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Solving Infeasibilities in Dynamic Optimization Problems

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Abstract: DRTO Systems sometimes present failures when solving dynamic optimization problems. There are situations where the infeasibilities are due to the initial conditions, changing of constraints during the operation, or even in presence of conflicts between some specifications. The proposed method consists in solving these infeasibilities by reformulating the DAOP as a multi-objective optimization problem by relaxing the constraints. The goal programming approach was used to solve the dynamic optimization problem. Two examples, exploring different characteristic of these kinds of problems, were used to illustrate the methodology. The results show the ability of the proposed approach in locating and solving the infeasibilities, increasing the robustness of DRTO systems.

Keywords: Dynamic Optimization, Infeasibility, Multi-objective optimizations, Optimal control.

1. INTRODUCTION

DRTO Systems (Dynamic Real-Time Optimization) are becoming more attractive to establish optimized politics in processes operation (Biegler, 2009; Kadam and Marquardt, 2007, Biegler & Zavala, 2009). When solving the dynamic optimization problem of a DRTO system it is possible to find some problems that compromise its effectivity, such as failures in finding the optimal solution. This can happen when the problem is infeasible or unbounded, has numeric difficulties, system errors, or even problems with the optimization model. In this paper, we will focus on infeasibility of dynamic optimization problems. When this kind of problems is solved in real time applications, there are some situations where the initial conditions stay in an infeasible region or tend inexorably to the constraints violation. There are other situations where the process recipes are changed between two stages during the operation, or some important disturbance can appear, forcing some abrupt change in the process operation. In this case, the problem may become infeasible (intentionally or not). Another common problem is the presence of conflicts between some specifications. It is not rare to find this situation in real time operation when the operators establish constraints that compete themselves, resulting in an infeasible solution of the dynamic optimization problem.

Since the 70's decade have appeared studies detecting infeasible sets of constraints in the optimization problem. At that time, the drive force was to find infeasibilities in linear programming problems (LP). The way to detect an infeasible set of constraints was the direct location using some heuristic, such as: lower bound greater than upper bound, top temperature larger than bottom temperature in a distillation column, etc.

During the 80's started to appear some systematic methods to detect infeasible sets of constraints and to find the causes of such infeasibilities in LP problems (Greenberg, 1993). Using this approach, it has been possible to detect the irreducible infeasible set of constraints (IIS) (Van Loon, 1981). This is a set of constraints where any chosen subset results in a feasible problem. However, it is possible to have more than one IIS, and their detection is a complex combinatorial problem. The methods for IIS detection usually employed to solve infeasibilities in NLP problems are the deletion filter, addition filter, elastic filter, and sensibility filter (Chinneck, 2008). Besides, sometimes is useful to combine different filters or to group some constraints in order to speed up the IIS searching. This approach has been used in MINOS (Chinneck, 1994) and CONOPT (Drud, 1994) softwares.

Recently, consensus constraint method has appeared to find infeasible points in NLP problems. This method computes the feasible distances for each constraint and generates the feasibility vectors (Chinneck, 2004). The bad directions of these vectors should not be included in a vector called consensus vector, which represents the mean feasibility for the violated constraints. This approach is not useful for finding feasibility in dynamic optimization problems due to the large number of possible combinations of IIS in discrete-time optimization problem, and due to the correlation of constrained state variables with their past values in continuous-time problem. This problem exists due to the sensitivity of the constraint with the control actions in the previous instants, similar to the behavior of convolution models, where a control action in the beginning of the optimization horizon has a strong influence in the state variables in an instant far ahead. This behavior suggests us to implement the control actions in a distant earlier time in order to avoid effectively the constraint violation. This kind of problem turns difficult the efficient using of this kind of technique.

It has also been proposed the solution for infeasible problem using goal programming where an original problem is reformulated as multi-objectives NLP problem (Tamiz et al., 1996). In this formulation, slack variables are introduced to relax the original optimization problem as follow:

$$\begin{aligned} &\min \ \gamma \\ &s.t. \\ &w_i s_i \le \gamma \\ &g_i(x) - s_i \le 0 \quad i = 1, \cdots, m \\ &s_i \ge 0 \end{aligned} \tag{1}$$

where $\sum_{i=1}^{m} w_i = 1$ and $w_i \ge 0$.

