



Solving dynamic optimization infeasibility problems

Euclides Almeida^a, Argimiro R. Secchi^{b,*}

^a Petrobras SA – Petróleo Brasileiro and PPGEQ/UFRGSBrazil

^b PEQ – COPPE – Universidade Federal do Rio de Janeiro, Brazil

ARTICLE INFO

Article history:

Received 29 July 2010

Received in revised form 17 June 2011

Accepted 5 July 2011

Available online 28 July 2011

Keywords:

Dynamic optimization

Infeasibility

Multi-objective optimization

Real-time optimization

Constraint relaxation

ABSTRACT

Dynamic real-time optimization (DRTO) systems sometimes fail when solving intrinsic optimization problems. There are situations where the solution is infeasible due to the initial conditions, constraint changes during operation, or even the presence of conflicts on constraint specifications. By using a goal programming approach, this work proposes a method to solve these infeasibilities by reformulating the differential-algebraic optimization problem as a multi-objective dynamic optimization problem with path constraint relaxations. Three examples were solved exploring the characteristics of such infeasibility problems. The results demonstrate the ability of the proposed method in identifying and relaxing the constraint violations, increasing the robustness of DRTO systems.

© 2011 Elsevier Ltd. All rights reserved.

1. Introduction

Dynamic real-time optimization (DRTO) systems and nonlinear model predictive control (NMPC) applications have been frequently used to establish optimal policies for process operations (Biegler, 2009; Biegler and Zavala, 2008; Kadam and Marquardt, 2007). The core of a DRTO system consists on solving a differential-algebraic optimization problem (DAOP), where the dynamic process behavior is described by a set of differential-algebraic equations (DAEs). The DAOP may have path, interior-point and end-time constraints. Moreover, the end time may be a free variable in the optimization problem.

A DRTO system is usually designed to run automatically in a closed loop mode. However, while a DRTO system seeks the solution of the optimization problem, failures may occur if the problem is infeasible or unbounded, has numerical difficulties, presents system errors, or even presents model-building errors. Furthermore, it is also possible to find situations where the initial conditions, normally provided by some state estimator in each DRTO cycle, are infeasible or tend inexorably to infeasibility. In all these cases, the optimizer will fail to find a solution, shutting down the DRTO system.

Academics have tried to solve infeasibility problems in different ways. Since the 70s there have been concerns in detecting the set of constraints that make constrained linear optimization problems

(LPs) infeasible. The approach used to detect infeasibility was direct location using heuristics, such as the lower limit greater than the upper limit of a variable, or the top temperature higher than the bottom temperature in a distillation column.

In the 80s, systematic methods for detection of infeasible constraint sets started to appear, which identify these sources of LP infeasibilities (Greenberg, 1993). Using ranking and elimination approach, an Irreducibly Inconsistent System (IIS) is detected (van Loon, 1981), where any chosen subset makes the problem feasible. There are some cases where it is possible to find more than one IIS in an optimization problem. This detection is a combinatorial problem procedure that increases the computational cost for finding the IIS. The existence of multiple IIS leads us to an unanswered question of what is the best choice of IIS to solve the optimization problem? There is an IIS set that results in the best value of the objective function, but it is necessary to test all IIS in order to find the best solution. The current IIS detection methods consist of the following filters: deletion, addition, elastic and sensitivity (Chinneck, 2008). In addition, the combination of these filters and constraint groupings can speed up the infeasible set detection process. The solvers MINOS (Chinneck, 1994) and CONOPT (Drud, 1994) have both used this approach.

Chinneck (2004) introduced the consensus methods to detect infeasibility of constrained nonlinear optimization problems (NLPs) by calculating the feasible distances from the original problems to obtain feasible vectors. The worst directions of these vectors should not be included into the “consensus vector”, which represents the average infeasibility for the violated constraints. The efficiency of this method is a function of the number of constraints in the optimization problem, and is not attractive for large-scale problems.

* Corresponding author at: PEQ-COPPE/UFRJ, Cx.P. 68502, CEP 21941-972 - Rio de Janeiro, RJ, Brazil. Tel.: +55 21 2562 8301; fax: +55 21 2562 8300.

E-mail addresses: ean@petrobras.com.br (E. Almeida), arge@peq.coppe.ufrj.br (A.R. Secchi).

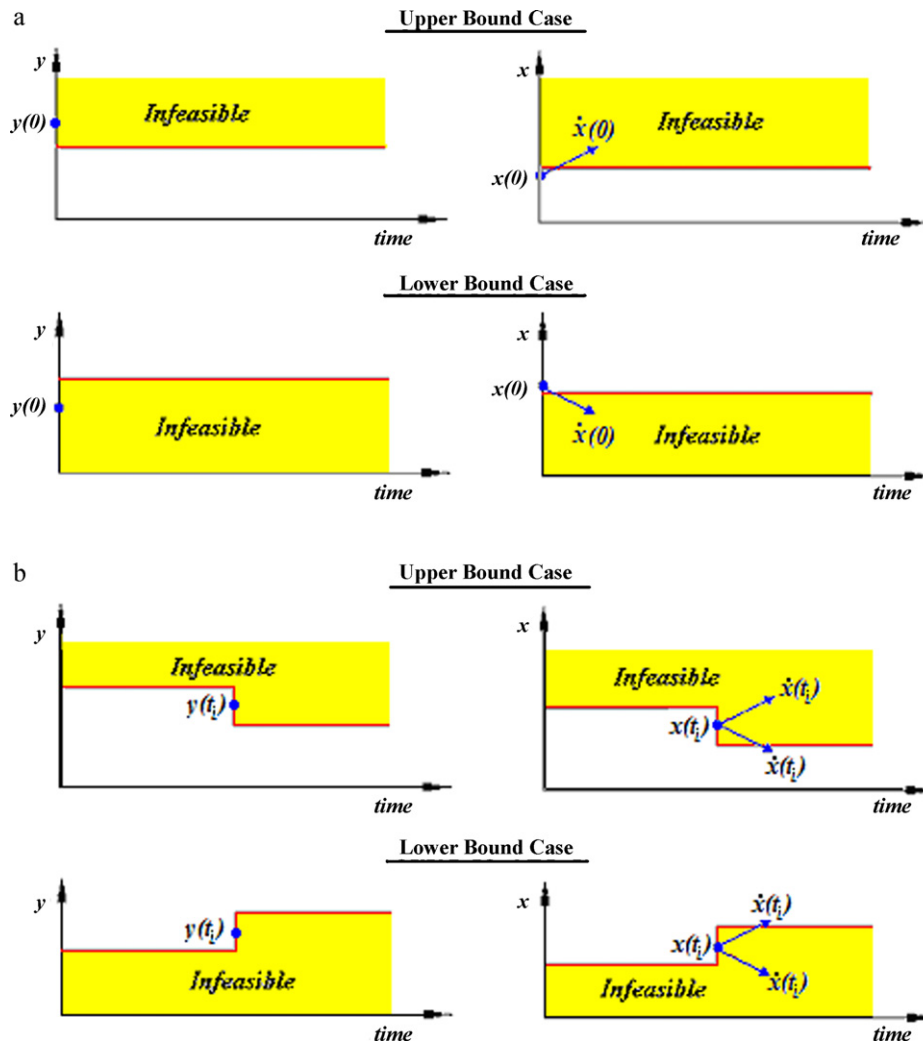


Fig. 1. (a) Initial infeasibility and tendency to infeasibility and (b) intermediate infeasibility or intermediate tendency to infeasibility.

