# A MultiObjective Optimization Approach for the Simultaneous Single Line Scheduling and Control of CSTRs

| | |
|---|---|
| Journal: | *Industrial & Engineering Chemistry Research* |
| Manuscript ID: | Draft |
| Manuscript Type: | Article |
| Date Submitted by the Author: | n/a |
| Complete List of Authors: | Tlacuahuac, Antonio; Universidad Iberoamericana, Chemical Engineering<br>Gutierrez-Limon, Miguel Angel; Universidad Iberoamericana, chemical Engineering<br>Grossmann, Ignacio; Carnegie Mellon University, Chemical Engineering |
| | |

# A MultiObjective Optimization Approach for the Simultaneous Single Line Scheduling and Control of CSTRs

Miguel Angel Gutiérrez-Limón, Antonio Flores-Tlacuahuac*

Departamento de Ingeniería y Ciencias Químicas, Universidad Iberoamericana,

Prolongación Paseo de la Reforma 880, México, D.F. 01219, México

Ignacio E. Grossmann

Department of Chemical Engineering, Carnegie-Mellon University,

5000 Forbes Avenue, Pittsburgh, Pennsylvania 15213

August 5, 2011

*To whom correspondence should be addressed. E-mail: antonio.flores@uia.mx

**Abstract**

A new multiobjective optimization formulation dealing with simultaneous scheduling and control issues in single line processing systems is proposed. Objective functions featuring economic profits and dynamic performance are considered because normally they are in conflict. Because integer, continuous variables and process dynamic behavior are involved the optimization problem is cast in terms of a Mixed-Integer Dynamic Optimization (MIDO) problem. The Pareto front of each problem is computed using the $\epsilon$-constraint method for handling multiobjective problems. The results indicate that improved optimal solutions can be obtained by using multiobjective optimization techniques instead of just simple merging all the target objective functions into a single objective. The proposed multiobjective approach for handling scheduling and control problems is illustrated using three CSTR examples of varying nonlinear behavior.

# 1 Introduction

With the ever world-wide increasing competition to improve economic profits new ways of addressing the solution of processing problems are required. In particular, in the field of process operations scheduling and control problems are a clear example of processing problems that can benefit from using new and integrated ways of solving such problems. In fact, scheduling and control problems are normally solved in a sequential manner [1], [2]. First transition times are fixed (i.e. process dynamics is neglected) and the optimal processing sequence is determined. Second, an optimal production sequence is fixed and then a set of control actions driving the process between all two products combination (as demanded by the sequence production) is computed. The result of solving the scheduling and control problem in this way is that the natural existing interactions between scheduling and control problems are not explicitly exploited leading to suboptimal solutions. Instead, when both problems are solved simultaneously improved optimal solutions have been reported for different kinds of processing systems [3] ,[4]. Moreover, there are some additional ways to get improved optimal solutions: (a) using a multiobjective optimization approach, (b) considering a real time scheduling and control approach and (c) taking into account process uncertain behaviour. In this work we explore the solution of scheduling and control problems taking into account the presence of several objective functions leading to the formulation of multiobjective scheduling and control optimization problems. Multiobjective scheduling optimization [5], [6] and control problems [7], [8], [9], [10], [11] have been treated separately. In this work we propose an optimization formulation to merge both problems. A recent review on scheduling and control issues can be found elsewhere [12].

Engineering problems normally feature several and conflicting design and/or operation objectives. Polymerization reactors are a good example of systems featuring conflicting design objectives. For instance, commonly in free radicals polymerization kinetics there is a trade-off between monomer conversion and molecular weight distribution [13] making difficult to achieve large monomer conversions and large molecular weight distributions simultaneously. Because of productivity targets normally large conversions are required, whereas for certain applications large values of the molecular weight distributions are also demanded. However, increasing conversion leads to decreased molecular weight and vice-versa. Hence, a trade-off between the two design variables must be formulated.

Although a common approach to address the design and operation of processing systems featuring several design objectives consists in merging all the objectives into a single one design objective [14], such an approach has several weaknesses: (a) it requires the selection of weighting functions that can be difficult to justify and (b) it may lead to sub-optimal solutions. Both problems can be removed, to a certain extent, by addressing such problems as true multiobjective design and optimization issues. Working along this line the selection of sometimes subjective weighting functions can be avoided and improved optimal solutions can be attained. In this work a Mixed-Integer Dynamic Optimization Non-Linear Programming (MIDO) formulation is used for addressing simultaneous scheduling and control problems. The problem to be tackled consists in computing simultaneously the best production sequence and optimal dynamic transition trajectories such that a set of production targets are met. The objective functions considered are the process economic profit and variables deviations from their desired steady-state values, since the systems work under continuous processing conditions. Ideally one would like to obtain scheduling and control process solutions featuring large economic profits while having small deviations from desired target points. Both are desirable and conflicting objectives because highly profitable systems usually present large deviation of state variables and vice versa. Therefore, the Pareto front between these two objectives is attained and several optimal solutions along this curve are shown and discussed. We have not addressed the selection of the best multiobjective optimal solution since this is not a fully solved problem whose consideration demands the intervention of an expert [15] or the deployment of algorithmic methods [16]. As far as we know no other multiobjective optimization formulations have been proposed in the research literature for dealing with simultaneous scheduling and control issues.

## 2 Problem Formulation

The problem to be solved can be formulated as follows: "Given is a set of products to be manufactured in a single CSTR and in a single processing line, product cost, inventory cost, raw material cost and product demands, the problem consists in the simultaneous determination of the best production cycle and optimal products transitions such that each one of the optimal solutions corresponds to a point along the Pareto front where the objective functions are the process economic profit and the dynamic performance of such a process". For each one of the optimal solution points located on the Pareto curve the major decision variables corresponds to: optimal production sequence, amounts to be manufactured of each product, production times, transition times, optimal transition trajectory and the optimal values of the control variables. Finally, as discussed in [3] we have used a production wheel with a cyclic schedule, which is a valid production strategy assuming that the product demand rates are constant.

## 3 Multiobjective Scheduling and Control Formulation

In previous works [3], [17] we have proposed an optimization formulation able to deal with simultaneous single line scheduling and control problems using a single objective function. Although multiobjective optimization problems are sometimes reformulated as single optimization problems [14], by proper weighting of the individual objective functions, they should be approached and solved as true multiobjective optimization problems using some of the methods proposed for this aim [18], [19]. There are at least two reasons to do so: (1) The subjective choice of weighting functions is avoided and (2) Improved optimal solutions can be obtained. However, a clear disadvantage of multiobjective optimization calculations is that, for complex systems, computational times can be large.

For dealing with single objective scheduling and control problems the following objective function ($\Omega$) was employed [3]:

$$\Omega = \varphi_1 - \varphi_2 \tag{1}$$

where the individual objective functions $\varphi_1$ and $\varphi_2$ read as follows,

$$\varphi_1 = \sum_{i=1}^{N_p} \frac{C_i^p W_i}{T_c} - \sum_{i=1}^{N_p} \frac{C_i^s (G_i - W_i/T_c)}{2\Theta_i} \tag{2}$$

$$\varphi_2 = \int_0^{t_f} \sum_i \Delta x_i(t)^2 dt \tag{3}$$

where the first part of the $\varphi_1$ term corresponds to the earnings concerning the sales of the products, whereas the second part represents the inventory costs and $\varphi_2$ 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. As can be noticed, $\varphi_1$ and $\varphi_2$ have different units. $\varphi_1$ has economic profit units, whereas $\varphi_2$ has the units in which the variable $x_i$ is measured. Originally [3] $\varphi_2$ was transformed into a transition cost by using a proper weighting function. As defined $\varphi_1$ and $\varphi_2$ are conflicting objectives. In fact, large $\varphi_1$ values mean systems with high profit that commonly lead to poor dynamic performance (i.e. large $\varphi_2$ values): more attention is paid to selecting a good scheduling strategy with less emphasis on process dynamics. Ideally, we would like to achieve large $\varphi_1$ values and small $\varphi_2$ values. Since this is not possible a trade-off between the two objectives ought to be established. In a multi objective optimization problem (MOO) there are at least two objectives involving a set of decision variables and constraints. These objectives are often conflicting. In such situations, there will be many optimal solutions to the MOO problem, all of which are equally good in the sense that each one of them is better than the rest in at least one objective. This implies that one objective improves while at least another objective becomes worse when one moves from one optimal solution to another. The solutions of a MOO problem are known as the Pareto-optimal solutions and give rise to an infinite set of points known as the Pareto front. In this work we have used the $\varepsilon$-constraint approach [20] for attaining the Pareto front although some other options are also available [18].