In this case, a unique solution is obtained instead the optimal Pareto set, and the weights w_i are chosen through a heuristic criterion (Yang, 2008). This approach turns to be more effective to locate and solve infeasibilities in NLP.

The known methods are focused on locating and solve infeasibility in LP and NLP problems. These methods have not been applied to identify and solve infeasibility in DAOP (Differential-Algebraic Optimization Problem). The techniques that remove or move constraints in LP and NLP problems are not effective for solving cases with infeasible initial conditions or tendency to infeasibility, and may lead the plant to unprofitable or even insecure conditions. Differently of stationary optimization, feasible solution of dynamic systems may depend on their initial conditions and the directions of the time derivatives. A state variable can be located in a feasible region, but the direction of the time derivative may point to an infeasible region where there are no control actions that avoid the constraint violation. This kind of infeasibility can happen when the process is close to bounds (usually after some running of the optimizer in real time). In the same way the initial infeasibility problem, it is possible to have some discontinuities in the optimization horizon during the operation (e.g., changing the specifications during process transition).

In order to efficiently solve the above infeasibility problems, it is proposed a methodology based on constraints relaxation through the solution of a multi-objectives dynamic optimization problem described in the following section.

2. SOLVING INFEASIBILITY PROBLEM

When using diagnosis tools, it should be verified not only if the initial conditions are feasible or not, but also if the directions of the state variables time derivatives tend to violate a constraint. However, these cannot be enough to solve the infeasibility problem, being also necessary to analyze the feasibility of all state and control variables profiles.

Optimization problem formulation

Dynamic optimization packages usually use a standardized problem formulation where bound constraints are imposed to state and control variables and model parameters. Therefore, the dynamics optimization problems are usually presented as following (Cervantes et al., 2000):

$$\begin{aligned} &\min_{u,p,t_i} \varphi\left(x\left(t_f\right)\right) \\ &s.t. \\ &F_i\left(\dot{x}(t), x(t), y(t), u(t), p, t\right) = 0 \quad t \in \left[t_0, t_f\right] \\ &x^L \le x(t) \le x^U \\ &y^L \le y(t) \le y^U \\ &u^L \le u(t) \le u^U \\ &p^L \le p \le p^U \end{aligned} \tag{2}$$

where *x(t)* are the differential variables, *y(t)* the algebraic variables, *u(t)* the control variables, and *p* the time independent model parameters. The process can have path constraints, interior point constraints, and final time constraints (t_f).

The proposed method consists in solving the infeasibilities by reformulating the DAOP as multi-objective optimization problem relaxing the constraints. This relaxation is performed through the inclusion of slack variables and the utopian objectives into the DAOP. The objective is to find the minimum movement of the problematic constraints while optimizing the original DAOP. The basic difference of this approach is the usage of soft and hard constraints at the same time of using the relaxation approach. This leads to the simultaneous solution of the optimization problem and constraints relaxation. Using this approach, it is simple to decide about the optimal constraints movements. In order to solve this problem, the minimization of constraints relaxations are formulated as additional objectives functions. The resulting multi-objective optimization problem is formulated as the following goal-programming problem:

