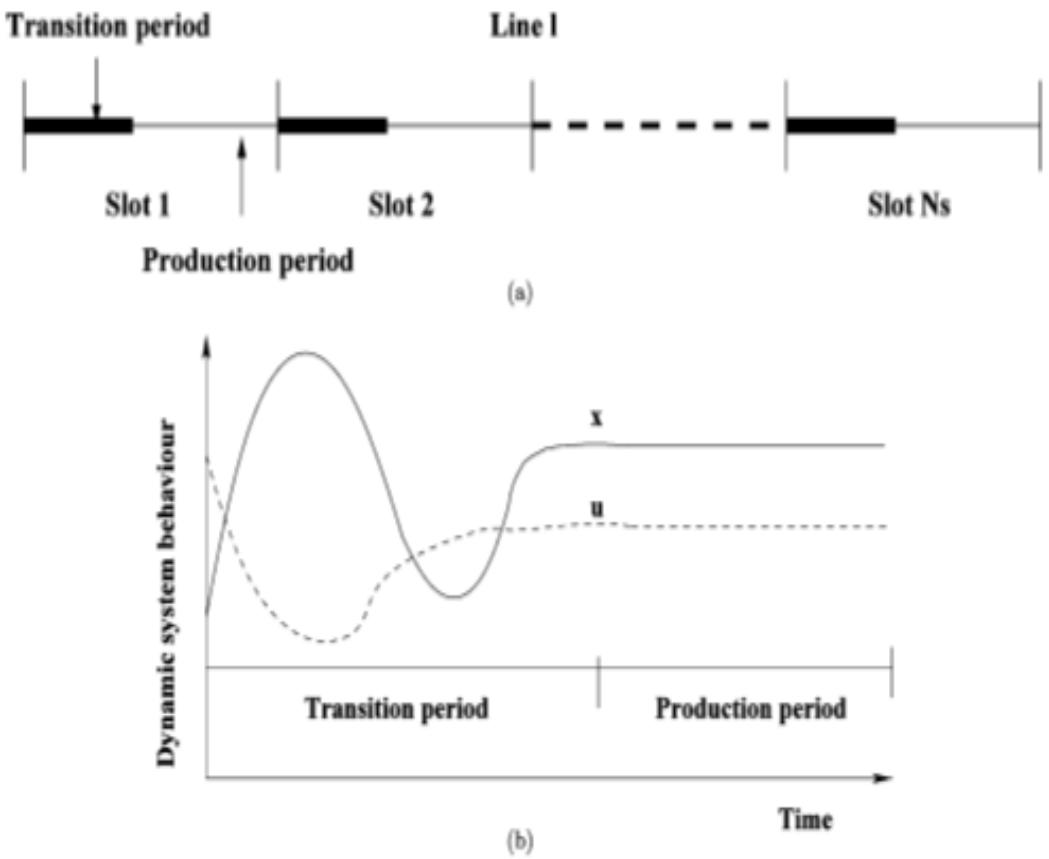


Figure 1. (a) Schematic of the process, consisting of l parallel production lines. At each line l, the cyclic time is divided into N_s slots. (b) When a change in the setpoint of the system occurs, there is a transition period, followed by a continuous production period.

Case Study 5: Two Series-Connected Nonisothermal CSTRs

$$\frac{dx_1}{dt} = (1-\lambda)x_2 - x_1 + Da_1(1-x_1)\exp\left[\frac{\theta_1}{1+(\theta_1/\gamma)}\right]$$

$$\frac{d\theta_1}{dt} = (1-\lambda)\theta_2 - \theta_1 + Da_1 B(1-x_1)\exp\left[\frac{\theta_1}{1+(\theta_1/\gamma)}\right] - \beta_1(\theta_1 - \theta_{c1})$$

$$\frac{dx_2}{dt} = x_1 - x_2 + Da_2(1-x_2)\exp\left[\frac{\theta_2}{1+(\theta_2/\gamma)}\right]$$

$$\frac{d\theta_2}{dt} = \theta_1 - \theta_2 + Da_2 B(1-x_2)\exp\left[\frac{\theta_2}{1+(\theta_2/\gamma)}\right] - \beta_2(\theta_2 - \theta_{c2})$$