Another approach that can be used for solving the infeasibility problem is the multi-objective formulation which introduces slack variables (s_i) to relax the constraints, as follows:

$$\begin{aligned} \min_{z,s} \quad & [s_1 \ \cdots \ s_m] \\ \text{s.t.} \quad & g_i(z) \leq s_i \quad i = 1, \dots, m \\ & s_i \geq 0 \end{aligned}$$

where an optimal solution from the Pareto set can be obtained by different approaches. Tamiz, Mardle, and Jones (1996). applied the following goal programming approach (Eq. (1)) for solving this multi-objective infeasibility problem.

$$\begin{aligned} \min_{z,s,\gamma} \quad & \gamma \\ \text{s.t.} \quad & w_i s_i \leq \gamma \\ & g_i(z) - s_i \leq \gamma \quad i = 1, \dots, m \\ & s_i \geq 0 \end{aligned} \quad (1)$$

where z are the state variables, γ is the objective function, $\sum_{i=1}^m w_i = 1$ and $w_i \geq 0$.

The optimal solution in the Pareto set is obtained by choosing the weights w_i according to a heuristic criterion (Yang, 2008). This approach identifies the infeasibility by solving the relaxed NLP.

Some techniques are available to soften the constraints in model predictive controllers (MPC). One of the first adopted techniques was the conversion of the original inequality constraint, $g(z) \leq 0$, to an equality constraint, $g(z) + s^2 = 0$, which incorporates a slack variable, s , and requires an additional term in the objective function, a cost function, $s^T Q s$, where Q is a positive definite matrix (Camacho and Bordons, 1999; Jacobson and Lele, 1969). Another technique applied to handle inequality path constraints in optimal control problems is based on the constraint violation measurement. It can be applied by adding new differential variables $\dot{w}(t) = [\max(0, g(z(t)))]^2$ and end-point constraints $w(t_f) \leq \varepsilon$ where ε is a very small positive value (Vassiliadis, Sargent, & Pantelides, 1994).

A successful DRTO system has to be efficient and robust to find a profitable optimal solution of the DAOP. One of the most important issues found during the DAOP solution is problem infeasibility. The main goal of the present work is to increase the robustness of DRTO systems by using an efficient and automatic methodology for solving DAOP infeasibilities. We have proposed a methodology based on DAOP path constraint relaxation by solving a multi-objective dynamic optimization problem (MODAOP) and dealing efficiently with infeasibilities.

In Section 2, we discuss the types of infeasibilities in dynamic optimization problems. Section 3 presents the proposed methodology to handle infeasibilities. In Section 4, we present case studies illustrating the proposed methodology and discuss the results.

2. Infeasibilities in dynamic optimization problems

Dynamic optimization packages usually adopt the following standard formulations of DAOP, with constraints only on state and control variables and parameters:

$$\begin{aligned}
 & \min_{u(t), p} \phi(x(t_f)) \\
 & \text{s.t.} \\
 & F(\dot{x}(t), x(t), y(t), u(t), p, t) = 0, \quad x(t_0) = x_0 \quad t \in [t_0, t_f] \\
 & x^L \leq x(t) \leq x^U \\
 & y^L \leq y(t) \leq y^U \\
 & u^L \leq u(t) \leq u^U \\
 & p^L \leq p \leq p^U
 \end{aligned} \tag{2}$$

where $\phi(x(t_f))$ is the objective function, $F(\bullet) \in \mathbb{R}^{nx+ny}$ is the DAE system, $x(t) \in \mathbb{R}^{nx}$ are the state variables, $y(t) \in \mathbb{R}^{ny}$ the algebraic variables, $u(t) \in \mathbb{R}^{nu}$ the control variables, and $p \in \mathbb{R}^{np}$ the time-independent model parameters. In this formulation, all inequality constraints appear as algebraic equations by introducing new variables bounded according to the original constraint.

Unlike stationary optimization, the feasibility of the DAOP solution also depends on the initial condition of the state variables and the directions of their time derivatives. There are cases where a given state variable is feasible, but its time derivative can point to an infeasible region, which drives the process to constraint violation without any possible control actions to avoid this, as will be shown in case 2 (dynamic optimization of a non-isothermal semi-batch reactor) of Section 4. This situation may occur when the process is close to its bounds. Moreover, the values of algebraic variables, evaluated by the optimizer startup procedure, can fall improperly outside the operating limits or even tend inexorably to infeasibility (Fig. 1a). In addition, there are other situations in which the process operation recipe is changed (e.g., changes on product specification) or when the forecast of an important disturbance requires an abrupt change of the process constraints. At that moment the problem may become infeasible (intentionally or not), see Fig. 1b. Therefore, it is necessary to deal with the infeasibilities resulting from these situations.

Another common issue is the presence of conflicts on constraint specifications. In real-time optimization, it is not rare to find situations where the operator establishes constraint positions that compete amongst themselves, resulting in an infeasible DAOP. Therefore, the tendency to initial and intermediate infeasibility, and conflicts on constraints specifications can also be factors contributing to the failure of the dynamic optimizers.

3. Solving the infeasibility problem

As mentioned in Section 1, there are usually two alternatives to solve infeasibilities: ranking and elimination, or identification and relaxation of the violated constraints.

The ranking and elimination approaches are not useful to detect infeasibility in dynamic optimization problems because the high number of constraints in the discrete-time domain may result in a very large number of IIS (each constraint in continuous-time domain results in a number of constraints equal to the number of discrete points). Another issue is the time correlation between state variables and the previous movements on the control variables, making a constraint violation in a given time sensitive to control actions in previous time instants. This behavior is similar to that found in convolution models, where a control action at the beginning of the time horizon has a strong influence on the state variables in subsequent time points far from the point in analysis,

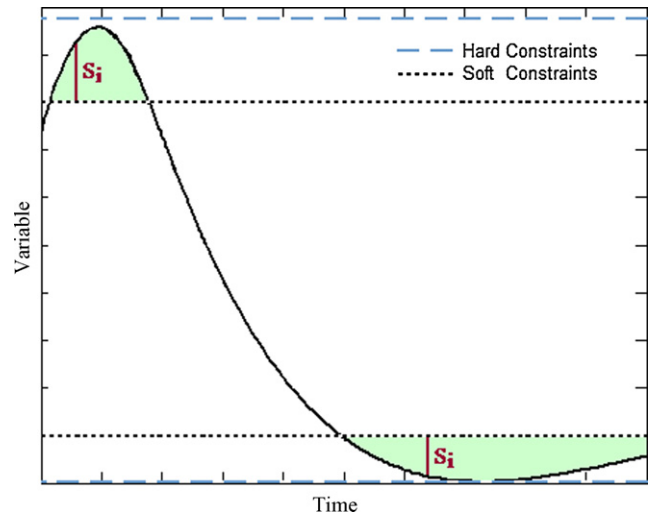


Fig. 2. Constraints relaxation minimization using integral of slack variables.

making it more effective to change control actions earlier in time to avoid constraint violations. This kind of behavior makes it difficult to use these techniques for finding infeasible set of constraints.

The techniques that identify and relax constraints on LPs and NLPs are not effective for solving infeasibilities or trends to infeasibilities on the initial conditions or intermediate time points in DAOP because they are NP-hard problems (non-deterministic polynomial time), where the computational cost is factorial or combinatorial because of the dynamic optimization problem complexity. Furthermore, the inherent use of heuristics to obtain the optimal solution may lead the plant to a non-profitable or even unsafe condition.