$$\begin{aligned} &\min_{u,\Delta\gamma,s^x,s^y,s^u,p,t_i} \gamma(t_f) \\ &s.t. \\ &F(\dot{x}(t), x(t), y(t), u(t), p, t) = 0 && where \ \ F(\bullet) \in \Re^{nx+ny}, t \in [t_0, t_f] \\ &\frac{d\gamma}{dt} = \Delta\gamma(t) \\ &\psi^{\phi}(t_f) = \gamma(t_f) w_0 - \phi(x(t_f)) + \phi^L \\ &\psi_i^{x}(t) = \Delta\gamma(t) - \left(\frac{s^x{}_i(t)}{\sigma^x{}_i}\right)^2 && where \ \ i = 1, \cdots, nx \\ &\psi_j^{y}(t) = \Delta\gamma(t) - \left(\frac{s^y{}_j(t)}{\sigma^y{}_j}\right)^2 && where \ \ j = 1, \cdots, ny \\ &\psi_k^{u}(t) = \Delta\gamma(t) - \left(\frac{s^u{}_k(t)}{\sigma^u{}_k}\right)^2 && where \ \ k = 1, \cdots, nu \\ &g^x(t) = x(t) + s^x(t) \\ &g^y(t) = y(t) + s^y(t) \\ &g^u(t) = u(t) + s^u(t) \\ &x^L \le g^x(t) \le x^U && where \ \ g^x(t) \in \Re^{nx} \\ &y^L \le g^y(t) \le y^U && where \ \ g^y(t) \in \Re^{ny} \\ &u^L \le g^u(t) \le u^U && where \ \ g^u(t) \in \Re^{nx} \\ &\psi^{\phi}(t) \ge 0; \psi^x(t) \ge 0; \psi^y(t) \ge 0; \psi^u(t) \ge 0; \end{aligned} \tag{3}$$

In order to eliminate the effects of the state and control variables magnitudes, the relaxations are normalized using the acceptable violation variance ($\sigma^{x}{}_i^{2}$).

There are two possible relaxation strategies: moving the constraint along the optimization horizon and introducing time-varying slack variables as a control variable. In the first case, the constraint may be relaxed in time points that would not be necessary and the control profiles may also change by this relaxation. This optimization problem formulation is equivalent to define slack variable as time-invariant parameters to be optimized. In the second strategy, the constraints are relaxed along the time intervals where the problem becomes infeasible. The manipulations of the slack variables follow the criterion of minimum relaxation that turns the problem feasible. This strategy is more complex but more appropriated, because it moves the constraints only in the time intervals necessary to remove the infeasibility of the optimization problem.

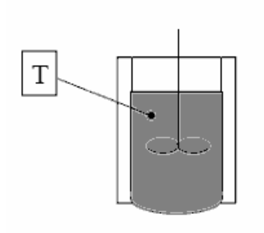
When optimization problems are solved in real-time mode, it is necessary to obtain a unique solution (in the Pareto set) to be implemented in the real plant. Due to this fact, evolutionary methods (Coello, Pulido & Montes, 2005) are not useful. The weighted sum approach (Marler & Arora, 2004) is effective only for problems with convex Pareto set. The ε-constraint approach (Marler & Arora, 2004), where the most important objective function is choose and all other objectives are constrained, is difficult to apply because in dynamic optimization problems the most important objective depends on the time interval and on the magnitude of the constraint violations. The use of multi-objectives optimization algorithm based on utopia (Logist et al., 2009) shows to be more interesting for the solution of dynamic optimization problems because the possibility to solve the feasibility and optimality problems simultaneously, and does not present the disadvantages of the other approaches.

3. CASE STUDIES, RESULTS AND COMMENTS

The DAOP's are usually solved by direct methods. The current approaches are: sequential methods – single-shooting, hybrid methods – multi-shooting and simultaneous methods. Biegler and Grossman (2004) wrote a comprehensive review about these methods. We adopted the single-shooting method, where the control variables were discretized as piecewise constant profiles, the DAE and sensitivity systems are integrated, and the resulting NLP problem is solved sequentially.

3.1 - Case 1 – Dynamic optimization of a batch reactor

Consider the following batch reaction process where the temperature is the control variable of the system (Ray, 1981; Cervantes et al., 2000). The initial conditions are: $C_A = 1.0$, $C_B = 0.0$, $C_C = 0.0$, $T = 780\ K$, and $\Delta T = 0.001\ K$. The production objective is the maximization of the component B concentration (C_B) at the final time. Besides, it should be avoided the production of the component C (C_C), because it is an undesirable component.



$$A \xrightarrow{1} B \xrightarrow{2} C$$

Fig. 1. Batch reactor scheme and reactions.