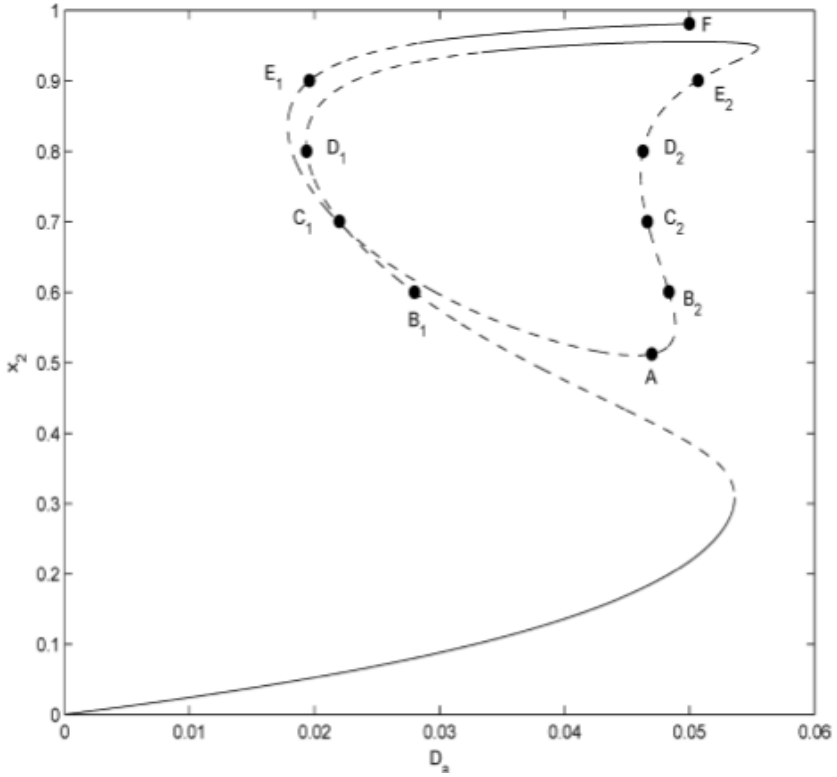


Table 5. Process Data for the Third Case Study[a]

product	conversion percentage	production rate [kg/h]	demand rate [kg/h]	product cost [$/kg]	inventory cost [$/kg]
A	51.25	450	30	1	1
B_1	60.01	600	40	3	1.5
B_2	60.08	700	45	4	1.8
C_1	70.08	900	36	2	2
C_2	70.04	850	30	4	1
D_1	80.02	700	44	3	2
E_2	90.05	800	50	5	1
F	98.09	750	40	4	1

[a] A, B_1, B_2, C_1, C_2, D_1, E_2, and F denote the eight products to be manufactured. Two production lines and four slots for each one of the production lines were used.