The proposed method consists in the solution of a DAOP where we reformulate the original problem as a multi-objective optimization using a time-varying constraint relaxation technique. The adopted strategy is the inclusion of time-varying slack variables and a utopian goal term in the DAOP. The solution of this problem leads to the minimum relaxation of problematic constraints. The main characteristic of this approach is the formulation of a both soft- and hard-constrained problem, leading to the simultaneous solution of the DAOP and the path constraints relaxation problems. In this approach, we do not need to choose which constraints should be relaxed unless it is clearly defined in the problem. In fact, the optimization algorithm makes the decision of which constraints should be relaxed, and by how much. Once the modified problem is solved, it is also possible to diagnose the infeasibility causes of the original DAOP.

Eq. (3) describes the mathematical formulation of the multi-objective optimization problem by relaxing the constraints with time-varying slack variables, $s(t)$.

$$\begin{aligned}
 & \min_{u, s^x, s^y, s^u, p} \left[\phi(x(t_f)), \int_0^{t_f} (s_i^x(t))^2 dt, \int_0^{t_f} (s_j^y(t))^2 dt, \int_0^{t_f} (s_k^u(t))^2 dt \right] \\
 & \text{s.t.} \\
 & F(\dot{x}(t), x(t), y(t), u(t), p, t) = 0 \quad , \quad x(t_f) = x_0 \quad t \in [t_0, t_f] \\
 & x^L \leq x(t) + s^x(t) \leq x^U \\
 & y^L \leq y(t) + s^y(t) \leq y^U \\
 & u^L \leq u(t) + s^u(t) \leq u^U \\
 & p^L \leq p \leq p^U \\
 & s_i^x \leq s^x(t) \leq s_u^x \quad \text{where } s^x(t) \in \mathbb{R}^{Sx} \\
 & s_j^y \leq s^y(t) \leq s_u^y \quad \text{where } s^y(t) \in \mathbb{R}^{Sy} \\
 & s_k^u \leq s^u(t) \leq s_u^u \quad \text{where } s^u(t) \in \mathbb{R}^{Su}
 \end{aligned} \tag{3}$$

where $i \in \{1, \dots, nx\}, j \in \{1, \dots, ny\}$ and $k \in \{1, \dots, nu\}$.

The integral of the constraint relaxations represents the amount of movements beyond their bounds that have to be minimized, as shown in Fig. 2.

The basic differences between this formulation and the original DAOP are the simultaneous usage of time-varying soft and hard constraints, and the simultaneous solution of the optimization problem and constraint relaxation.

The solution of the multi-objective DAOP (Eq. (4)) is a Pareto set. For DRTO applications, it is desirable to obtain a single optimum value of the objective function instead of an optimal set. In order to obtain a unique solution, we reformulated the original DAOP using a goal programming approach as follows:

$$\begin{aligned}
 & \min_{u, \Delta\gamma, s^x, s^y, s^u, p} \gamma(t_f) \\
 & \text{s.t.} \\
 & F(\dot{x}(t), x(t), y(t), u(t), p, t) = 0, \quad x(t_0) = x_0 \quad t \in [t_0, t_f] \\
 & \frac{d\gamma}{dt} = \Delta\gamma(t), \quad \gamma(t_0) = 0 \\
 & \phi(x(t_f)) - \phi^L \leq \gamma(t_f)w_0 \\
 & \left(\frac{s_i^x(t)}{\sigma_i^x}\right)^2 \leq \Delta\gamma(t) \quad \text{where } i \in \{1, \dots, nx\} \\
 & \left(\frac{s_j^y(t)}{\sigma_j^y}\right)^2 \leq \Delta\gamma(t) \quad \text{where } j \in \{1, \dots, ny\} \\
 & \left(\frac{s_k^u(t)}{\sigma_k^u}\right)^2 \leq \Delta\gamma(t) \quad \text{where } k \in \{1, \dots, nu\} \\
 & x^L \leq x(t) + s^x(t) \leq x^U \\
 & y^L \leq y(t) + s^y(t) \leq y^U \\
 & u^L \leq u(t) + s^u(t) \leq u^U \\
 & s_L^x \leq s^x(t) \leq s_U^x \quad \text{wheres}^x(t) \in \mathfrak{N}^{Sx} \\
 & s_L^y \leq s^y(t) \leq s_U^y \quad \text{wheres}^y(t) \in \mathfrak{N}^{Sy} \\
 & s_L^u \leq s^u(t) \leq s_U^u \quad \text{wheres}^u(t) \in \mathfrak{N}^{Su}
 \end{aligned} \tag{4}$$

In Eq. (4), $\gamma(t_f)$ is the new objective function, $\Delta\gamma(t)$ is the maximum degree of constraint violations at each time instant, ϕ^L is a utopian value of the objective function of the original DAOP and w_0 is its under-attainment weight, $(\sigma_i^z)^2$ is the allowed variance of the constraint violation $s_i^z(t)$ of $z_i(t)$, $z \in \{x, y, u\}$, that can be obtained by statistical analysis of plant historical data, and s_L^z and s_U^z are the minimum and maximum allowed constraint violations, respectively, based on process analysis of the DAOP.

The meaning of the new variable γ is the larger of two values: (1) the integral of the worst squared relaxation weighted by the reciprocal of the allowed variance of the constraint violation at each time instant or (2) the distance between the original objective function and its utopian value. All relaxations are constrained and the original constraints are relaxed in the infinite-dimensional DAOP. The utopian value is chosen based on its physical meaning. For instance, if the objective is the maximization of a component molar fraction, then the utopian value may be 1 ($\phi^L = -1$, since Eq. (4) is a minimization problem). The under-attainment weight w_0 ($0 \leq w_0 \leq 1$) focuses on the feasibility aspect at the expense of the original objective function. When the minimization of constraint violations is very important, small values of w_0 should be used, such as $w_0 = 0.1$. It is important to note that it is not necessary to relax all variables $z(t)$ as will be shown in the case studies in Section 4, which avoids the generation of large optimization problems. If variables are bounded on their domains or cannot be relaxed due to other reasons, then their constraints may not be reformulated by including slack variables.

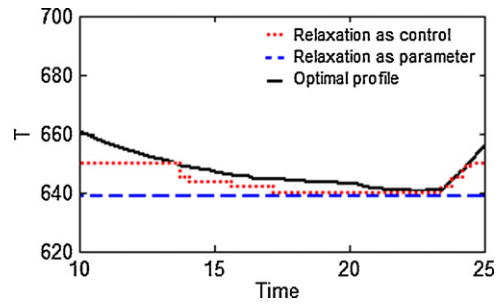


Fig. 3. Constraints relaxation using slack variables as parameter or control variable.

