

SCHEDULING AND CONTROL USING MULTIOBJECTIVE OPTIMIZATION APPROACH

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Abstract

A new multiobjective optimization formulation dealing with simultaneous scheduling and control issues is proposed. Objective functions featuring economic profits and dynamic performance are deployed 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 addressed problem is computed using the ϵ -technique for handling multiobjective problems. The results indicate that better optimal solutions can be attained by deploying 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 a CSTR example with nonlinear behavior.

Keywords

MULTIOBJECTIVE, SCHEDULING, CSTR

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 be benefited from using new and integrated ways of solving such problems. In fact, industrially scheduling and control problems are normally solved in a sequential manner (Richards et al., 2002), (Allcock et al., 2002). First 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 consequence of solving the scheduling and control problem along this way is that the natural existing interactions between scheduling and control problems are not exploited leading to

suboptimal solutions. When both problems are solved simultaneously improved optimal solutions have been reported for different kinds of processing systems (Flores-Tlacuahuac and Grossman, 2006), (Terrazas-Moreno et al., 2007). However, there are some additional ways to get better 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 (Zhenya and Ierapetritou, 2007), (Baez Senties, 2010) and control problems (Tsoukas et al., 1982), (Kerrigan et al., 2000),

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(Zambrano and Camacho, 2002), (Gambier, 2008), (Bemporad and Munoz de la Pena., 2009) 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 (Harjunoski et al., 2009).

Science and Engineering problems normally feature several and contradictory design and/or operation objectives. For instance, during the design of a given system commonly economic performance is stressed neglecting key issues such as the generation and release of pollutants. So, highly profitable systems may lead to large pollution levels. On the other hand, minimum pollutant concentration may require large economic inversions reducing system profit. It seems hard to achieve simultaneously large economic profits and low pollutant levels. Therefore, a trade-off between such design objectives ought to be established. Polymerization reactors are another 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 (Maner, 1996) making hard to achieve large monomer conversions and large molecular weight distributions simultaneously. Because of productivity targets normally large conversions are required, whereas for certain applications also large values of the molecular weight distributions are also demanded. However, increasing conversion leads to decrease molecular weight and vice-versa. Hence, a trade-off between the two design variables must be formulated. Finally, in modern biofuel production systems conflicting and competing objectives also arise. For bioethanol production from cellulosic residues a pretreatment process is required. In this step glucose, xylose, xylane and some undesired products are formed. We would like to design the cellulose pretreatment process in such a way such that, for instance, maximum concentration of xylose is obtained while simultaneously producing minimum amounts of the undesired products. The above three examples are intended

to illustrate that modern market economy and sustainability issues, among other factors, demand the simultaneous consideration of several, and often conflicting, design objectives and that a trade-off solution among such objectives must be attained so all the objectives are met in a certain proportion.

Although a common approach to address the design and operation of processing systems featuring several design objectives lies in merging all the objectives into a single one design objective (Das and Dennis, 1997), 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 suboptimal 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 desired steady-state values, since the systems works under continuous processing conditions. Therefore, the Pareto curve 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 (Vafaeyan and Thibault, 2009) or the deployment of algorithmic methods (Grossmann et al., 1982). 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.

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, 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". 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 (Flores-Tlacuahuac and Grossman, 2006) we have used a production wheel with a cycle schedule which is a valid production strategy assuming that the product demand rates are constant.