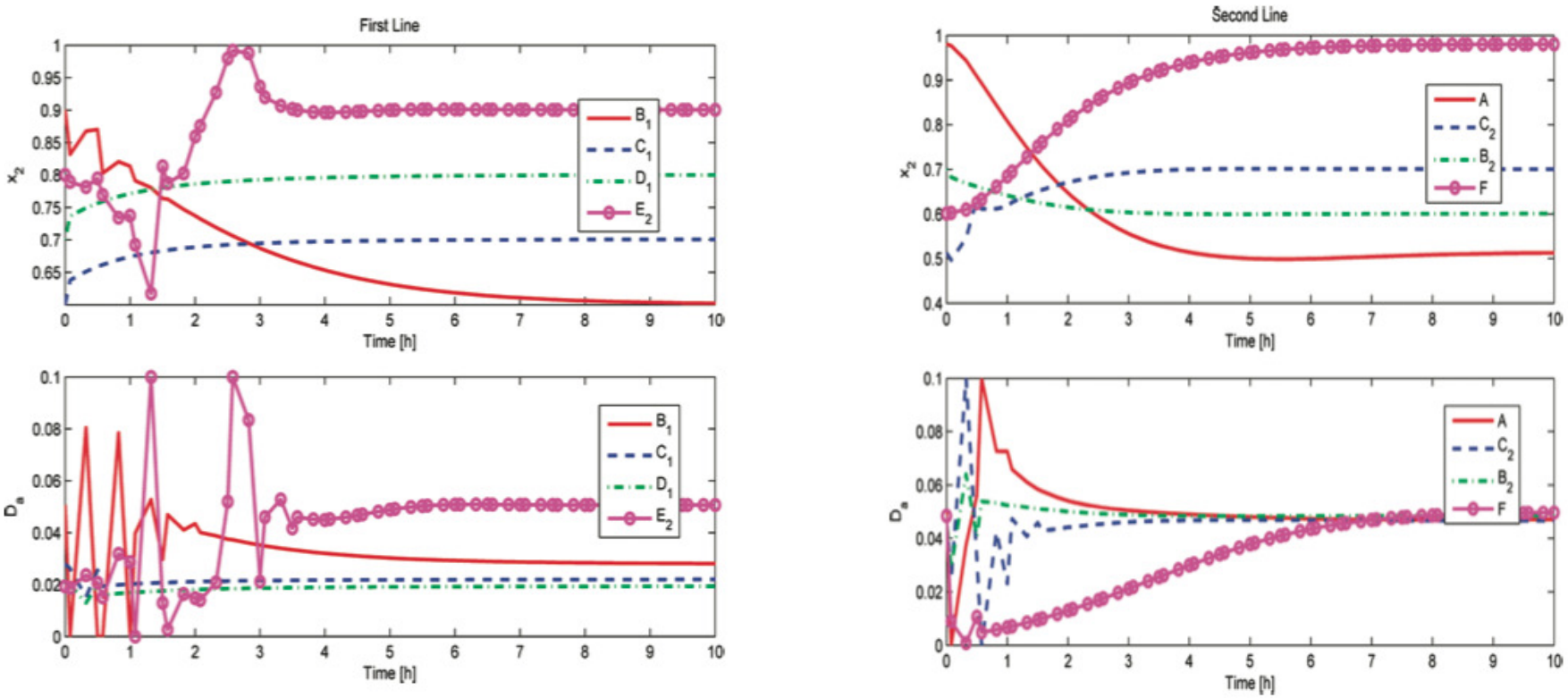
Table 6. Optimal Scheduling and Control Results for the Third Case Study[a]

	Steady-State Values					w [kg]		Processing Time, PT [h]		Optimal Transition Time, θ [h]	
product	x_1	θ_1	x_2	θ_2	Da	L_1	L_2	L_1	L_2	L_1	L_2
A	0.3629	2.3480	0.5125	1.8795	0.047		1537.64		13.42		4.8
B_1	0.0979	0.4049	0.6001	3.8178	0.028	2083.4		13.48		8.7	
B_2	0.3566	2.2594	0.6008	2.5435	0.04837		2306.45		13.3		3.9
C_1	0.0985	0.3596	0.7008	4.5371	0.022	1875.06		12.09		5.3	
C_2	0.3799	2.3774	0.7004	3.1421	0.04664		1537.64		11.81		4.1
D_1	0.1048	0.3553	0.8002	5.2180	0.01937	2291.74		13.28		4.2	
E_2	0.3533	2.0872	0.9005	4.7090	0.0507	2604.25		13.26		3.9	
F	0.9722	6.4840	0.9809	2.2257	0.05		2050.18		12.74		6.7

[a] Profit = $1848/h. Cyclic times are 52.085 and 51.254 h for the first and second production lines, respectively; w is the amount manufactured, and L_1 and L_2 stand for the first and second production lines, respectively.