Rewriting Eq. (4) in standard form (similar to Eq. (2)), we get the following problem:

$$\begin{aligned}
 & \min_{u, \Delta\gamma, s^x, s^y, s^u, p} \gamma(t_f) \\
 & \text{s.t.} \\
 & F(\dot{x}(t), x(t), y(t), u(t), p, t) = 0, \quad x(t_0) = x_0 \quad t \in [t_0, t_f] \\
 & \frac{d\gamma}{dt} = \Delta\gamma(t), \quad \gamma(t_0) = 0 \\
 & \psi^\phi(t_f) = \gamma(t_f)w_0 - \phi(x(t_f)) + \phi^L \\
 & \psi_i^x(t) = \Delta\gamma(t) - \left(\frac{s_i^x(t)}{\sigma_i^x}\right)^2 \quad \text{where } i \in \{1, \dots, nx\} \\
 & \psi_j^y(t) = \Delta\gamma(t) - \left(\frac{s_j^y(t)}{\sigma_j^y}\right)^2 \quad \text{where } j \in \{1, \dots, ny\} \\
 & \psi_k^u(t) = \Delta\gamma(t) - \left(\frac{s_k^u(t)}{\sigma_k^u}\right)^2 \quad \text{where } k \in \{1, \dots, nu\} \\
 & g^x(t) = x(t) + s^x(t) \\
 & g^y(t) = y(t) + s^y(t) \\
 & g^u(t) = u(t) + s^u(t) \\
 & x^L \leq g^x(t) \leq x^U \quad \text{where } g^x(t) \in \mathfrak{N}^{Sx} \\
 & y^L \leq g^y(t) \leq y^U \quad \text{where } g^y(t) \in \mathfrak{N}^{Sy} \\
 & u^L \leq g^u(t) \leq u^U \quad \text{where } g^u(t) \in \mathfrak{N}^{Su} \\
 & s_L^x \leq s^x(t) \leq s_U^x \quad \text{where } s^x(t) \in \mathfrak{N}^{Sx} \\
 & s_L^y \leq s^y(t) \leq s_U^y \quad \text{where } s^y(t) \in \mathfrak{N}^{Sy} \\
 & s_L^u \leq s^u(t) \leq s_U^u \quad \text{where } s^u(t) \in \mathfrak{N}^{Su} \\
 & \psi^\phi(t) \geq 0, \quad \psi^x(t) \geq 0, \quad \psi^y(t) \geq 0, \quad \psi^u(t) \geq 0
 \end{aligned} \tag{5}$$

There are two possible relaxation strategies: (1) shift the constraint by a constant value throughout the optimization horizon. The disadvantage of this strategy is that the constraints are also relaxed at time instants where the relaxations are not necessary and, consequently, these relaxations may affect the optimization of the control profiles. This strategy is equivalent to optimizing a model parameter in the optimization problem; (2) consider the slack variables as control variables. In this case, the constraints

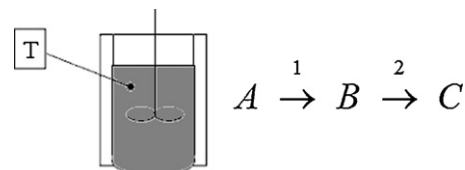


Fig. 4. Scheme and reactions of a batch reactor.

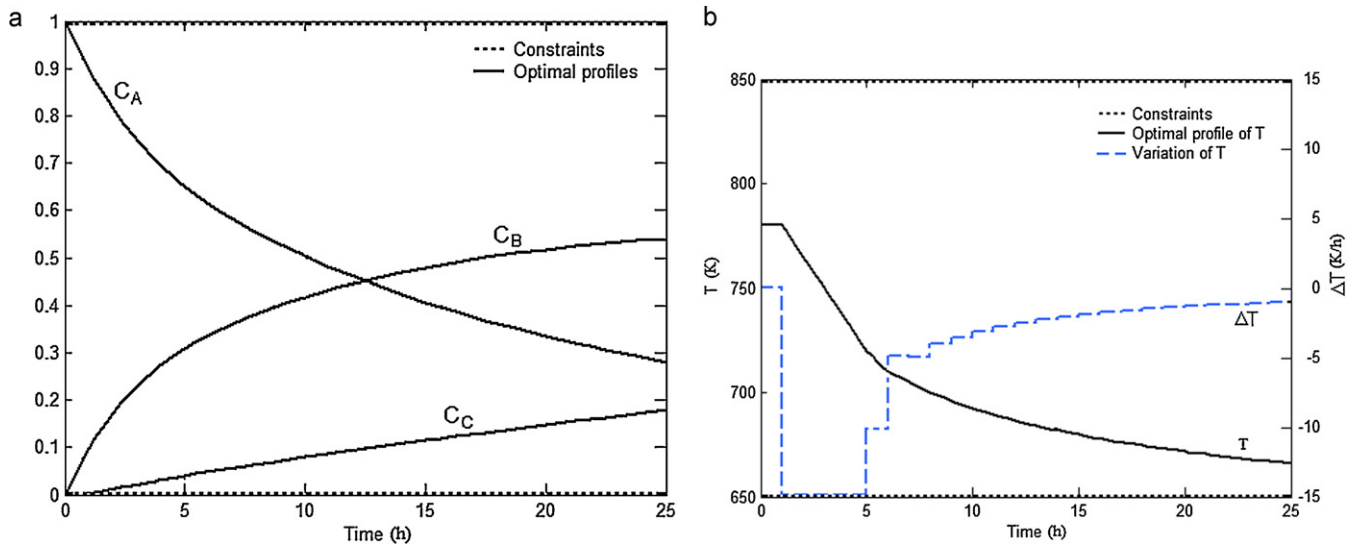


Fig. 5. Optimal solution of the original problem. Trajectories of (a) C_A , C_B and C_C , (b) T and ΔT .

are relaxed only in time intervals in which the problem becomes infeasible. The manipulations of the slack variables follow the criterion of minimum relaxation of these variables in order to make the problem feasible, as shown in Fig. 3. This strategy is more com-

plex but more efficient, and is used in the proposed methodology. When using DRTO application, it is possible to replace a sequence of small relaxations by a single relaxation in a defined interval of the optimization horizon.