Multiobjective Scheduling and Control Formulation

In previous works (Flores-Tlacuahuac and Grossman, 2006), (Flores-Tlacuahuac and Grossmann, 2006a) we have proposed an optimization formulation able to deal with scheduling and control problems using a single objective function. As mentioned above, many Science and Engineering problems commonly feature several, and sometimes conflicting, objective functions. Although multiobjective optimization problems are sometimes reformulated as single optimization problems (Das and Dennis, 1997) 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 (Chinchuluun and Pardalos., 2007), (Das and Dennis, 1998). 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 attained. 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 (Ω) was deployed (Flores-Tlacuahuac and Grossman, 2006):

$$\Omega = \varphi_1 - \varphi_2 \quad (1)$$

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

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

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

where the first part of the φ_1 term has to do with 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. As can be noticed φ_1 and φ_2 have different measurement units. φ_1 has economic profit units, whereas φ_2 has the units in the variable x_i is measured. Originally (Flores-Tlacuahuac and Grossman, 2006) φ_2 was transformed into a transition cost by using a proper weighting function. Solving the multiobjective optimization problem as a single objective optimization problem can lead us to obtain sub optimal solutions. Taking explicitly into account the nature of the different contributions to the objective function will help us to obtain better optimal solutions. 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 they are plotted in a diagram known as Pareto curve. In this work we have used the ε -constraint approach (Haimes et al., 1971) for attaining the Pareto front although some other options are also available (Chinchuluun and Pardalos., 2007).

In the ε -constraint method one of the objectives (f_l) is selected to be optimized and the others (f_j) are converted into constraints. Hence,

$$\begin{aligned} &\text{minimize } f_l(x) \\ &\text{subject to } f_j(x) \leq \varepsilon_j, \quad \text{for all } j = 1, \dots, N, j \neq l \end{aligned} \quad (4)$$

where ε_j are upper bounds for the objectives f_j , $j \neq l$ and N stands for the number of objective functions. The solution

of this problem is always weakly Pareto optimal and Pareto optimal if it is unique. An advantage of the ε -constraint method over the weighting method to solve MOO problems is that the ε -constraint method can find any Pareto optimal solution even for non convex problems. Following the ε -constraint approach, we separated the original objective function and formed the next MOO problem

$$\max \quad \Omega = \varphi_1 \quad (5)$$

$$\text{Subject to } \varphi_2 \leq \varepsilon \quad (6)$$

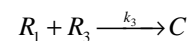
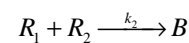
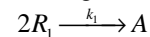
In this way, the MOO problem has been transformed into a single objective optimization problem (SOO) by considering the function φ_2 as an additional inequality constraint. We must emphasize that φ_2 is a little bit different in its present form in relationship to its original form (Flores-Tlacuahuac and Grossman, 2006) but it has no more the weighting factor included as part of its past definition. Of course the MOO problem is also subject to the constraints associated to the scheduling and dynamics behavior of the problem. Because those constraints have been deeply discussed in previous works (Flores-Tlacuahuac and Grossman, 2006) they are not 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 (Biegler, 2010) 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 (Bonami, 2007).

Case Study.

In the next example, it can be distinguished a two-step procedure to achieve a Pareto Diagram. This can be outlined as follows. First we chose a range of values of ε , and then we solved the SOO problem, which is a Mixed-Integer Dynamic Optimization (MIDO) problem, just as described above for each value of ε . That is, each point in the Pareto diagram represents the solution of a MIDO problem, a difficult task per se.

CSTR with Simultaneous Reactions and Input Multiplicities

In this example, the following set of reactions:



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:

$$\frac{dC_{R_1}}{dt} = \frac{(Q_{R_1} C_{R_1}^i - QC_{R_1})}{V} + \mathcal{R}_{r_1} \quad (7)$$

$$\frac{dC_{R_2}}{dt} = \frac{(Q_{R_2} C_{R_2}^i - QC_{R_2})}{V} + \mathcal{R}_{r_2} \quad (8)$$

$$\frac{dC_{R_3}}{dt} = \frac{(Q_{R_3} C_{R_3}^i - QC_{R_3})}{V} + \mathcal{R}_{r_3} \quad (9)$$