Statistics: 5011 equations, 5995 cont. vars, 64 discrete vars, 1 h CPU time, Sbb

Case Study 5: Two Series-Connected Nonisothermal CSTRs



A Multiobjective Optimization Approach for SC problems

- Many Engineering problems feature conflicting objectives
- Until now dynamic transitions have been *converted* into economic profits by using weighting functions so a single objective function was used
- However improved optimal solutions can be obtained by solving SC problems as Multiobjective optimization problems and the subjective choice of weighting functions is avoided
- Instead of computing a single optimal solution the Pareto front is computed
- The designer chooses his/her preferred optimal solution
- Other measurements such as minimum distance from Utopia region to a point on the Pareto front can be used

A Multiobjective Optimization Approach for SC problems

For dealing with single objective scheduling and control problems the following objective function (Ω) was employed:

$$\Omega = \varphi_1 - \varphi_2$$

where the individual objective functions φ_1 and φ_2 read as follows,

$$\begin{aligned} \varphi_1 &= \sum_{i=1}^{N_p} \frac{C_i^p W_i}{T_c} - \sum_{i=1}^{N_p} \frac{C_i^s (G_i - W_i / T_c)}{2\Theta_i} \\ \varphi_2 &= \int_0^{t_f} \sum_i \Delta x_i(t)^2 dt \end{aligned}$$

where the first part of the φ_1 term corresponds to the earnings concerning the sales of the products, whereas the second part represents the inventory costs and φ_2 is a function related with the off-set or deviation from the target steady-states and it is a measure of the dynamic performance of the processing system.

A Multiobjective Optimization Approach for SC problems

- φ_1 and φ_2 are conflicting objectives
- Large φ_1 values mean systems with high profit that commonly lead to poor dynamic performance (i.e. large φ_2 values): more attention is paid to selecting a good scheduling strategy with less emphasis on process dynamics
- Ideally, we would like to achieve large φ_1 values and small φ_2 values
- Since this is not possible a trade-off between the two objectives ought to be established
- Although there are some methods for computing the Pareto front, the ε-constraint method was used due to is simplicity

A Multiobjective Optimization Approach for SC problems

- In the ε-constraint method one of the objectives is selected to be optimized and the others are converted into constraints bounded by a parameter ε
- An advantage of the ε-constraint method over the weighting method to solve Multiobjective problems is that the ε-constraint method can find a Pareto optimal solution even for non convex problems
- Following the ε-constraint approach, we separated the original objective function and formed the next Multiobjective optimization problem

$$\max \quad \Omega = \varphi_1$$

subject to

$$\begin{aligned} \varphi_2 &\leq \varepsilon \\ g(x, y, u) &\leq 0 \end{aligned}$$

$$(1)\ 2R_1 \xrightarrow{k_1} A; \quad (2)\ R_1 + R_2 \xrightarrow{k_2} B; \quad (3)\ R_1 + R_3 \xrightarrow{k_3} C$$

$$\begin{aligned}
\frac{dC_{R_1}}{dt} &= \frac{(Q_{R_1} C^i_{R_1} - QC_{R_1})}{V} + \Re_{r_1} \\
\frac{dC_{R_2}}{dt} &= \frac{(Q_{R_2} C^i_{R_2} - QC_{R_2})}{V} + \Re_{r_2} \\
\frac{dC_{R_3}}{dt} &= \frac{(Q_{R_3} C^i_{R_3} - QC_{R_3})}{V} + \Re_{r_3} \\
\frac{dC_A}{dt} &= \frac{Q(C^i_A - C_A)}{V} + \Re_A \\
\frac{dC_B}{dt} &= \frac{Q(C^i_B - C_B)}{V} + \Re_B \\
\frac{dC_C}{dt} &= \frac{Q(C^i_C - C_C)}{V} + \Re_C \\
\Re_A &= k_1 C^2_{R_1}, \Re_B = k_2 C_{R_1} C_{R_2} \\
\Re_C &= k_3 C_{R_1} C_{R_3}, \Re_{r_1} = -\Re_A - \Re_B - \Re_C \\
\Re_{r_2} &= -\Re_B, \Re_{r_3} = -\Re_C \\
Q &= Q_{R_1} + Q_{R_2} + Q_{R_3}
\end{aligned}$$

where Q_{R_1}, Q_{R_2}, and Q_{R_3} are the feed stream volumetric flow rates of reactants R_1, R_2, and R_3, respectively.