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

$$\max \quad \Omega = \varphi_1 \tag{4}$$

subject to

$$\varphi_2 \leq \varepsilon \tag{5}$$

$$g(x, y, u) \leq 0 \tag{6}$$

In this way, the MOO problem has been transformed into a single objective optimization problem (SOO) by considering the function $\varphi_2$ as an additional inequality constraint. Even when the MOO problem was transformed into a SOO problem no arbitrary weighting functions were used for this purpose. We must emphasize that $\varphi_2$ is somewhat different in its present form in relationship to its original form [3] and no longer requires a weighting function. Of course the MOO problem is also subject to the constraints associated to the scheduling and dynamics behavior of the problem given by Equation 6 where $x$ stands for the continuous variables, $y$ represents the binary variables and $u$ stands for the manipulated variables. Because those constraints have been discussed in detail in previous works [3] they are not explicitly mentioned in the present work. We only highlight that the MOO problem turns out to be a Mixed-Integer Dynamic Optimization (MIDO) problem. To solve the MIDO problem we use a simultaneous discretization approach [21] to transform the MIDO problem into a Mixed-Integer Non-Linear problem (MINLP) that can be solved by standard techniques aimed to solve non-convex MINLPs [22]. Specifically, in this work the Sbb MINLP solver available in Gams [23] was used.

# 4 Case Studies

In this section 3 CSTRs case studies were undertaken for illustrating the MOO approach proposed in the present work. We have previously used the same examples for addressing single line and single objective scheduling and control problems [3]. In the next examples a two-steps procedure to attain a Pareto front for each case is shown. First we chose a range of values of $\varepsilon$, and then we solved the SOO problem, which is a Mixed Integer Dynamic Optimization (MIDO) problem, just as described above for each value of $\varepsilon$ and represented by Equations 4-6. That is, each point in the Pareto front represents the solution of a MIDO problem, a difficult task per se.

## 4.1 CSTR with a Simple Irreversible Reaction.

The first example consists of a CSTR featuring quasi-linear behavior. The model is simple enough for testing the multi-objective scheduling and control methodology previously proposed, but it has embedded nonlinear behavior to make it a challenging problem. Consider the following reaction taking place in an isothermal, constant holdup CSTR for manufacturing five different products, $A, B, C, D$ and $E$:

$$3R \xrightarrow{k} P, -\Re_R = kC_R^3 \tag{7}$$

The isothermal dynamic composition model is given by

$$\frac{dC_R}{dt} = \frac{Q}{V}(C_0 - C_R) + \Re_R \tag{8}$$

where $C_R$ is the reactant composition, $V$ is the reactor volume, $C_0$ stands for the feed stream composition, $k$ is the reaction rate and $Q$ is the feed stream volumetric flow rate which is also the manipulated variable for the transition between the involved products. Table 1 shows the steady state values of $Q$ and $C_R$ leading to the manufacture of the different products as well the demand rate, product and inventory costs. The numerical value of the system parameters are: $C_0 = 1$ mol/L, $V = 5000$ L, $k = 2$ L$^2$/ (mol$^2$-h). We solved the MOO problem as a series of single objective problems, as previously stated. The range of values of $\phi_2$ varied from 73 to 128 and the Pareto curve is shown in Figure 1.

Table 1: Operating Conditions for Manufacturing Products and Design and Kinetic Parameters for First Case Study.

| Product | $Q$ (L/h) | $C_R$ (mol/L) | Demand rate (Kg/h) | Product Cost ($/Kg) | Inventory cost ($/Kg) |
|---|---|---|---|---|---|
| $A$ | 10 | 0.0967 | 3 | 200 | 1.0 |
| $B$ | 100 | 0.2 | 8 | 150 | 1.5 |
| $C$ | 400 | 0.3032 | 10 | 130 | 1.8 |
| $D$ | 1000 | 0.393 | 10 | 125 | 2.0 |
| $E$ | 2500 | 0.5 | 10 | 120 | 1.7 |

It is clear that any point along the Pareto front represents an optimal solution of the simultaneous scheduling and control problem. From this point of view no point is better or worse than the remaining points, and it is up to the designer to pick up a given optimal solution as the best solution for the purposes at hand. There are in the

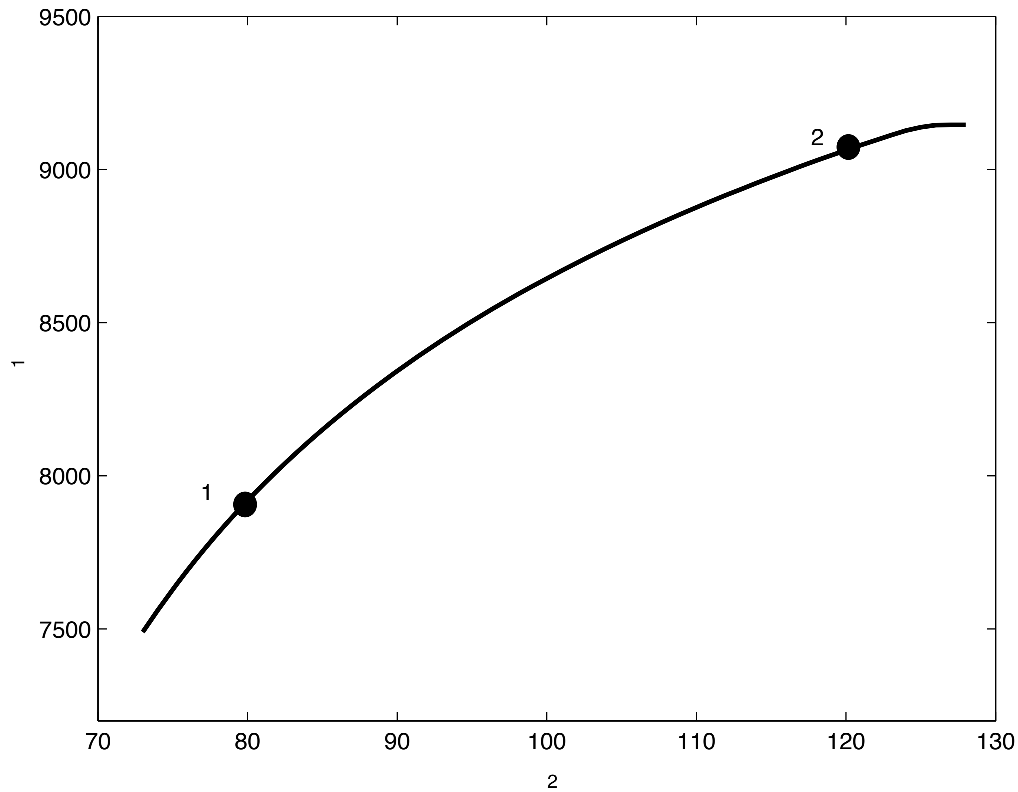


Figure 1: Pareto front for First Case Study. The coordinates for the first and second points are: $[\phi_2,^1 \phi_1^1] = [80, 7919]$ and $[\phi_2^2, \phi_1^2] = [120, 9063]$, respectively.

literature some methods based on heuristics [15] and in algorithmic procedures [16] to help to select the best optimal point. However, in all the examples addressed in this work we arbitrarily selected two optimal points along the Pareto front to discuss and compare the quality of the scheduling and control optimal solutions. Accordingly, in Tables 2 and 3 the optimal scheduling and control results for points 1 and 2 of the corresponding Pareto front (see Figure 1) are shown. As noticed, in the first point of the Pareto front the optimal production sequence turns out to be: $D \rightarrow C \rightarrow B \rightarrow A \rightarrow E$, whereas in the second point of the Pareto front the optimal sequence is: $E \rightarrow D \rightarrow C \rightarrow B \rightarrow A$. Because of the assumption of a cyclic production wheel, actually both optimal sequences turn out to be the same sequence. The CPU times are 36 and 49 sec for the first and second points, respectively, whereas the number of constraints for both cases is 1270. All the problems were solved deploying the Sbb MINLP solver available in Gams [23].