The process model equations are given as:

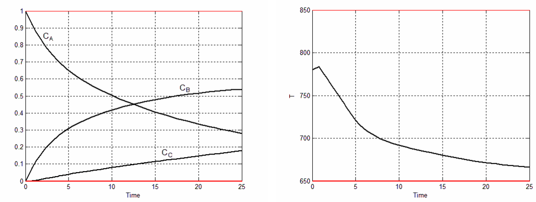
$$\begin{aligned}
\frac{dC_A}{dt} &= -k_1 C_A \\
\frac{dC_B}{dt} &= k_1 C_A - k_2 C_B \\
C_A + C_B + C_C &= 1 \\
k_1 = k_{1,0} e^{\left(\frac{-E_1}{RT}\right)}&;\ k_2 = k_{2,0} e^{\left(\frac{-E_2}{RT}\right)}
\end{aligned} \tag{4}$$

where C_A, C_B e C_C are the mol fractions of the components A, B, and C respectively, T the reaction temperature in K; and k_1, k_2, E_1, and E_2 are the kinetic parameters of the reactions 1 and 2.

With this case study, three problems were solved: the original problem without bounds on the composition and $T \geq 650\ K$; the infeasible problem with constraints on reaction temperature and on composition of C; and the problem with relaxation on these constraints.

Original Problem

The original problem has a feasible solution. The batch reaction is optimized with a final (t_f) time of 25 hours, and the optimal profiles are shown in Figure 2.



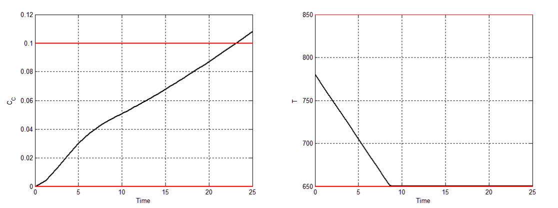
(a) (b)

Fig. 2. Optimal solution of the original problem. State profiles C_A, C_B and C_C (a) and control profile T (b).

The lower bound of the reaction temperature was not reached, and the final composition of B and C were 0.5406 and 0.1789, respectively, where the later should be as lower as possible.

Infeasible Problem

Suppose now an upper bound in the composition of C (undesired co-product) is imposed, where the maximum allowed value is 0.1. Due to this fact, the upper bound of the C composition and the lower bound of the reaction temperature T compete each other, because they cannot be satisfied at the same time points. In this case, the infeasible problem is found due to conflicting specifications.



(a) (b)

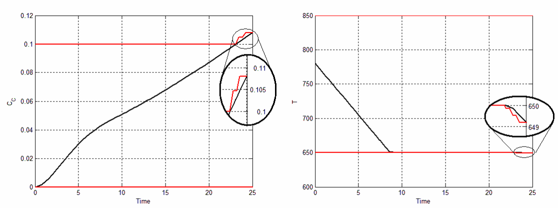
Fig. 3. Solution of the infeasible problem. State profile of C_C (a) and control profile T (b).

As it can be seen in Fig. 3, the optimizer reduced the reaction temperature with the maximum negative rate. Notice that the final concentration of C (0.1081) violated the constraint and the reaction temperature reached the lower bound (650 K). It is impossible to find a feasible solution using this problem formulation. The only possible solution would be to relax the upper bound of the concentration of C and/or the lower bound of the reaction temperature.

Relaxed Problem

In this case, the multi-objective dynamic optimization problem is solved as mentioned before. The objectives that compete each other are: maximize C_B at final time and minimize the relaxation of the constraints C_C and T. Using this formulation, three control variables are added $\Delta\gamma$, s_{CC}, and s_T with piecewise constant profiles.

The optimizer found a feasible optimal solution, shown in Fig. 4, where the relaxation of the minimum reaction temperature and maximum concentration of C were minimized. Notice that the maximum concentration of C reached was 0.1080, and the minimum temperature was 649.1962 K.