Table: Operating Conditions Leading to the Manufacture of the A, B, and C Products of the Second Case Study

Product	Demand rate (Kg/h)	Product cost ($/Kg)	Inventory cost ($/Kg)
A	5	500	1.0
B	10	400	1.5
C	15	600	1.8

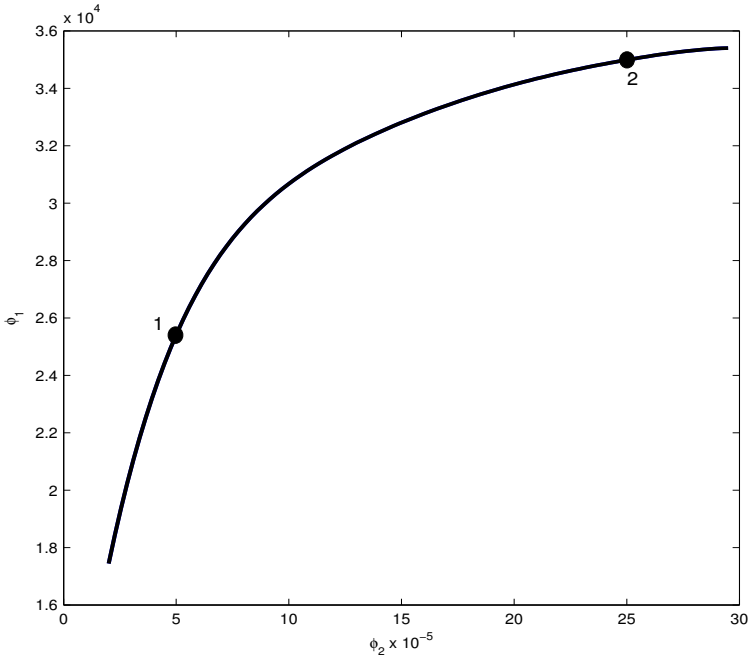


Figure: Pareto curve for the second case of study. The coordinates for the first and second points are: $[\phi_2^1, \phi_1^1] = [5\text{x}10^{-5}, 25590]$ and $[\phi_2^2, \phi_1^2] = [2.5\text{x}10^{-4}, 35250]$, respectively.

Table: Results for the the first optimal operating point. The objective function values are: $\phi_2^1 = 5\text{x}10^{-5}$ and $\phi_1^1 = 25590$.Total cycle time is 659.3 h.

Slot	Prod	Process time (min)	Prod rate (Kg/min)	w (Kg)	Transition time (min)	T start (min)	T end (min)
1	A	49.423	66.700	3296.519	10	0.000	59.423
2	B	92.456	71.310	6593.038	10	59.423	161.879
3	C	447.425	89.520	40053.458	50	161.879	659.304

Table: Results for the the second optimal operating point. The objective function values are: $\phi_2^2 = 2.5\text{x}10^{-4}$ and $\phi_1^2 = 35250$.Total cycle time is 327.8 h.

Slot	Prod	Process time (min)	Prod rate (Kg/min)	w (Kg)	Transition time (min)	T start (min)	T end (min)
1	B	45.969	71.310	3278.079	10	0.000	55.969
2	A	24.573	66.700	1639.039	10	55.969	90.543
3	C	227.265	89.520	20344.778	10	90.543	327.808