$$\frac{dC_A}{dt} = \frac{Q(C_A^i - C_A)}{V} + \mathcal{R}_A \quad (10)$$

$$\frac{dC_B}{dt} = \frac{Q(C_B^i - C_B)}{V} + \mathcal{R}_B \quad (11)$$

$$\frac{dC_C}{dt} = \frac{Q(C_C^i - C_C)}{V} + \mathcal{R}_C \quad (12)$$

$$\mathcal{R}_A = k_1 C_{R_1}^2 \quad (13)$$

$$\mathcal{R}_B = k_2 C_{R_1} C_{R_2} \quad (14)$$

$$\mathcal{R}_C = k_3 C_{R_1} C_{R_3} \quad (15)$$

$$\mathcal{R}_{r_1} = -\mathcal{R}_A - \mathcal{R}_B - \mathcal{R}_C \quad (16)$$

$$\mathcal{R}_{r_2} = -\mathcal{R}_B \quad (17)$$

$$\mathcal{R}_{r_3} = -\mathcal{R}_C \quad (18)$$

$$Q = Q_{R_1} + Q_{R_2} + Q_{R_3} \quad (19)$$

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 is the reactant concentration, C is the product concentration, 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 (Flores-Tlacuahuac and Grossman, 2006), whereas demand rate, product and inventory costs are shown in Table 1. With the provided design information the whole Pareto front is attained as depicted in Figure 1. The coordinates of the first and second points are $[\varphi_2^1; \varphi_1^1] = [5 \times 10^{-5}, 25590]$ and $[\varphi_2^2; \varphi_1^2] = [2.5 \times 10^{-4}, 35250]$, respectively. 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 seen in the first point of 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 1:42.6 and 0:43.1 min 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 better economic profit (\$35250) when compared to the profit attained from 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 2 and 3 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 requested product demand can be met deploying 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 2 and 3 the dynamic optimal transition profiles for the two points in the Pareto front are depicted. Because in both cases the value of the φ_2 objective function turns out to be rather small the dynamic transition profiles exhibit smooth dynamic behavior.

Table 1: Operating Conditions Leading to the Manufacture of the A, B, and C Products of the Case Study

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

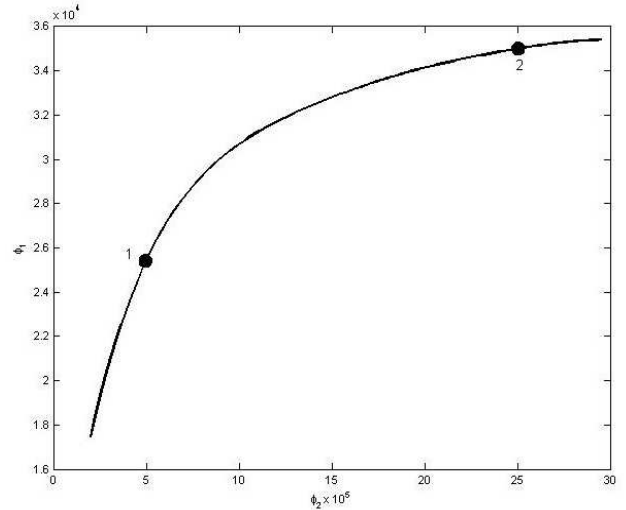


Figure 1: Pareto curve for the case of study. Coordinates for the first and second points are: $[\varphi_2^1; \varphi_1^1] = [5 \times 10^{-5}, 25590]$ and $[\varphi_2^2; \varphi_1^2] = [2.5 \times 10^{-4}, 35250]$, respectively.

Conclusions

In this work we proposed an optimization formulation for dealing with multiobjective scheduling and control problems. The formulation assumes that the approached problems are solved off-line and without taking into account process uncertainty. The results attained in the present work clearly demonstrates the advantages of deploying 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 by the time being they tend to require large CPU times. On the contrary, multiobjective optimization techniques are simpler to deploy and they 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 (Flores-Tlacuahuac et al., 2011), (Zavala and Flores-Tlacuahuac, 2011) because a multiobjective control strategy is required for this purpose.