Table 2: First Case Study: Scheduling and Control results for the the first optimal operating point. The objective function values are: $\phi_2^1 = 80$ and $\phi_1^1 = 7919$. Total cycle time is 132 h.

| Slot | Product | Process time (h) | Production rate (Kg/h) | $w$ (Kg) | Transition time (h) | T start (h) | T end (h) |
|---|---|---|---|---|---|---|---|
| 1 | $D$ | 2.169 | 607.000 | 1316.852 | 5.000 | 0.000 | 7.169 |
| 2 | $C$ | 4.725 | 278.720 | 1316.852 | 7.119 | 7.169 | 19.013 |
| 3 | $B$ | 13.169 | 80.000 | 1053.481 | 20.994 | 19.013 | 53.176 |
| 4 | $A$ | 43.735 | 9.033 | 395.055 | 5.000 | 53.176 | 101.910 |
| 5 | $E$ | 24.775 | 1250.000 | 30968.407 | 5.000 | 101.910 | 131.685 |

However, in terms of the value of the objective functions, both optimal production sequences are not completely equivalent. In fact, the second point of the Pareto front features higher economic profit but worse dynamic performance ( $\phi_2^2 = 120$, $\phi_1^2 = 9063$) in comparison to the first point of the same Pareto front which exhibits worse economic profit but slightly better dynamic performance ($\phi_2^1 = 80$, $\phi_1^1 = 7919$). These results clearly indicate that both objective functions are in conflict: improving the economic profit would lead to poorer dynamic performance and vice versa. The optimal dynamic transitions are depicted in Figures 2 and 3. As noticed from these Figures, and for this reason they are included in this case study, differences in dynamic performance are hardly evident although they exist. However, even when from a dynamic behavior point of view, both processing

Table 3: First Case Study: Scheduling and Control results for the the second optimal operating point. The objective function values are: $\phi_2^2 = 120$ and $\phi_1^2 = 9063$.Total cycle time is 126.3 h.

| Slot | Product | Process time (h) | Production rate (Kg/h) | w (Kg) | Transition time (h) | t start (h) | t end (h) |
|---|---|---|---|---|---|---|---|
| 1 | $E$ | 23.984 | 1250.00 | 29980.158 | 5.000 | 0.000 | 28.984 |
| 2 | $D$ | 2.080 | 607.00 | 1262.344 | 5.000 | 28.984 | 36.064 |
| 3 | $C$ | 4.529 | 278.72 | 1262.344 | 5.000 | 36.064 | 45.693 |
| 4 | $B$ | 12.623 | 80.00 | 1009.875 | 20.994 | 45.693 | 79.310 |
| 5 | $A$ | 41.924 | 9.03 | 378.703 | 5.000 | 79.310 | 126.234 |

systems look similar the proposed MOO approach allowed us to detect improved optimal solutions.

## 4.2 CSTR with Simultaneous Reactions and Input Multiplicities

In this example, the following set of reactions:

$$2R_1 \xrightarrow{k_1} A$$
$$R_1 + R_2 \xrightarrow{k_2} B$$
$$R_1 + R_3 \xrightarrow{k_3} C$$

is carried out in an isothermal CSTR for manufacturing products $A$, $B$, and $C$ starting from the reactants $R_1$, $R_2$, and $R_3$. The dynamic mathematical model and kinetic rate expressions read as follows:

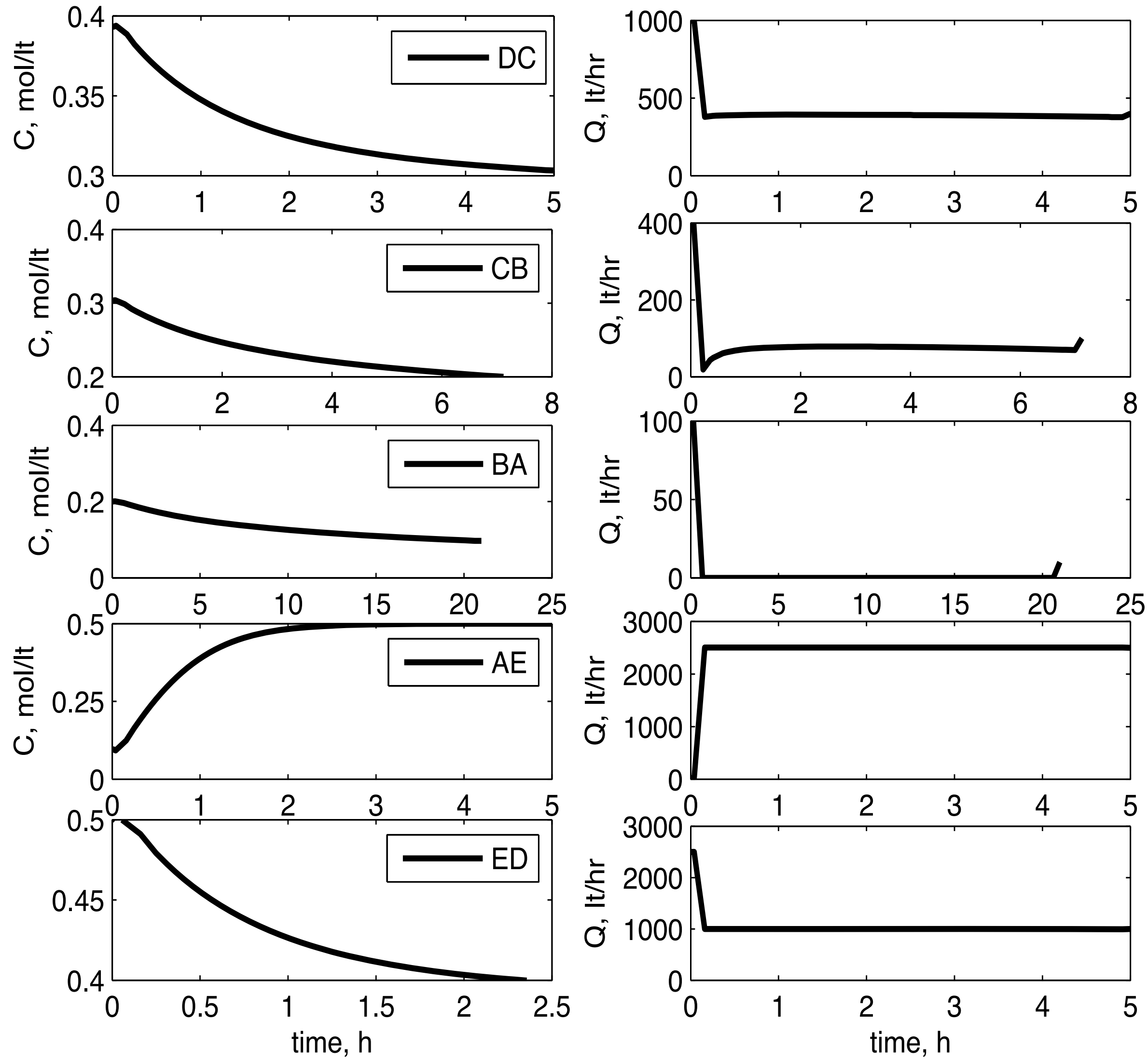


Figure 2: First Case Study: Optimal dynamic transition profiles for reactor concentration and volumetric flow rate for the first point of the Pareto front.