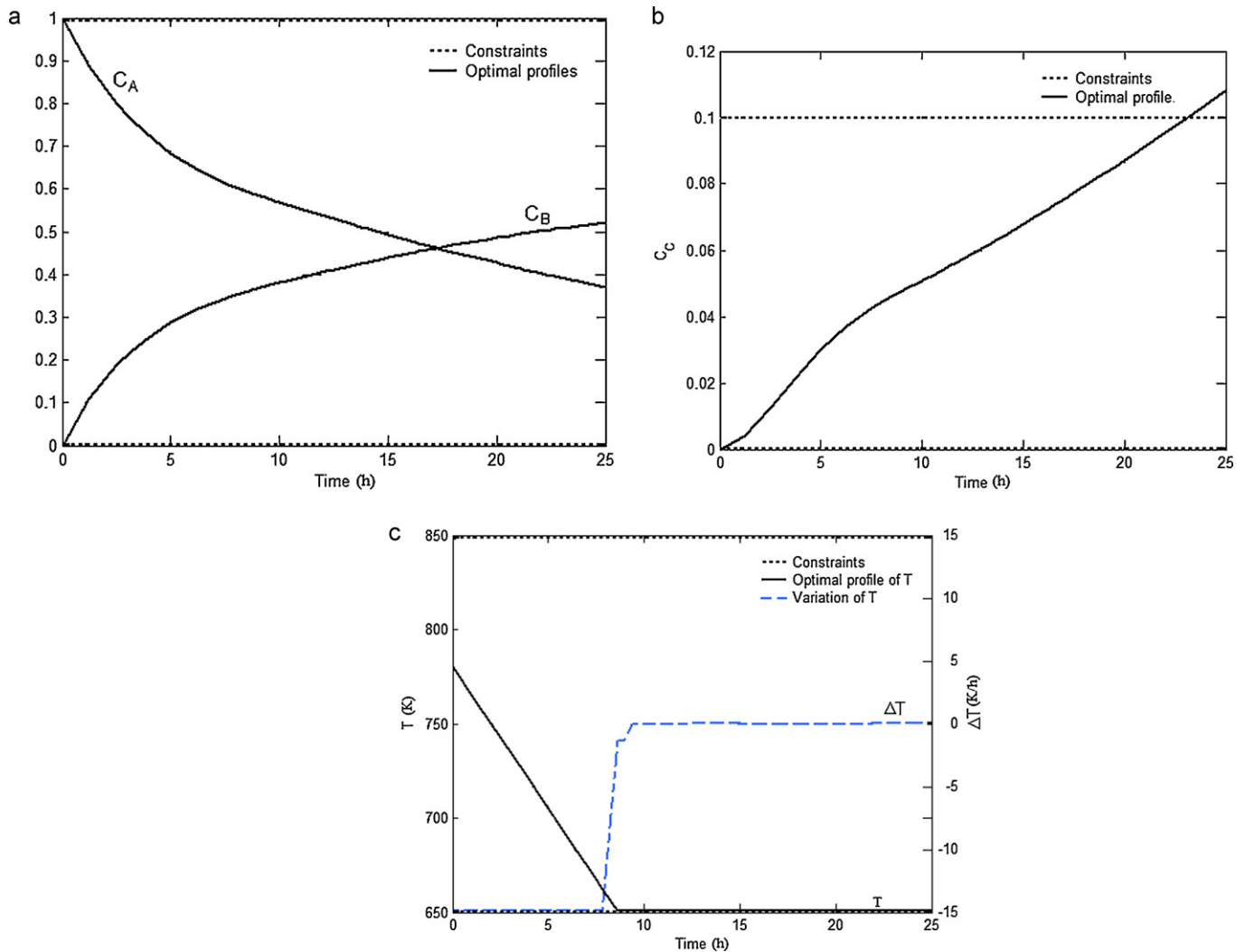


Fig. 6. Best result of the infeasible problem. Trajectories of (a) C_A and C_B , (b) C_C , (c) T and ΔT .

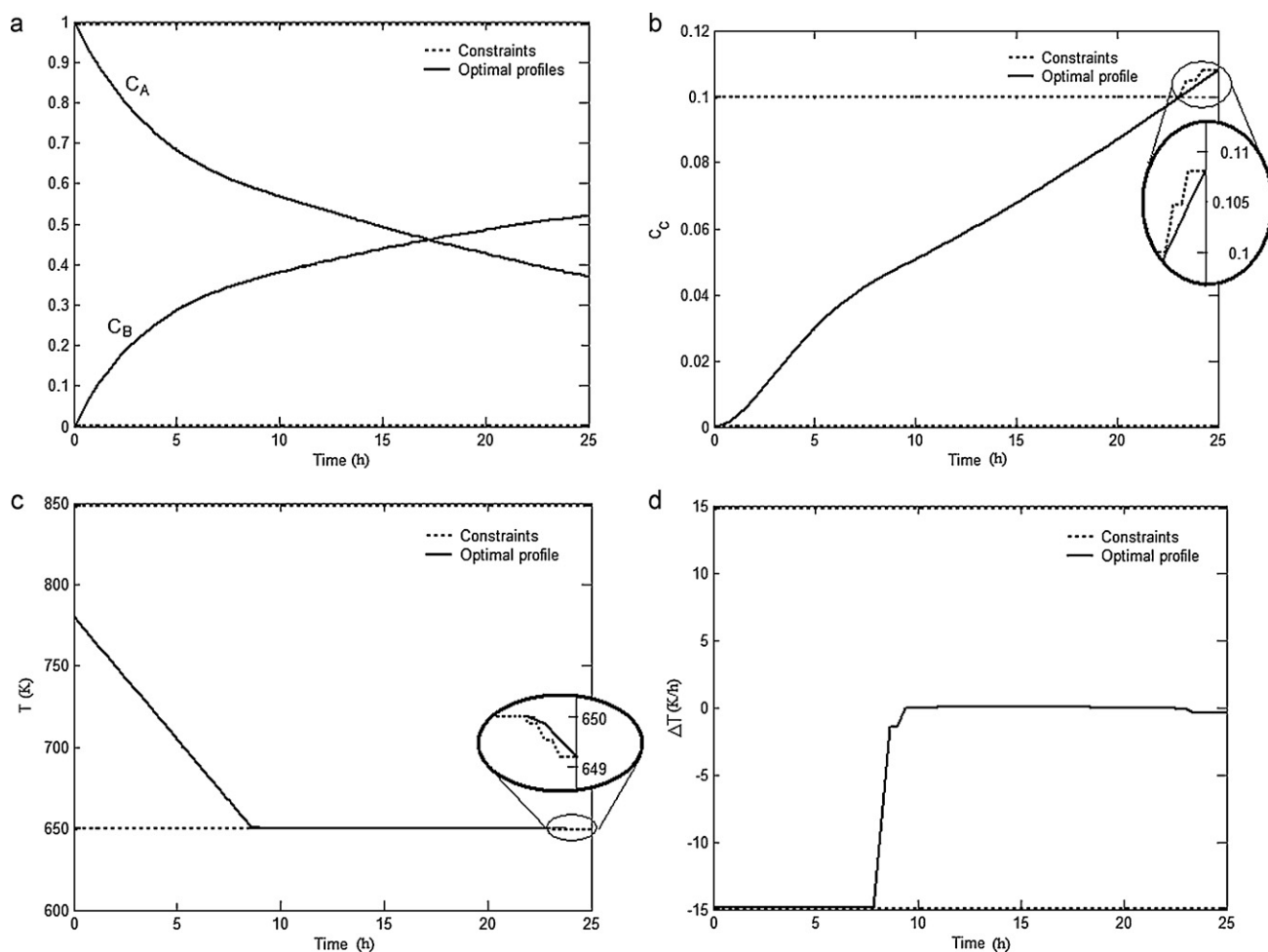


Fig. 7. The relaxed problem solution. Trajectories of (a) C_A and C_B , (b) C_C , (c) T , and (d) variation of T .

4. Case studies, results and comments

In this section, we present three cases showing the features of the proposed methodology, discussing issues such as conflict between specifications, initial infeasibility, tendency to initial infeasibility, and intermediate infeasibility. In each case, we studied three situations: the original problem (feasible solution), the infeasible problem, and the relaxed feasible problem. When solving the original DAOP and the infeasible DAOP we have used the original standard formulation presented in Eq. (2). In the relaxation case, we have replaced the original DAOP by the relaxed reformulation described by Eq. (5). The same relaxed formulation has been used for all dynamic optimization packages.

In this study, the NLP is solved using the interior point method implemented in IPOPT (Wächter and Biegler, 2006) for the simultaneous approach through the package DynoPC (Lang and Biegler, 2007), and a quasi-Newton method implemented in SNOPT (Gill, Murray, & Saunders, 2005) for the sequential approach through the package DyOS (Schlegel and Marquardt, 2006). Both packages (DynoPC and DyOS) provided similar results for all case studies, and therefore only the results using DyOS are presented. The NLP solver and the integrator used in DyOS runs are SNOPT (Gill et al., 2005) and extended LIMEX (Schlegel, Marquardt, Ehrig, & Nowak, 2004), respectively. DyOS package has a wavelet-based mesh adaptation strategy (Binder, Cruse, Villas, & Marquardt, 2000). We used the multi-shooting direct method for solving DAOP using DyOS. The initial number of grid points used in all cases was 8 elements, and the relative and absolute tolerances adopted for both NLP solver and integrator were 10^{-6} .