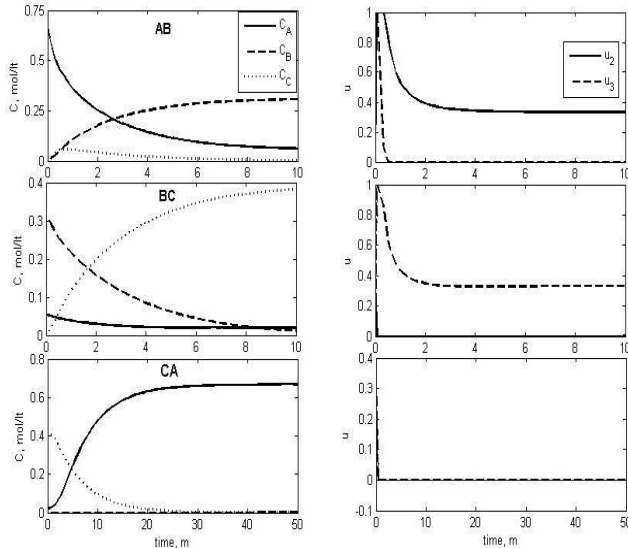


Figure 2: Optimal dynamic transition profiles for reactor concentration and volumetric flow rate for the first point of the Pareto front.

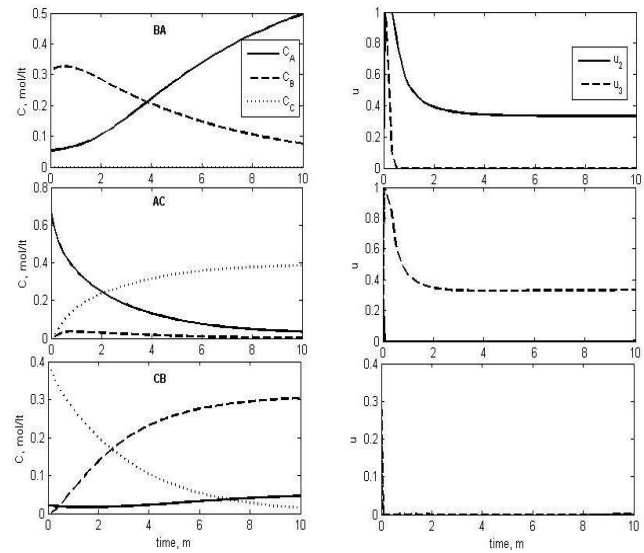


Figure 3: Optimal dynamic transition profiles for reactor concentration and volumetric flow rate for the second point of the Pareto front.

Table 2: Scheduling and Control results for the first optimal operating point. The objective function values are: $\varphi_2^1 = 5 \times 10^{-5}$ and $\varphi_1^1 = 25590$. 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	659.034

Table 3: Scheduling and Control results for the second optimal operating point. The objective function values are: $\varphi_2 = 2.5 \times 10^{-4}$ and $\varphi_1 = 35250$. 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