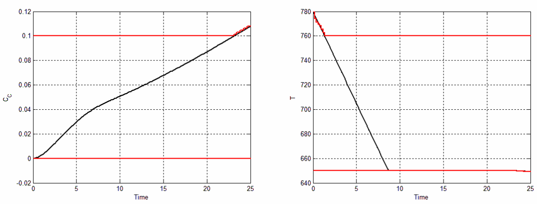


(a) (b)

Fig. 4. Solution of the relaxed problem. State profile of C_C (b) and control profile T (c).

Consider now we have a problem with initial condition infeasibility where the temperature upper bound is moved from 800 to 760 K. This situation is not rare when running the dynamic optimization of an actual plant, because usually the initial conditions cannot be chosen. In this case, we have the following modified constraint of the relaxed problem: $-30 \le s_T(t) \le 30.0$ and $650 \le g_T(t) \le 760$. The relaxed solution gives the profiles shown in Fig. 5, which is the same solution as in the previous case, despite the relaxation of the upper bound at beginning of the time horizon.

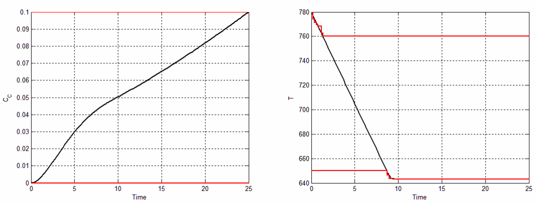
Another studied situation was solving the problem without relaxing the maximum composition of C. In this case, the profile of the reaction temperature is changed to compensate this hard constraint. Notice, in Fig. 6, that there was a larger relaxation in the minimum reaction temperature of 7 K.



(a) (b)

Fig. 5. Solution of relaxed problem - upper bound of T = 760 K. State profile of C_C (a) and control profile T (b).

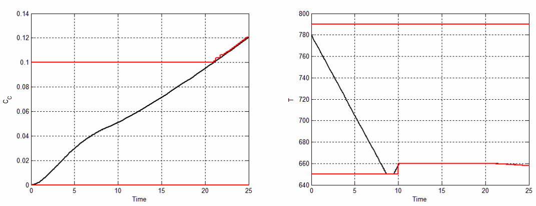
If that relaxation is acceptable, it is better to relax only one constraint. In this case, the first running of the optimizer is performed with relaxation in all constraints. When noting it is possible to have an alternative solution, a second running can be performed where the concentration of C becomes a hard constraint.



(a) (b)

Fig. 6. Solution of the partially relaxed problem. State profile of C_C (a) and control profile T (b).

In a second case, we have a problem of intermediate infeasibility where the lower bound is moved from 650 K to 660 K at 10 hours during the reactor operation. In this case, the problem becomes infeasible inside the optimization horizon. It is possible to find this situation in operation of real plants when a recipe is changed during the operation where the constraints specifications are changed. In this case, we have the following constraints of the relaxed problem: $650 \le g_T(t) \le 760$ for $t \in [0, 10]$ and $660 \le g_T(t) \le 760$ for $t \in (10, 25]$. The relaxed solution gives the optimal profiles shown in Fig. 7.



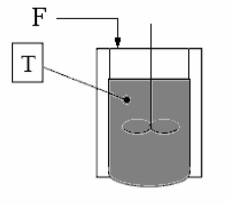
(a) (b)

Fig. 7. Solution of the relaxed problem – intermediate infeasibility. State profile of C_C (b) and control profile T (c).

Notice that the optimizer found a feasible solution by anticipating the process transition when the recipe was changed. The bounds in reaction temperature and the composition of C were appropriately relaxed during the process operation.