4.1. Case 1 – dynamic optimization of a batch reactor

Consider the following batch process (Fig. 4), where the control variable is the reaction batch temperature (Cervantes, Waechter, Tutuncu, & Biegler, 2000; Ray, 1981). The initial conditions of this process are $C_A = 1.0$, $C_B = 0.0$, $C_C = 0.0$, given in mole fractions, and $T = 780$ K. The production objective is to maximize the concentration of the desired product, component B (C_B), avoiding the production of the undesired component C (C_C).

The mathematical model that describes this process is the following:

$$\begin{aligned} \frac{dC_A}{dt} &= -k_1(T)C_A \\ \frac{dC_B}{dt} &= k_1(T)C_A - k_2(T)C_B \\ C_A + C_B + C_C &= 1 \end{aligned} \quad (6)$$

where $k_1(T) = k_{01} e^{-E_1/RT}$ and $k_2(T) = k_{02} e^{-E_2/RT}$, $k_{01} = 65.5 \text{ h}^{-1}$ and $E_1/R = 5027.7 \text{ K}$ are the kinetic parameters of reactions 1, $k_{02} = 1970 \text{ h}^{-1}$ and $E_2/R = 8044.31 \text{ K}$ are the kinetic parameters of reactions 2, and T the reaction temperature in K.

In this work, this example was divided in three cases: (1) the original problem with domain constraints on concentrations, (2) the infeasible problem due to the constraints on reaction temperature and concentration of component C, and (3) problem with constraint relaxation.

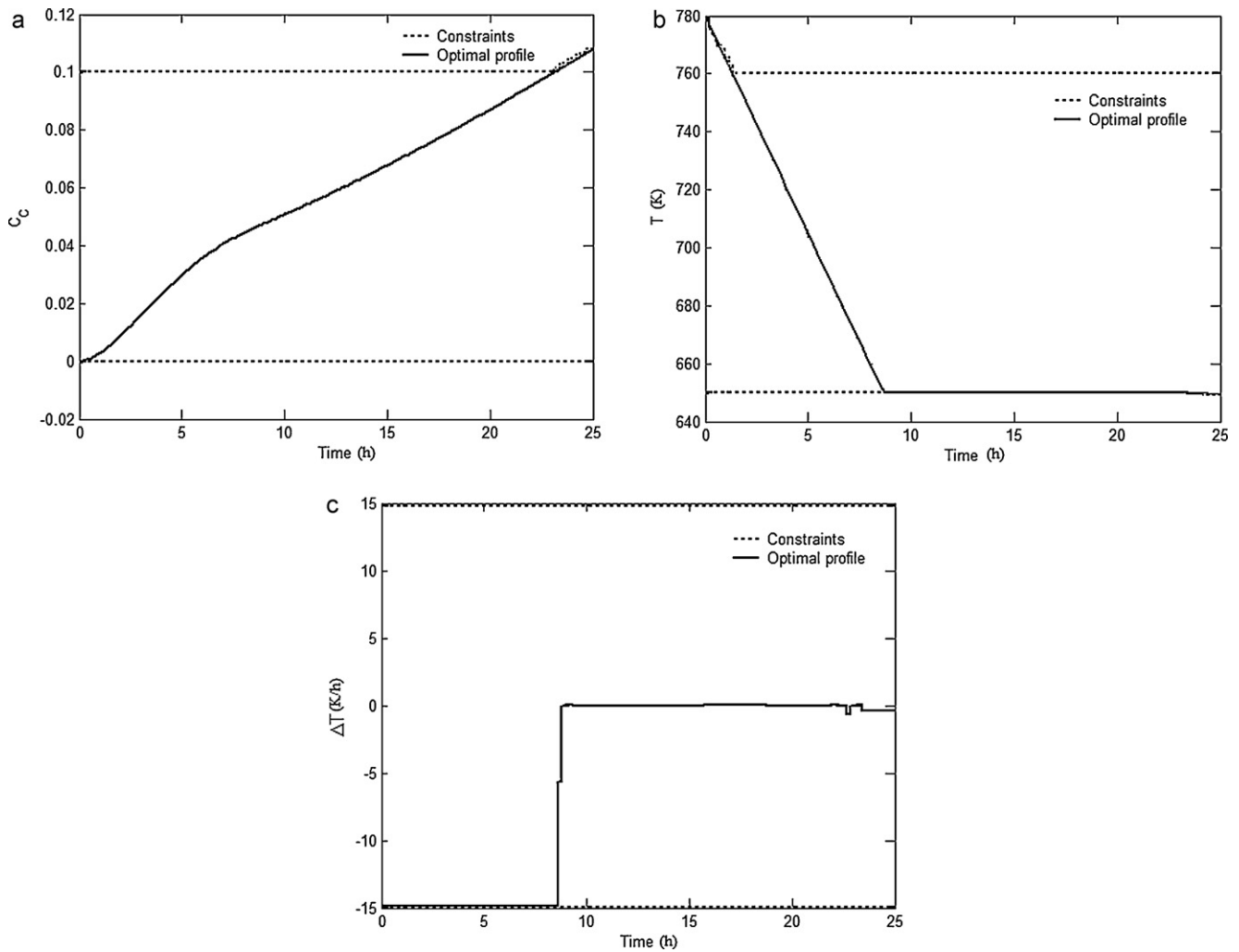


Fig. 8. The relaxed problem solution – upper bound of $T = 760$ K. Trajectories of (a) C_C , (b) T , and (c) variation of T .

4.1.1. Original problem

The original problem has a feasible solution in which the optimizer maximizes the concentration of B at the final time (t_f) of 25 h, and is described as follows:

$$\begin{aligned}
 & \max_{\Delta T(t)} C_B(t_f) \\
 & \text{s.t.} \\
 & \frac{dC_A}{dt} = -k_1(T)C_A \quad C_A(0) = 1.0 \\
 & \frac{dC_B}{dt} = k_1(T)C_A - k_2(T)C_B \quad C_B(0) = 0.0 \\
 & C_A + C_B + C_C = 1 \\
 & 0 \leq C_A, C_B, C_C \leq 1 \\
 & \frac{dT}{dt} = \Delta T \quad T(0) = 780 \text{ K} \\
 & 650 \leq T(t) \leq 850 \\
 & -15 \leq \Delta T(t) \leq 15
 \end{aligned} \tag{7}$$

where $k_1(T) = k_{01} e^{-E_1/RT}$ and $k_2(T) = k_{02} e^{-E_2/RT}$.

The optimal solution (Fig. 5) is obtained by imposing a piecewise constant profile to the control variable ΔT and binding the value of T and its variation. A piecewise constant profile over ΔT corresponds to a piecewise linear profile in T (the original manipulated variable). In industry, many manipulated variables present

some dynamics and cannot be set directly to an arbitrary value, or the control actions are implemented in form of limited steps changes. Therefore the best way to mimic real world operation is to represent the manipulated variables as state variables and impose step changes their time derivatives. Higher order profiles are not usually implemented in industry.

The optimization found a feasible solution where the final concentration of B was 0.5406 and the reaction temperature was above its minimum value. Also note that the final concentration of byproduct C, which must be as low as possible, was 0.1789.

4.1.2. Infeasible problem

In this problem, a limit of 0.1 on the maximum allowed concentration of undesirable byproduct C is defined. This implies a conflict between the constraint on maximum concentration of C and minimum reaction temperature since they cannot be satisfied simultaneously. In this case, the imposed constraint $0 \leq C_C \leq 0.1$ results in an infeasible problem and highlights the conflicts in constraint specifications.