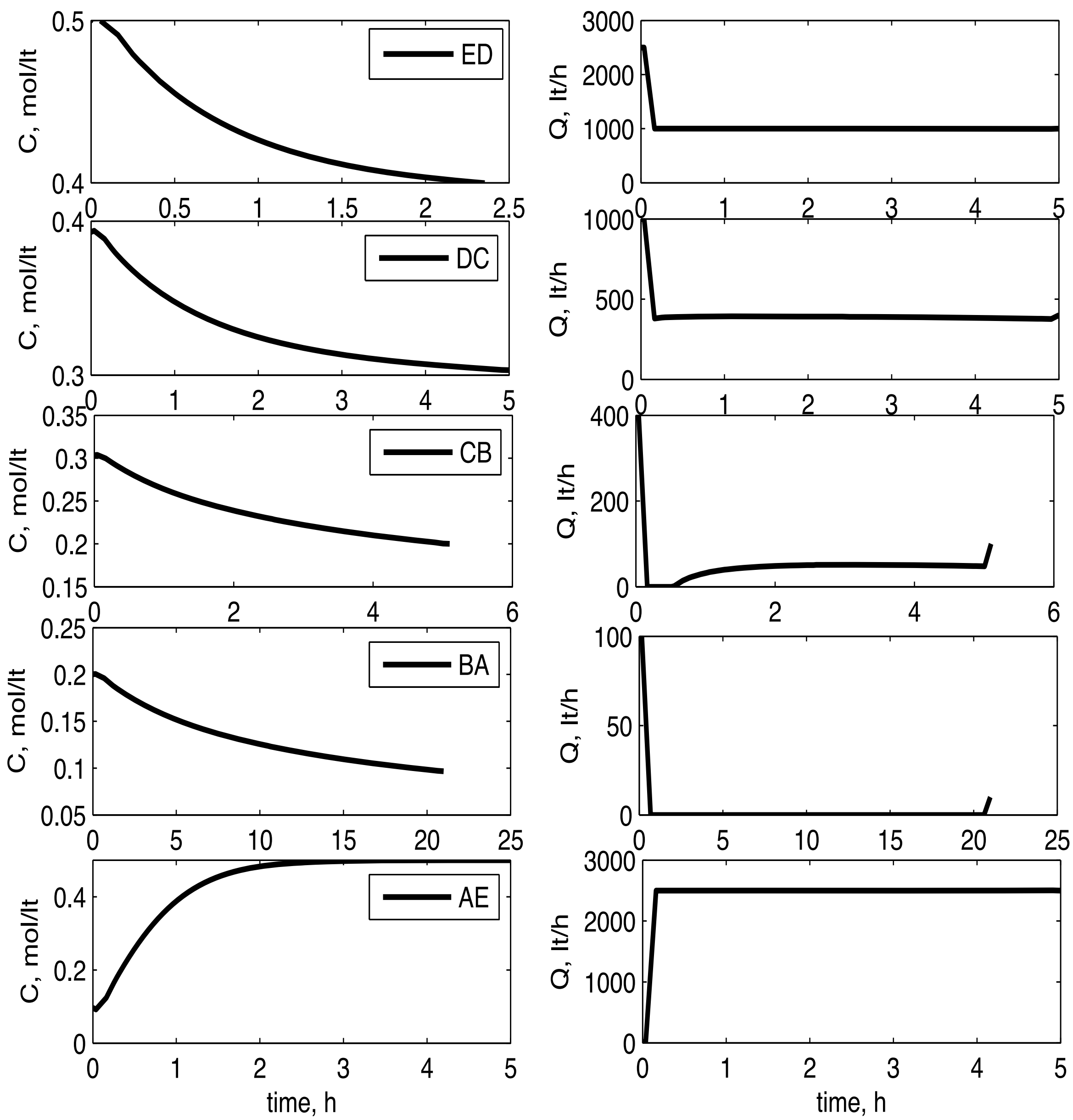


Figure 3: First Case Study: Optimal dynamic transition profiles for reactor concentration and volumetric flow rate for the second point of the Pareto front.

$$\frac{dC_{R_1}}{dt} = \frac{(Q_{R_1}C^i_{R_1} - QC_{R_1})}{V} + \Re_{r_1} \quad (9)$$

$$\frac{dC_{R_2}}{dt} = \frac{(Q_{R_2}C^i_{R_2} - QC_{R_2})}{V} + \Re_{r_2} \quad (10)$$

$$\frac{dC_{R_3}}{dt} = \frac{(Q_{R_3}C^i_{R_3} - QC_{R_3})}{V} + \Re_{r_3} \quad (11)$$

$$\frac{dC_A}{dt} = \frac{Q(C^i_A - C_A)}{V} + \Re_A \quad (12)$$

$$\frac{dC_B}{dt} = \frac{Q(C^i_B - C_B)}{V} + \Re_B \quad (13)$$

$$\frac{dC_C}{dt} = \frac{Q(C^i_C - C_C)}{V} + \Re_C \quad (14)$$

$$\Re_A = k_1 C^2_{R_1} \quad (15)$$

$$\Re_B = k_2 C_{R_1} C_{R_2} \quad (16)$$

$$\Re_C = k_3 C_{R_1} C_{R_3} \quad (17)$$

$$\Re_{r_1} = -\Re_A - \Re_B - \Re_C \quad (18)$$

$$\Re_{r_2} = -\Re_B \quad (19)$$

$$\Re_{r_3} = -\Re_C \quad (20)$$

$$Q = Q_{R_1} + Q_{R_2} + Q_{R_3} \quad (21)$$

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. $C^i_j$ is the feed stream concentration, $C_j$ is the product concentration both for $j = R_1, R_2, R_3, A, B, C$, $V$ is the reactor volume, and $k_1$, $k_2$, and $k_3$ are the kinetic constants. $Q$ is the total feed stream volumetric flow rate. The value of the design parameters and steady-state processing conditions can be found in Tables 5 and 6 in [3], whereas demand rate, product and inventory costs are shown in Table 4. With the provided design information the whole Pareto front is attained as depicted in Figure 4. The coordinates of the first and second points are: $[\phi^1_2, \phi^1_1]$ = [5x10$^{-5}$, 25590] and $[\phi^2_2, \phi^2_1]$ = [2.5x10$^{-4}$, 35250], respectively.