3.2 - Case 2 – Dynamic optimization of a non-isothermal semi-batch reactor

Consider a non-isothermal semi-batch reactor with two exothermic reactions in sequence subject to the heat removal constraint, Fig. 8. This problem has two control variables, the feed flow rate F and the reactor temperature (Srinivasan et al., 2003). The optimization objective is to maximize the amount of the component C produced during the time horizon. There are some constraints imposed to this process: maximum reaction heat rate generated along the time horizon and maximum final reactor volume. The initial conditions of the process are: $C_A(t_0)$ = 10.0 *mol/l,* $C_B(t_0)$ = 1.1685 *mol/l,* $C_C(t_0)$ = 0.0 *mol/l,* $C_{B,In}$= 20.0 *mol/l,* $V(t_0)$ = 1 *l,* $F(t_0)$ = 0.5 *l/h* and $T(t_0)$ = 35 ^oC.



$$A + B \xrightarrow{1} C \xrightarrow{2} D$$

Fig. 8. Semi-batch reactor scheme and reactions.

The model equations of this problem are given as:

$$\begin{aligned}
\dot{c}_A &= -k_1 c_A c_B - \frac{F}{V} c_A \\
\dot{c}_B &= -k_1 c_A c_B + \frac{F}{V}\left(c_{B,In} - c_B\right) \\
\dot{c}_C &= k_1 c_A c_B - k_2 c_C + \frac{F}{V} c_C \qquad (6) \\
\dot{V} &= F \\
Q &= (-\Delta H_1) k_1 c_A c_B + (-\Delta H_2) k_2 c_C V \\
c_A &+ c_B + c_C + c_D = 1 \\
k_1 &= k_{1,0} e^{\left(-\frac{E_1}{R(T+273)}\right)}; k_2 = k_{2,0} e^{\left(-\frac{E_2}{R(T+273)}\right)}
\end{aligned}$$

where k_1, k_2, E_1, and E_2 are the kinetic parameters of the reactions 1 and 2; T is the reaction temperature in ^{o}C; c_A, c_B, c_C, and c_D are the concentrations of components *A*, *B*, *C*, and *D*, respectively (mol fractions); $c_{B,In}$ the feed composition of *B; F* the feed flow rate; V the reactor volume; Q is the heat rate generated by the reactions; and ΔH_1 and ΔH_2 are the reaction heat of reactions 1 and 2, respectively. The model parameters are: $k_{1,0}$ = 4.0 *l/mol.h,* E_1 = 6000 *kJ/mol,* $k_{2,0}$ = 800 *l/mol.h,* E_2 = 20000 *kJ/mol,* ΔH_1 = -30 *kJ/mol,* ΔH_2 = -10 *kJ/mol* and *R* = 8.31 *J/mol.K*

Similar to the previous case, three different problems were solved with this case study: the original problem, without concentration constraints; the infeasible problem due to the constraints in the reaction temperature and concentration of C; and the problem with relaxation of these constraints.

Original Problem
The system was optimized up to the final time (t_f) of 0.5 hours. In this case, the constraints are the maximum feed flow rate, the maximum variation of this flow rate, the reaction temperature, maximum variation of this temperature, the maximum heat rate generated by the reactions, and the maximum reaction volume. There are no constraints on the reagents and products concentrations.

In this case, a well-known feasible solution was obtained. The upper limit of the reactor heat rate was reached, and a feasible solution shown in Fig. 9 was obtained on the dynamic optimization problem. Notice that the maximum concentration of B was 1.65 *mol/l*.

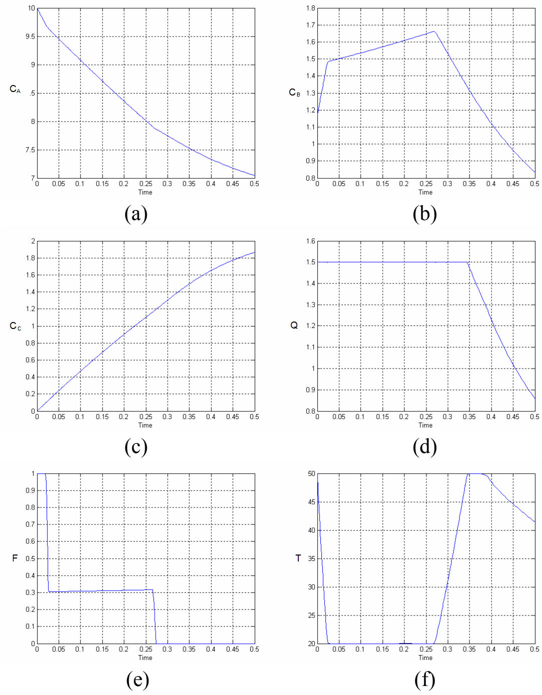


Fig. 9. Solution of the original problem. State profiles of C_A (a) and C_B (b); state profiles of C_C (b) and Q (d); and control profiles of F (e) and T (f).