As can be seen in Fig. 6, the optimizer attempts to reduce the reaction temperature with its maximum rate of negative variation. Note that the final concentration of C (0.1081) violates its upper bound, while the reaction temperature (650 K) reaches its lower bound during some intervals of the optimization horizon. When using this constraint configuration it is not possible to find any feasible solution, generating a fault in the optimizer. A profitable solution is the relaxation of the constraints related to maximum

concentration of C, the minimum reaction temperature and the maximum variation of temperature.

4.1.3. Relaxed problem

In the proposed methodology, we reformulated the problem as a multi-objective optimization problem where the first two constraints mentioned above are relaxed, considering the third one as a physical limitation of the process. The competing goals are to maximize $C_B(t_f)$ while minimizing the constraint relaxations in C_C and T . We formulated the multi-objective problem in its standard form, Eq. (5), where we added slack variables as control variables $\Delta\gamma$, s_{C_C} , and s_T with piecewise constant profiles as follows:

$$\begin{aligned} & \min_{\Delta T, \Delta\gamma, s_T, s_{C_C}} \gamma(t_f) \\ & \text{s.t.} \\ & \frac{dC_A}{dt} = -k_1(T)C_A \quad C_A(0) = 1.0 \\ & \frac{dC_B}{dt} = k_1(T)C_A - k_2(T)C_B \quad C_B(0) = 0.0 \\ & C_A + C_B + C_C = 1 \\ & \frac{dT}{dt} = \Delta T \quad T(0) = 780 \text{ K} \\ & \frac{d\gamma}{dt} = \Delta\gamma \quad \gamma(0) = 0.0 \\ & g_{C_C}(t) = C_C - s_{C_C} \\ & g_T(t) = T - s_T \\ & \phi(t_f) = -C_B(t_f) \\ & \psi_\phi = w^\phi \gamma(t_f) - \phi(t_f) + \phi_L \\ & \psi_\phi \geq 0 \\ & \psi_{C_C} = \Delta\gamma - \left(\frac{s_{C_C}}{\sigma_{C_C}}\right)^2 \\ & \psi_{C_C} \geq 0 \\ & \psi_T = \Delta\gamma - \left(\frac{s_T}{\sigma_T}\right)^2 \\ & \psi_T \geq 0 \\ & 0 \leq C_A, C_B \leq 1 \\ & 0 \leq g_{C_C}(t) \leq 0.1 \\ & 650 \leq g_T(t) \leq 850 \\ & -15 \leq \Delta T \leq 15 \\ & -0.1 \leq s_{C_C} \leq 0.1 \\ & -10 \leq s_T \leq 10 \end{aligned} \quad (8)$$

Fig. 7 shows that the optimizer finds a feasible solution which minimizes the relaxation of both the lower bound of the reaction temperature and the upper bound of the concentration of component C at the end of the batch process. The bounds of the slack variables were chosen based on tolerances defined by the process analysis of the DAOP. The standard deviation values for the relaxed constraints are $\sigma_{C_C} = 0.01$ and $\sigma_T = 1 \text{ K}$. The optimizer obtained a maximum concentration of C of 0.1080 and a minimum temperature of 649.19 K, but more important was the fact that the optimizer did not fail.

Next, an initial infeasibility problem was obtained by reducing the upper bound of the reaction temperature to 760 K. In this case, the problem becomes infeasible due to its inadequate initial condition. This situation is not rare in dynamic optimization problems in real plants, since the initial conditions of some variables cannot be chosen freely. In this case, we modified the following constraints

on the relaxed problem: $-30 \leq s_T(t) \leq 30$ and $650 \leq g_T(t) \leq 760$. The relaxed solution provides the profiles shown in Fig. 8.

An alternative scenario was obtained by not relaxing the maximum concentration of C. In this case, the optimizer changed the reaction temperature profile to compensate for this condition. Note that, in Fig. 9, there was a relaxation in the minimum reaction temperature of around 7 K, which is larger than the one shown in Fig. 8b. If this relaxation is acceptable, it may be preferable to apply it in a single constraint. In this case, in a first run, we could execute the optimizer relaxing all constraints. If it is possible to have another solution that is more convenient to the process operation, we could perform a second run setting hard constraints on some variables, as shown in this example using the concentration of C. This is a clear situation of the application of the proposed methodology for diagnosis purposes, instead of just increasing the robustness of the DRTO system.

In a second case, there was an intermediate infeasibility problem where the lower bound of the reaction temperature was raised from 650 K to 660 K after 10 h of batch operation. The problem becomes infeasible within the optimization horizon, which is a common situation found in dynamic optimization of real plants where the recipe can be altered during the batch process. To solve this case, we modified the following constraint on the relaxed problem: $650 \leq g_T(t) \leq 790$ for $t \in [0, 10]$ and $660 \leq g_T(t) \leq 790$ for $t \in (10, 25]$. The relaxed solution provides the optimum profiles shown in Fig. 10.

Note that the optimizer has avoided the infeasible solution due to the recipe change after 10 h by anticipating the temperature transition. Moreover, the temperature and the maximum concentration of C were relaxed at the end of the optimization horizon in order to enable a feasible solution.

4.2. Case 2 – dynamic optimization of a non-isothermal semi-batch reactor

Consider a non-isothermal semi-batch reactor with exothermic reactions in series subject to heat removal limitations, as shown in Fig. 11. This system has two control variables, the feed flow rate F of reagent B and the reactor temperature (Srinivasan, Palanki, and Bonvin, 2003). The production objective is the maximization of the amount of component C produced during a predefined optimization horizon. We must obey the upper bound of the heat rate produced by the reaction along the time horizon. We have imposed an upper bound for the final volume in the reactor of 1.1 L. The initial conditions of the process are $C_A(t_0) = 10.0 \text{ mol/L}$, $C_B(t_0) = 1.1685 \text{ mol/L}$, $C_C(t_0) = 0.0 \text{ mol/L}$, $V(t_0) = 1.0 \text{ L}$, $F_0 = 0.5 \text{ L/h}$, and $T_0 = 35^\circ \text{C}$, and the feed concentration is $C_{B,In} = 20.0 \text{ mol/L}$.

The mathematical model that describes this process is the following:

$$\begin{aligned} \frac{dC_A}{dt} &= -k_1 C_A C_B - \frac{F}{V} C_A \\ \frac{dC_B}{dt} &= -k_1 C_A C_B + \frac{F}{V} (C_{B,In} - C_B) \\ \frac{dC_C}{dt} &= k_1 C_A C_B - k_2 C_C - \frac{F}{V} C_C \\ \frac{dV}{dt} &= F \\ Q &= (-\Delta H_1) k_1 C_A C_B V + (-\Delta H_2) k_2 C_C V \end{aligned} \quad (9)$$

$$\begin{aligned} k_1 &= k_{01} e^{\left(\frac{E_1}{R(T+273)}\right)} \quad k_{01} = 4.0 \text{ L}/(\text{mol h}), \\ E_1 &= 6000 \text{ J/mol}, \quad R = 8.31 \text{ J/mol K} \\ k_2 &= k_{02} e^{\left(\frac{E_2}{R(T+273)}\right)} \\ k_{02} &= 800.0 \text{ L}/(\text{mol h}), \quad E_2 = 20,000 \text{ J/mol} \end{aligned}$$