Table 4: 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 |

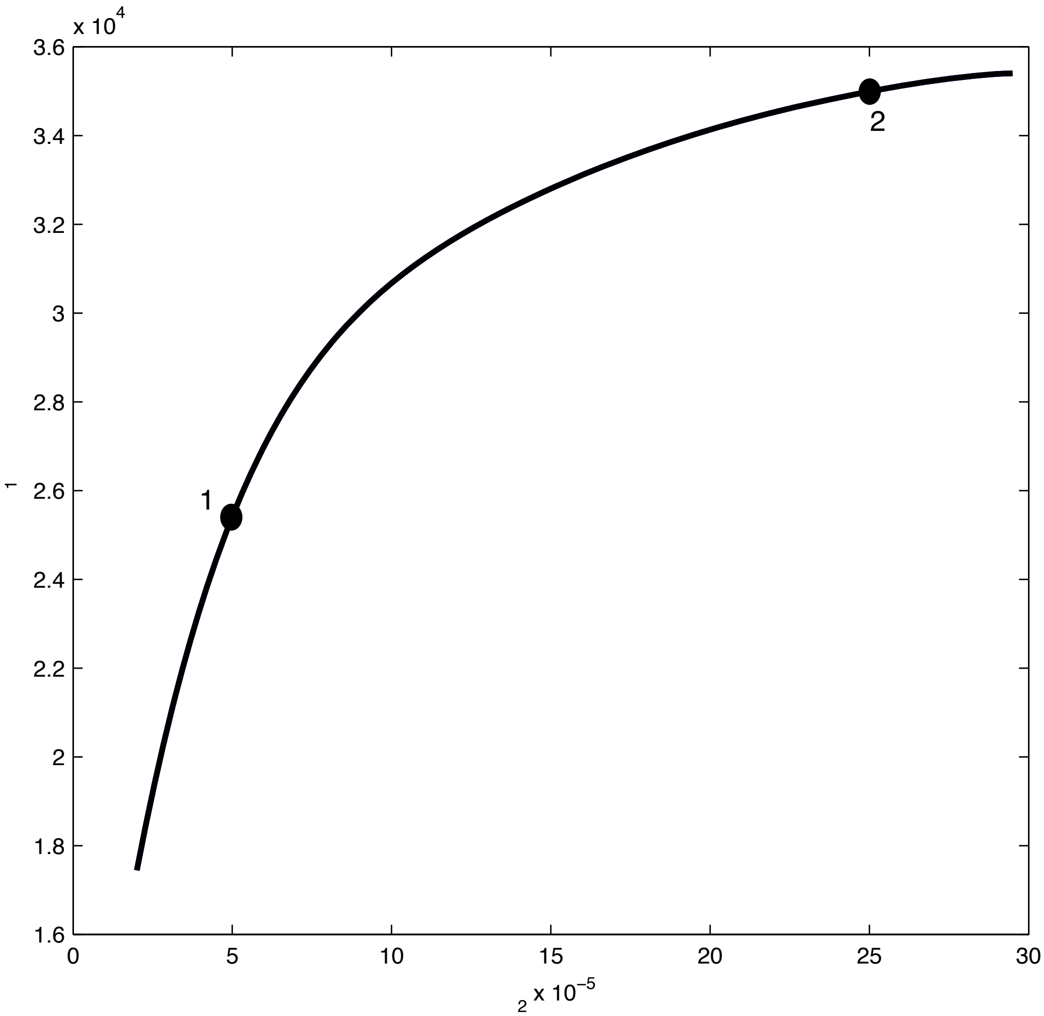


Figure 4: Pareto curve for the second case of study. The coordinates for the first and second points are: $[\phi_2^1, \phi_1^1] = [5\text{x}10^{-5}, 25590]$ and $[\phi_2^2, \phi_1^2] = [2.5\text{x}10^{-4}, 35250]$, respectively.

In Tables 5 and 6 the optimal scheduling and control results for points 1 and 2 of the corresponding Pareto front (see Figure 4) are shown. As seen, in the first point of

Table 5: Second Case Study: Scheduling and Control 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 | Product | Process time (min) | Production 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 6: Second Case Study: Scheduling and Control 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 | Product | Process time (min) | Production 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 |

the Pareto front the optimal production sequence is given by: $A \rightarrow B \rightarrow C$, whereas in the second point of the Pareto front the optimal sequence is: $B \rightarrow A \rightarrow C$. The CPU times are 1:42 min and 43.1 sec for the first and second points, respectively, whereas the number of constraints for both cases is 2831. As noticed, the second optimal solution features a higher economic profit ($35250) when compared to the profit attained at the first point ($25590). As a matter of fact, the cyclic time (327.8 h) of the second point turns out to be approximately half of the corresponding cyclic time (659.3 h) of the first point. As seen from results shown in Tables 5 and 6 the process time and the amount produced ($w$) also keep the same ratio between the two optimal operating points. This observation is important because it clearly states that the required product demand can be met using shorter processing times and increasing the economic profit. This fact also highlights the importance of the multi-objective optimization approach for scheduling and control problems: without computing the Pareto front it would be difficult to assess the advantage/disadvantage of a given optimal solution. The results from the Pareto front allow us to pick up an optimal point featuring target behavior. In Figures 5 and 6 the dynamic optimal transition profiles for the two points in the Pareto front are depicted. Because in both cases the value of the $\phi_2$ objective function turns out to be rather small the dynamic transition profiles exhibit smooth dynamic behavior.

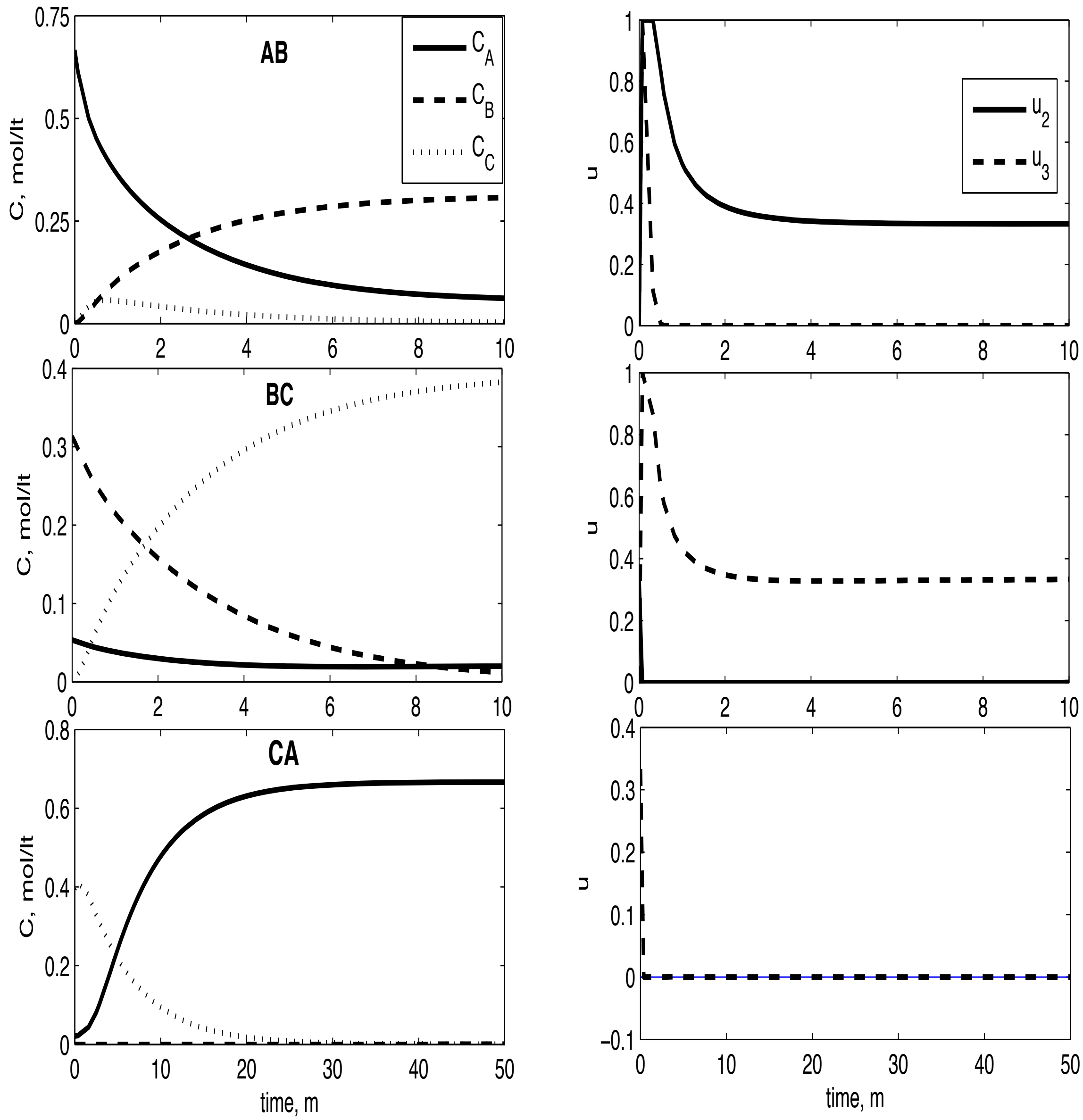


Figure 5: Second Case Study: Optimal dynamic transition profiles for reactor concentration and volumetric flow rate for the first point of the Pareto front.