References

- Allcock, A.C., Mahadevan, R. and Doyle III, F.J. (2002). Scheduling of Polymer Grade Transitions. *AIChE J.*, 48, 1754.
- Baez Senties, O., Azzaro-Pantel, C., Pibouleau, L., and Domenech, S. (2010) Multiobjective scheduling for semiconductor manufacturing plants. *Comput. Chem. Eng.*, 34, 555.
- Bemporad, A. and Munoz de la Pena, D. (2009) *Multiobjective model predictive control*. *Automatica*, 35, 2823.
- Biegler, L. T. (2010). Nonlinear Programming: Concepts, Algorithms, and Applications to Chemical Processes. *SIAM*, 2010.
- Bonami, P., Biegler, L., Conn, A., Cornuejols, G., Grossmann, I., Laird, C., Lee, J., Lodi, A., Margot, A., Nicolas, S. and Waechter, A. (2007) An algorithmic framework for convex mixed integer nonlinear programs. *Discrete Optimization*, i:10.1016/j.disopt.2006.10.011.
- Chinchuluun, A., and Pardalos, P. M. (2007). A survey of recent developments in multiobjective optimization. *Ann Oper Res*, 154:29.
- Das, I. and Dennis, J.E. (1997). A closer look at drawbacks of minimizing weighted sums of objectives for pareto set generation in multicriteria optimization problems. *Structural Optim.*, 14, 63.
- Das, I. and Dennis, J.E. (1998). Normal-boundary intersection: A new method for generating the pareto surface in nonlinear multicriteria optimization problems. *SIAM J. OPTIM.*, 8(3), 631.
- Flores-Tlacuahuac, A. and Grossman, I.E. (2006). Simultaneous Cyclic Scheduling and Control of a Multiproduct CSTR. *Ind. Eng. Chem. Res.*, 45, 6175.
- Flores-Tlacuahuac, A. and Grossman, I.E. (2006a). An Effective MIDO Approach for the Simultaneous Cyclic Scheduling and Control of Polymer Grade Transition Operations. In W. Marquardt and C. Pantelides, editors, *16th European Symposium on Computer Aided Process Engineering and 9th International Symposium on Process System Engineering*, 1221. Elsevier, 28.
- Flores-Tlacuahuac, A., Morales, P. and Rivera-Toledo, M. (2011). Multiobjective Non-Linear Model Predictive Control of a Class of Chemical Reactors. *Submitted for publication to Journal of Process Control*, 2011.
- Gambier, A. (2008) MPC and PID control based on multi-objective optimization. *Proceedings of the American Control Conference*, 4727.
- Grossman, I.E., Drabbant, R. and Jain, R.K. (1982). Incorporating toxicology in the synthesis of industrial chemical complexes. *Chemical Engineering Communications*, 17, 151.
- Haimes, Y. Y., Lasdon, L. S. and Wismer, D. A. (1971). On a bicriterion formulation of the problems of integrated system identification and system optimization. *IEEE Transactions on Systems, Man and Cybernetics*, 296.
- Harjunkski, I., Nystrom, R. and Horch, A. (2009) Integration of Scheduling and Control: Theory or Practice? *Comput. Chem. Eng.*, 33, 1909.
- Kerrigan E., Bemporad, A., Mignone, D., Morari, M., and Maciejowski, J. M. (2000). Multiobjective prioritisation and reconfiguration for the control of constrained hybrid systems. *Proceedings of the American Control Conference*, 1694.
- Maner, B.R., Doyle, F.J., Ogunnaike, B.A. and Pearson. R.K. (1996). Nonlinear model predictive control of a simulated multivariable polymerization reactor using second-order Volterra models. *Automatica*, 32, 1285.
- Richards, J.R., Congalidis, J.P. and Ray, W.H. (2002). Scheduling of Polymer Grade Transitions. *AIChE J.*, 48, 1754.
- Terrazas-Moreno, S., Flores-Tlacuahuac A., and Grossmann I.E. (2007). Simultaneous scheduling and control in polymerization reactors. *AIChE J.*, 53, 2301.
- Tsoukas. A., Tirrell, M., and Stephanopoulos G. (1982). Multiobjective dynamic optimization of semibatch copolymerization reactors. *Chemical Engineering Science*, 37, 1785.
- Vafaeian, V. and Thibault, J. (2009) Selection of pareto-optimal solutions for process optimization using rough set method: A new approach. *Computers and Chemical Engineering*, 30, 1155.
- Zambrano, D. and Camacho, E. (2002). Application of MPC with multiple objective for a solar refrigeration plant. *Proceedings of the IEEE Conference on Control Applications*, 1230.
- Zavala, V. M. and Flores-Tlacuahuac, A. (2011) Stability of Multi-Objective Predictive Control: An Utopia-Tracking Approach. *Submitted for publication to Automatica*, 2011.
- Zhenya, J. and Ierapetritou, M.G. (2007) Generate pareto optimal solutions of scheduling problems using normal boundary intersection technique. *Comput. Chem. Eng.*, 31, 268.