Infeasible Problem

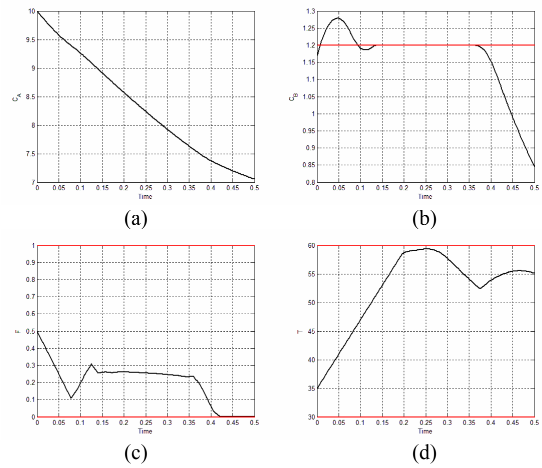


Fig. 10. Solution of the infeasible problem. State profiles of C_A and C_B (a) and control profiles of F (c) and T (d).

Consider that an upper bound on composition of the undesirable co-product B is imposed, where the maximum allowed concentration is 1.2 *mol/l*, and the maximum reactor heat rate Q is 1.6 *kJ/h*. This problem formulation causes competition and conflicting between these constraints, because they cannot be satisfied at the same time, as shown in the results of Fig. 10.

Relaxed Problem

In this case, the multi-objective dynamic optimization problem is solved as mentioned before. The objectives that compete between themselves are: maximize C_B at final time, minimize the relaxation of the constraints C_B, Q, and T. The results are presented in Fig. 11. Notice that the optimizer only has relaxed C_B, maintaining the bounds of Q and T in their original positions.

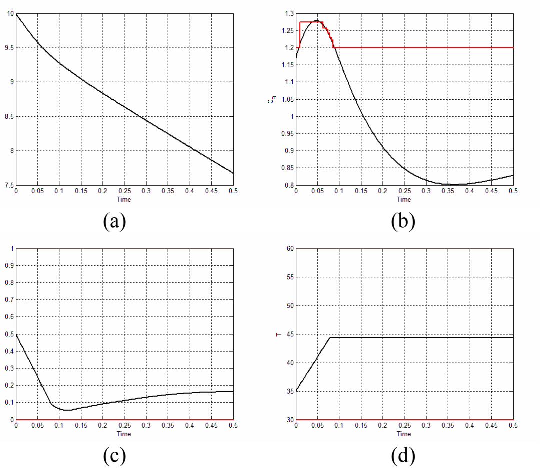


Fig. 11. Solution of the relaxed problem. State profiles of C_A (a) and C_B (b) and control profiles of F (c) and T (d).

4. CONCLUSIONS

This work presented a methodology for solving infeasible dynamic optimization problems through the constraints relaxation technique. This technique has been implemented in a different way that usually is implemented in NLP problems. In order to demonstrate these characteristics, two case studies of reactions systems were presented, where initial and intermediate infeasibilities and conflict between constraints specifications are explored.

The results shown this approach is efficient to obtain feasible relaxed optimal control problems when these are structurally infeasible. The proposed technique turns DRTO systems more robust, contributing with their effectiveness. We can also observe on the results that the proposed relaxations to make the problem feasible have minimum movement of the constraints.

Furthermore, we suggest using a sequential strategy in order to relax only some constraints while keeping the others in their original positions. This can be done by combining two techniques: isolation of infeasible constraints and the proposed technique.

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