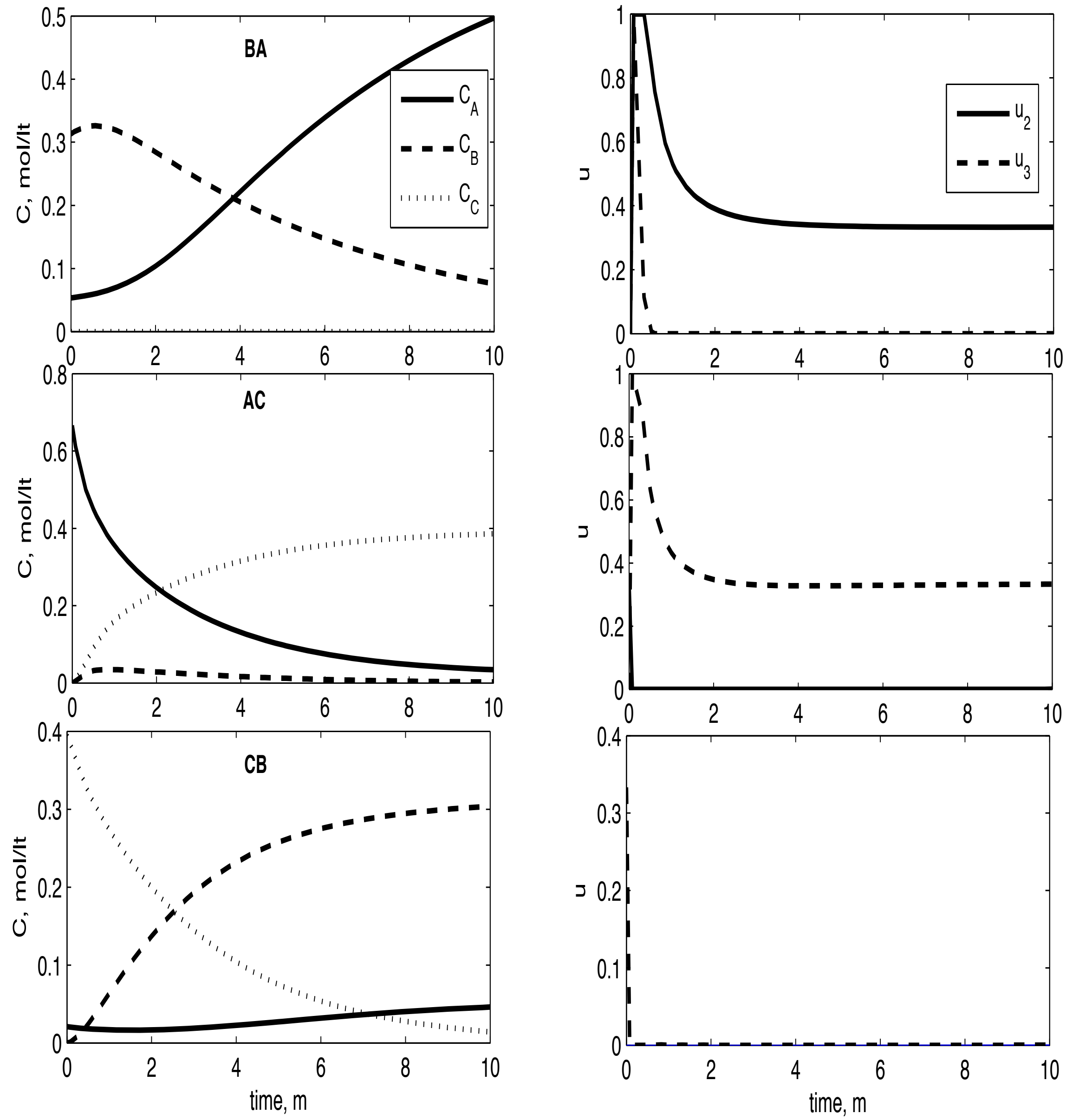


Figure 6: Second Case Study: Optimal dynamic transition profiles for reactor concentration and volumetric flow rate for the second point of the Pareto front.

## 4.3 CSTR with Output Multiplicities

The third example deals with highly non linear operating regions. The model was originally proposed by Hicks and Ray [24] and some of the original parameters were modified in order

Table 7: Parameters Values for the Third Case Study

| | | | | | |
|---|---|---|---|---|---|
| $\theta$ | 20 | residence time | $T_f$ | 300 | feed temperature |
| $J$ | 100 | $(-\Delta H)/(\rho C_p)$ | $k_{10}$ | 300 | pre exponential factor |
| $c_f$ | 7.6 | feed concentration | $T_c$ | 290 | coolant temperature |
| $\alpha$ | 1.95x10$^{-4}$ | dimensionless heat transfer area | $N$ | 5 | $E_1/(RJc_f)$ |

to end up with a multiplicity map. The model in its dimensionless form reads as:

$$\frac{dy_1}{dt} = \frac{1-y_1}{\theta} - k_{10}e^{-N/y_2}y_1 \tag{22}$$

$$\frac{dy_2}{dt} = \frac{y_f-y_2}{\theta} + k_{10}e^{-N/y_2}y_1 - \alpha u(y_2-y_c) \tag{23}$$

where $y_1$ denotes the dimensionless concentration $(c/c_f)$, $y_2$ is the dimensionless temperature $(T/Jc_f)$, $y_c$ is the dimensionless coolant temperature $(T_c/Jc_f)$, $y_f$ is the dimensionless feed temperature $(T_f/Jc_f)$, and $u$ is the coolant flow rate. Table 7 shows the numerical values of the parameters used for this example. Our purpose is to manufacture products $A$, $B$, $C$, and $D$ having as manipulated variable the feed stream flowrate $(u)$. Operating conditions leading to these products are shown in Table 8; demand rate, product and inventory costs are also provided. Using the design information the whole Pareto front is attained and depicted in Figure 7. The coordinates of the first and second points are: $[\phi_2^1, \phi_1^1] = [8.06,2700]$ and $[\phi_2^2, \phi_1^2] = [14.69,9300]$, respectively.

Table 8: Operating Conditions Leading to Products $A, B, C$ and $D$ of the third Case Study

| Product | $y_1$ | $y_2$ | $u$ | Demand rate (Kg/h) | Product ($/Kg) | Inventory cost ($/Kg) |
|---|---|---|---|---|---|---|
| $A$ | 0.0944 | 0.7766 | 340 | 110 | 100 | 1 |
| $B$ | 0.1367 | 0.7293 | 390 | 80 | 50 | 1.3 |
| $C$ | 0.1926 | 0.6881 | 430 | 87 | 30 | 1.4 |
| $D$ | 0.2632 | 0.6519 | 455 | 40 | 80 | 1.1 |

In Tables 9 and 10 the optimal scheduling and control results for points 1 and 2 of the corresponding Pareto front (see Figure 7) are shown. In the first point of the Pareto