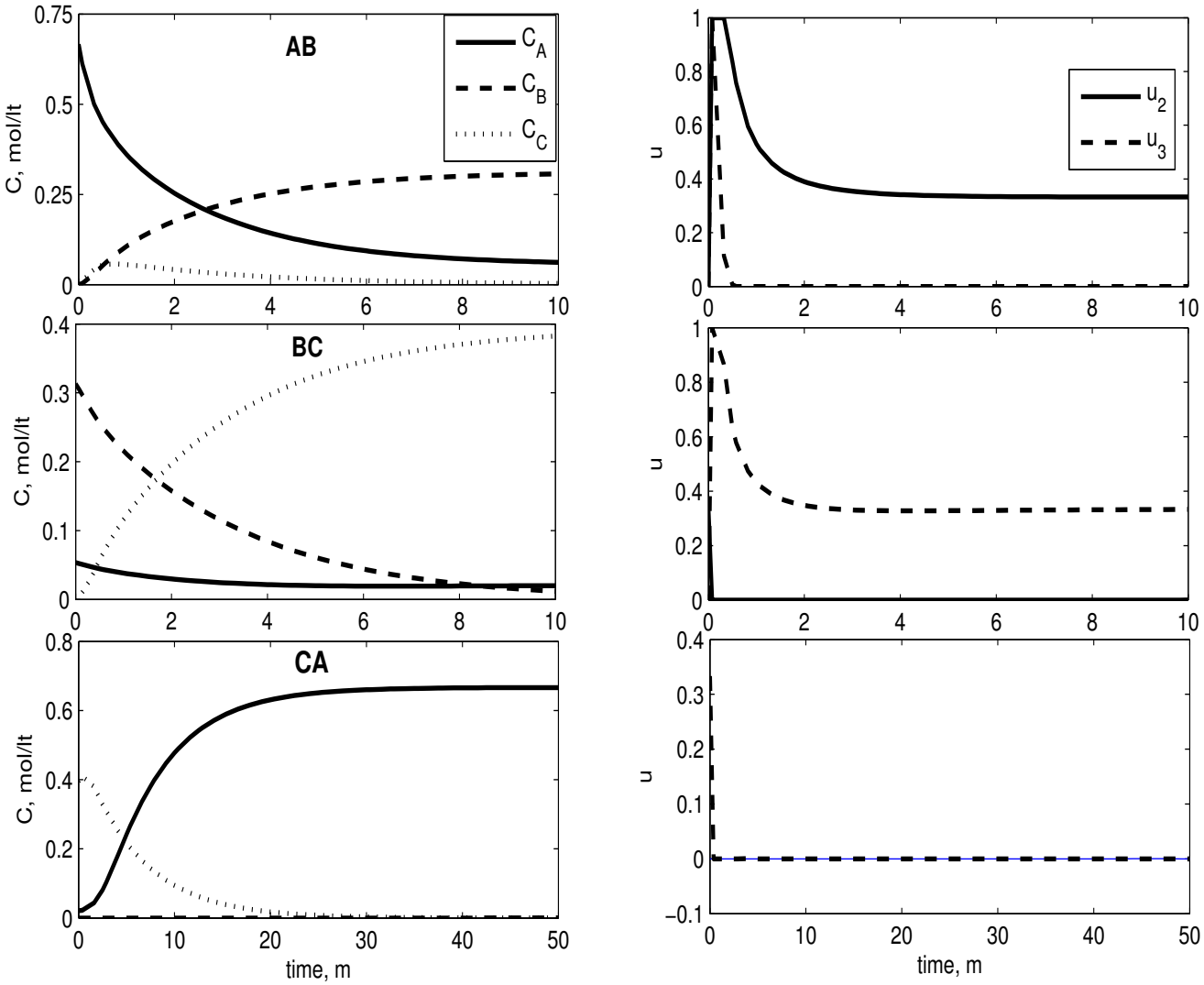


Figure: Optimal dynamic transition profiles for reactor concentration and volumetric flow rate for the first point of the Pareto front.