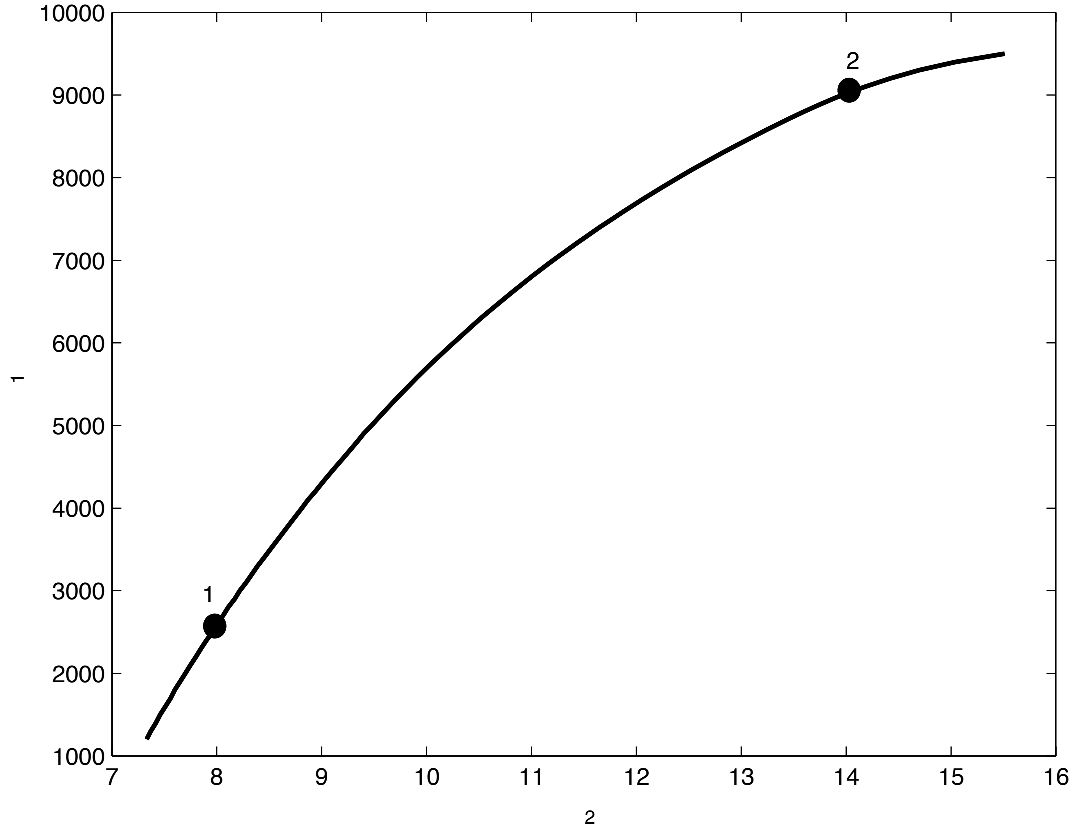


Figure 7: Pareto curve for the third case of study.The coordinates for the first and second points are: $[\phi_2,^1 \phi_1^1] = [8.06,2700]$ and $[\phi_2^2, \phi_1^2] = [14.69,9300]$, respectively.

Table 9: Third Case Study: Scheduling and Control results for the the first optimal operating point. The objective function values are: $\phi_2^1 = 8.06$ and $\phi_1^1 = 2700$.Total cycle time is 160 h.

| Slot | Product | Process time (h) | Production rate (Kg/h) | $w$ (Kg) | Transition time (h) | T start (h) | T end (h) |
|---|---|---|---|---|---|---|---|
| 1 | $D$ | 11.423 | 559.968 | 6396.627 | 10 | 0.000 | 21.423 |
| 2 | $A$ | 56.723 | 688.256 | 39039.728 | 10 | 21.423 | 88.146 |
| 3 | $B$ | 19.499 | 656.108 | 12793.254 | 11.504 | 88.146 | 119.149 |
| 4 | $C$ | 22.673 | 613.624 | 13912.664 | 18.094 | 119.149 | 159.916 |

front the optimal production sequence is given by: $D \rightarrow A \rightarrow B \rightarrow C$, whereas in the second point of the Pareto front the optimal sequence is: $B \rightarrow C \rightarrow D \rightarrow A$. The CPU times are 10.9 and 46.4 sec for the first and second points, respectively, whereas the

Table 10: Third Case Study: Scheduling and Control results for the the second optimal operating point. The objective function values are: $\phi_2^2 = 14.69$ and $\phi_1^2 = 9300$.Total cycle time is 119.4 h.

| Slot | Product | Process time (h) | Production rate (Kg/h) | $w$ (Kg) | Transition time (h) | T start (h) | T end (h) |
|---|---|---|---|---|---|---|---|
| 1 | $B$ | 14.552 | 656.108 | 9547.834 | 10 | 0.000 | 24.552 |
| 2 | $C$ | 16.921 | 613.624 | 10383.27 | 10 | 24.552 | 51.473 |
| 3 | $D$ | 8.525 | 559.968 | 4773.917 | 10 | 51.473 | 70.000 |
| 4 | $A$ | 39.349 | 688.256 | 27082.277 | 10 | 70.000 | 119.348 |

number of constraints for both cases is 2223. As noticed, because of the assumption of a cyclic production wheel, the two production sequences are actually the same. Despite this observation, the optimal solution of the second point of the Pareto front exhibits a higher economic profit ($9300) compared to the economic profit ($2700) attained from the first optimal point. It is clear that the second optimal solution is better than the first one because a reduction of the total cycle time: from 160 to 119.4 h. It is interesting to note that actually the amount produced of each product ($w$) becomes also smaller. This means that for each product $w$ is larger in the first optimal solution. However, process profit depends not only on $w$ but also on the magnitude of the transition times. The difference in dynamic performance between the solutions is not large. Therefore, the two solutions should display the same optimal dynamic transition behavior. Because of this reason only the optimal dynamic transitions for the second point of the Pareto fronts are depicted in Figure 8.

# 5 Conclusions and Future Work

In this work we proposed an optimization formulation for dealing with multiobjective simultaneous single line scheduling and control problems. The formulation assumes that the addressed problems are solved off-line and without taking into account process uncertainty. The results obtained in the present work clearly demonstrates the advantages of

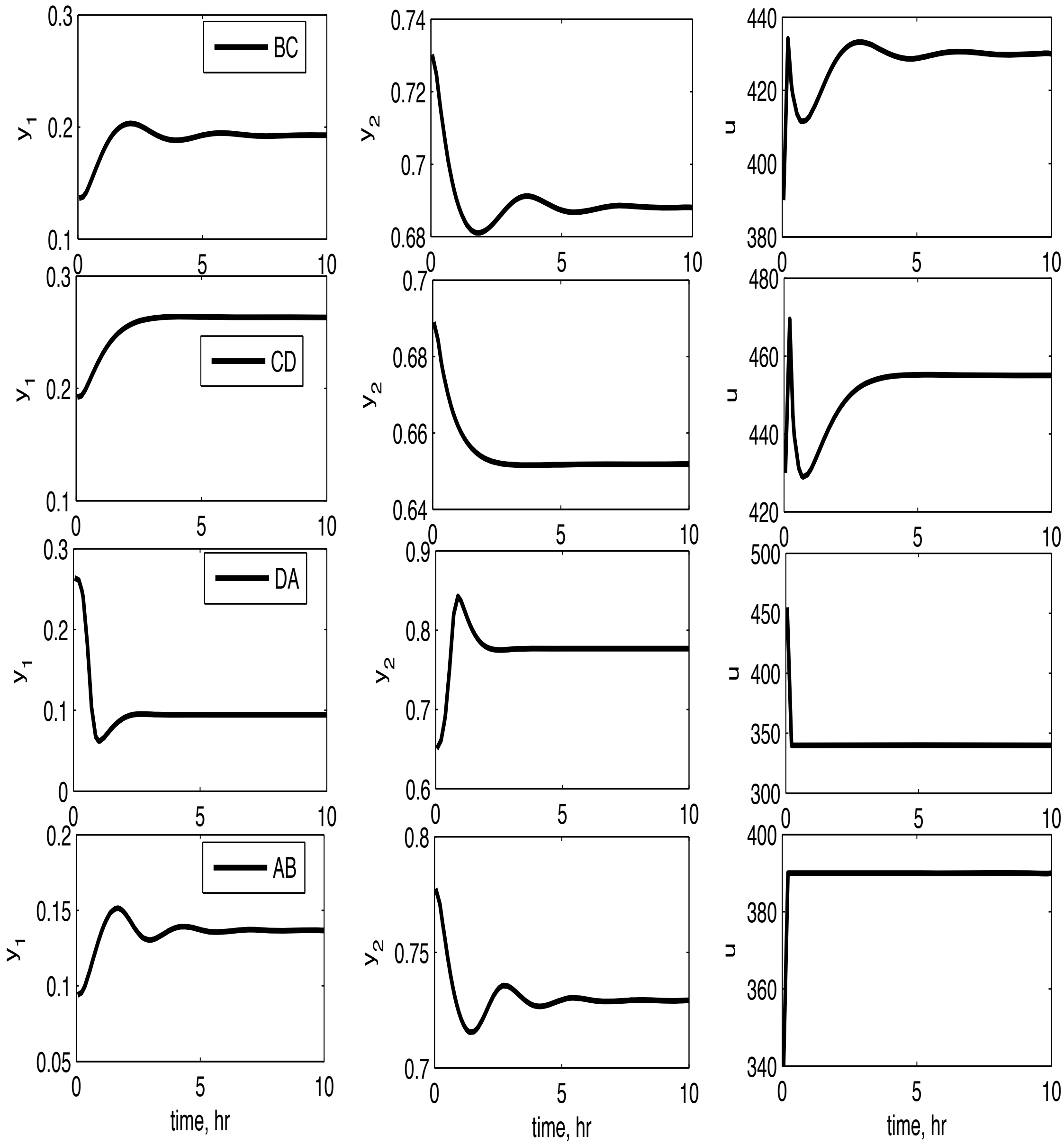


Figure 8: Third Case Study: Optimal dynamic transition profiles for dimensionless reactor concentration and temperature rate for the second point of the Pareto front.