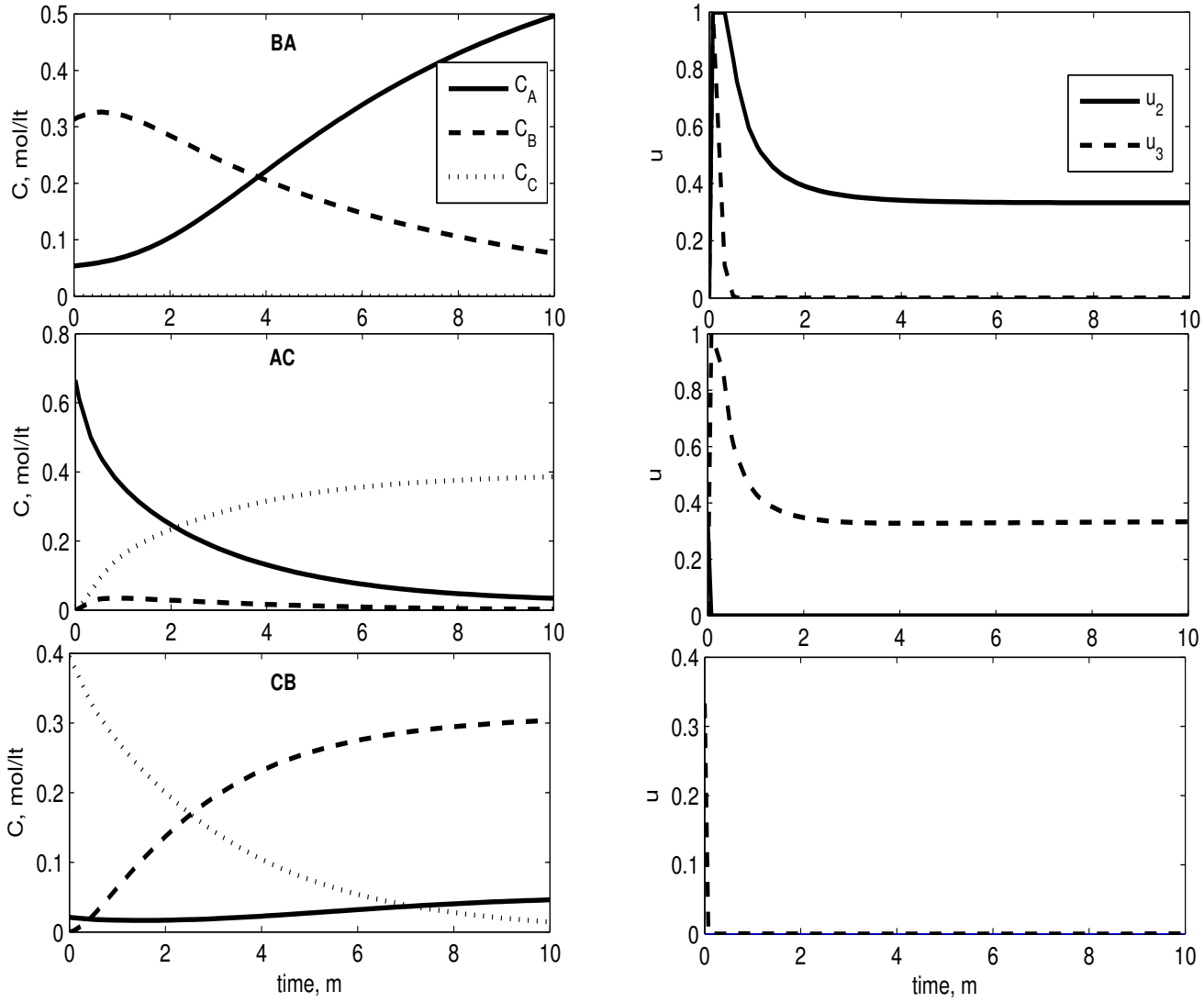


Figure: Optimal dynamic transition profiles for reactor concentration and volumetric flow rate for the second point of the Pareto front.

Conclusions

- An algorithmic framework for addressing Scheduling and Control problems using a MIDO formulation was presented
- The SC MIDO formulation was successfully applied to several case studies of varying complexity such as chemical reactors featuring strong nonlinear behavior, bifurcation points, unstable operating regions, multiple steady-states
- Presently the SC MIDO formulation only computes off-line optimal control policies, no consideration of the effect of uncertainties or disturbances

Future Work

- Real-Time Optimization for Scheduling and Control
- Stochastic Scheduling and Control
- Large-Scale Scheduling and Control
- Integration of Planning, Scheduling and Control

1. Antonio Flores-Tlacuahuac, I.E. Grossmann, "An Effective MIDO Approach for the Simultaneous Cyclic Scheduling and Control of Polymer Grade Transition Operations", In W. Marquardt and C. Pantelides, editors. In *16th European Symposium on Computer Aided Process Engineering and 9th International Symposium on Process System Engineering*, pages 1221-1226, Elsevier, 2006. ISBN: 978-0-444-52970-1.
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