considering a multiobjective approach for the addressed issues since full access to most of the optimal solutions is obtained. From an optimization point of view all the solutions are equally good and it is up to the designer to pick up the correct one according to certain design targets. Moreover, no other multiobjective scheduling and control optimization formulations have been proposed in the research literature. Of course, it could be stated that global optimization techniques can also handle these type of problems with the advantage of locating the best solution. The point with global optimization techniques for MINLP problems is that they require large CPU times and produce a single optimal solution. In contrast, multiobjective optimization techniques are simpler to implement and represent a good alternative to the use of global optimization techniques. Moreover, global optimization techniques normally feature a single objective function. Future work will deal with real-time scheduling and control problems using model predictive control techniques. Some work is in progress [25], [26] because a multiobjective control strategy is required for this purpose.

# Nomenclature

*Indices*

$i$, $p$=1,...,$N_p$: products

*Decision Variables*

$G_i$ =production rate

$T_c$ =total production wheel time

$W_i$ =amount produced of each product

$\Theta_i$ =total processing time of product $i$

*Parameters*

$N_p$ =Number of products

$C_i^p$ =price of products

$C_i^s$ =cost of inventory

$C^r$ =cost of raw material

$h_{fck}$ =length of finite element $f$ in slot $k$

$\Omega_{N_{cp},N_{cp}}$ =matrix of Radau quadrature weights

# References

[1] J.R. Richards J.P. Congalidis and W.H. Ray. Scheduling of Polymer Grade Transitions. *AIChE J.*, 48(8):1754–1764, 2002.

[2] A.C. Allcock R. Mahadevan, F.J. Doyle III. Scheduling of Polymer Grade Transitions. *AIChE J.*, 48(8):1754–1764, 2002.

[3] A. Flores-Tlacuahuac and I.E. Grossmann. Simultaneous Cyclic Scheduling and Control of a Multiproduct CSTR. *Ind. Eng. Chem. Res.*, 45(20):6175–6189, 2006.

[4] S. Terrazas-Moreno, A. Flores-Tlacuauhuac, and I.E. Grossmann. Simultaneous scheduling and control in polymerization reactors. *AIChE J.*, 53(9):2301–2315, 2007.

[5] J. Zhenya and M.G. Ierapetritou. Generate pareto optimal solutions of scheduling problems using normal boundary intersection technique. *Comput. Chem. Eng.*, 31(4):268–280, 2007.

[6] O. Baez Senties, C. Azzaro-Pantel, L. Pibouleau, and S. Domenech. Multiobjective scheduling for semiconductor manufacturing plants. *Comput. Chem. Eng.*, 34(4):555–566, 2010.

[7] Athanasios Tsoukas, Matthew Tirrell, and George Stephanopoulos. Multiobjective dynamic optimization of semibatch copolymerization reactors. *Chemical Engineering Science*, 37(12):1785 – 1795, 1982.

[8] E. Kerrigan, A. Bemporad, D. Mignone, M. Morari, and J. M. Maciejowski. Multiobjective prioritisation and reconfiguration for the control of constrained hybrid systems. *Proceedings of the American Control Conference*, pages 1694–1698, 2000.

[9] D. Zambrano and E. Camacho. Application of MPC with multiple objective for a solar refrigeration plant. *Proceedings of the IEEE Conference on Control Applications*, pages 1230–1235, 2002.

[10] A. Gambier. MPC and PID control based on multi-objective optimization. *Proceedings of the American Control Conference*, pages 4727–4732, 2008.

[11] A. Bemporad and D. Munoz de la Pena. Multiobjective model predictive control. *Automatica*, 35:2823–2830, 2009.

[12] I. Harjunkoski, R. Nystrom, and A. Horch. Integration of Scheduling and Control: Theory or Practice? *Comput. Chem. Eng.*, 33(12):1909–1918, 2009.

[13] B.R. Maner, F.J. Doyle, B.A. Ogunnaike, and R.K. Pearson. Nonlinear model predictive control of a simulated multivariable polymerization reactor using second-order volterra models. *Automatica*, 32(9):1285–1301, 1996.

[14] I. Das and J.E. Dennis. A closer look at drawbacks of minimizing weighted sums of objectives for pareto set generation in multicriteria optimization problems. *Structural Optim.*, (14):63–69, 1997.

[15] V. Vafaeyan and J. Thibault. Selection of pareto-optimal solutions for process optimization using rough set method: A new approach. *Computers and Chemical Engineering*, 30:1155–1168, 2009.

[16] I.E. Grossmann, R. Drabbant, and R.K. Jain. Incorporating toxicology in the synthesis of industrial chemical complexes. *Chemical Engineering Communications*, 17:151–170, 1982.

[17] Antonio Flores-Tlacuahuac and 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, *$16^{th}$ European Symposium on Computer Aided Process Engineering and $9^{th}$ International Symposium on Process System Engineering*, pages 1221–1226. Elsevier, 2006.

[18] A. Chinchuluun, , and P.M. Pardalos. A survey of recent developments in multiobjective optimization. *Ann Oper Res*, 154:29–50, 2007.

[19] I. Das and J.E. Dennis. Normal-bundary intersection: A new method for generating the pareto surface in nonlinear multicriteria optimization problems. *SIAM J. OPTIM.*, 8(3):631–657, 1998.

[20] Y.Y. Haimes, L.S. Lasdon, and D.A. Wismer. On a bicriterion formulation of the problems of integrated system identification and system optimization. *IEEE Transactions on Systems, Man and Cybernetics*, pages 296–297, 1971.

[21] L.T. Biegler. *Nonlinear Programming: Concepts, Algorithms, and Applications to Chemical Processes*. SIAM, 2010.

[22] P. Bonami, L.T. Biegler, A. Conn, G. Cornuejols, I.E. Grossmann, C. Laird, J. Lee, A. Lodi, F. Margot, N. Sawaya, and A. Waechter. An algorithmic framework for convex mixed integer nonlinear programs. *Discrete Optimization*, 5(2):186–204, 2008.

[23] A. Brooke, D. Kendrick, Meeraus, and R. A. Raman. *GAMS: A User's Guide*. GAMS Development Corporation, 1998, http://www.gams.com.

[24] G.A. Hicks and W.H. Ray. Approximation Methods for Optimal Control Synthesis. *Can. J. Chem. Eng.*, 40:522–529, 1971.

[25] A. Flores-Tlacuahuac, P. Morales, and M. Rivera-Toledo. Multiobjective Non-Linear Model Predictive Control of a Class of Chemical Reactors. Submitted for publication to *Industrial and Engineering Chemistry Research*, 2011.

[26] V.M Zavala and A. Flores-Tlacuahuac. Stability of Multi-Objective Predictive Control: An Utopia-Tracking Approach. Submitted for publication to *Automatica*, 2011.