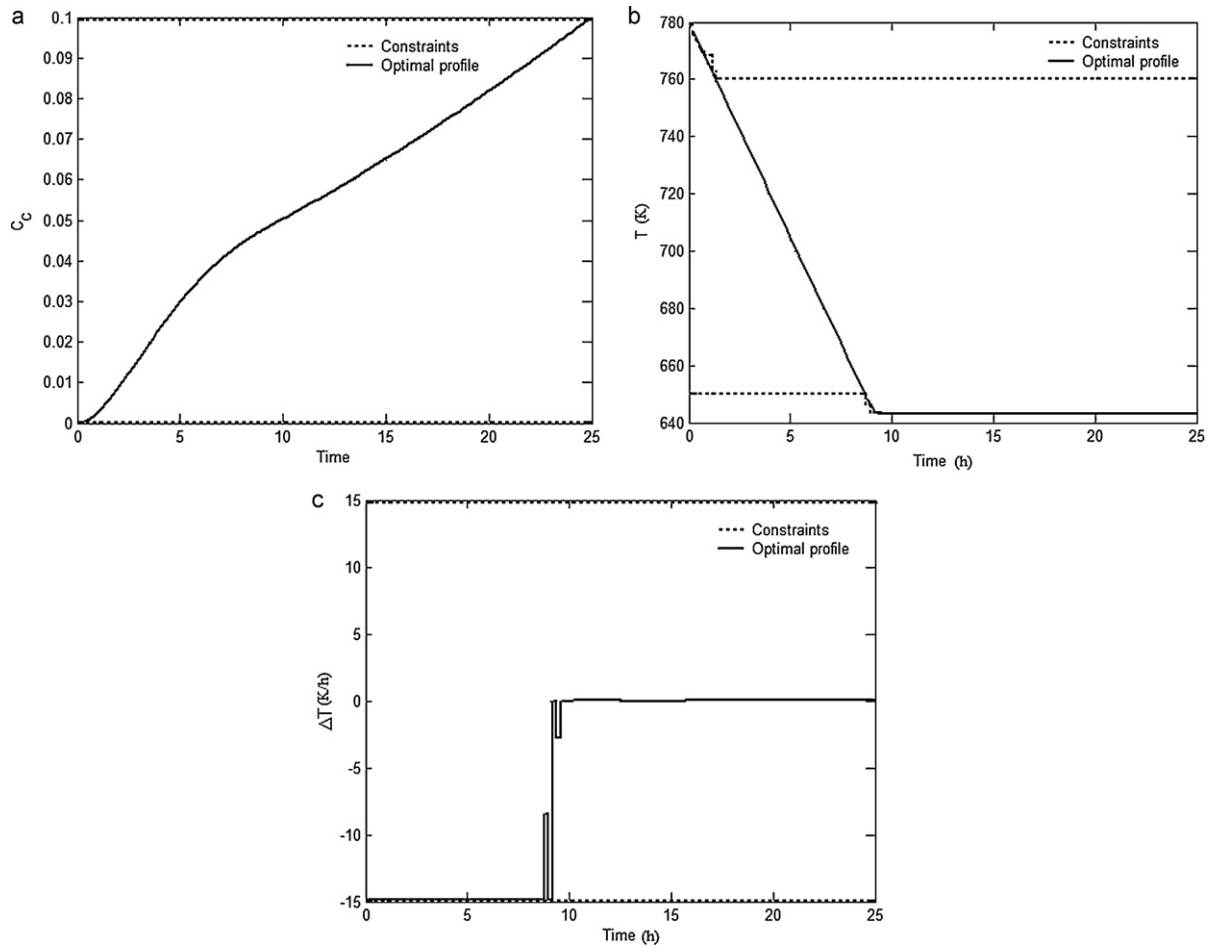


Fig. 9. Solution of the partially relaxed problem. Trajectories of (a) C_C , (b) T , and (c) variation of T .

where k_1 , E_1 , k_2 , and E_2 are the kinetic parameters of reactions 1 and 2, respectively. T is the reaction temperature in °C, C_A , C_B , and C_C are the concentrations of components A, B, and C, respectively. $C_{B,IN}$ is the feed concentration of B, F is the feed flow rate of reactant B, V is the reaction volume, Q is the heat rate produced by the reactions, $\Delta H_1 = -30,000$ J/mol and $\Delta H_2 = -10,000$ J/mol are the heat of reactions 1 and 2, respectively.

As in the previous case, we converted the original manipulated variables into differential state variables whose variations are manipulated by the optimizer. This transformation makes the problem more closely related to the ones found in industry, where feed flow rates and temperatures are manipulated obeying a ramp pattern. Thus, we add the following equations into the optimization model:

$$\frac{dF}{dt} = \Delta F \quad \text{and} \quad \frac{dT}{dt} = \Delta T \quad \text{where } F(t_0) = F_0 \quad \text{and} \quad T(t_0) = T_0 \quad (10)$$

In online DRTO applications, the digital control systems (DCS) supply the initial conditions of the real plant, which thus are not free variables for the optimization problem. Therefore, it is reasonable to state that F_0 and T_0 are given conditions for the process operation. In cases where the optimizer is used for planning purposes of a batch operation, F_0 and T_0 can be free variables. These planning cases are not the focus of this work.

Similar to the previous case, this example was divided into three cases: (1) the original problem, without constraints on component concentrations, (2) the infeasible problem due to bounds on reaction temperature and concentration of component C, and (3) constraint relaxation problem.

4.2.1. Original problem

The original problem has a feasible solution in which the optimizer maximizes the amount of product C at the final time (t_f) of 0.5 h, imposing piecewise constant profiles to the control variables ΔF and ΔT , and is formulated as follows:

$$\begin{aligned} & \max_{\Delta T(t), \Delta F(t)} C_C(t_f) V(t_f) \\ & \text{s.t.} \\ & \frac{dC_A}{dt} = -k_1 C_A C_B - \frac{F}{V} C_A \quad C_A(0) = 10.0 \text{ mol/L} \\ & \frac{dC_B}{dt} = -k_1 C_A C_B + \frac{F}{V} (C_{B,IN} - C_B) \quad C_B(0) = 1.1685 \text{ mol/L} \\ & \frac{dC_C}{dt} = k_1 C_A C_B - k_2 C_C - \frac{F}{V} C_C \quad C_C(0) = 0.0 \text{ mol/L} \\ & \frac{dV}{dt} = F \quad V(0) = 1.0 \text{ L} \\ & \frac{dF}{dt} = \Delta F \quad F(0) = 0.50 \text{ L/h} \\ & \frac{dT}{dt} = \Delta T \quad T(0) = 35.0 \text{ }^\circ\text{C} \\ & Q = (-\Delta H_1) k_1 C_A C_B V + (-\Delta H_2) k_2 C_C V \\ & 0.0 \leq Q(t) \leq 140 \text{ J/h} \\ & 0.0 \leq V(t_f) \leq 1.1 \text{ L} \\ & 20 \leq T(t) \leq 50 \text{ }^\circ\text{C} \\ & 0.0 \leq F(t) \leq 1.0 \text{ L/h} \\ & -100 \leq \Delta F(t) \leq 100 \text{ L/h}^2 \\ & -1000 \leq \Delta T(t) \leq 1000 \text{ }^\circ\text{C/h} \end{aligned} \quad (11)$$

In this case, there are bounds for the feed flow rate and its variation, as well as the reaction temperature and its variation. The jacket cooling duty and maximum reaction volume are also con-

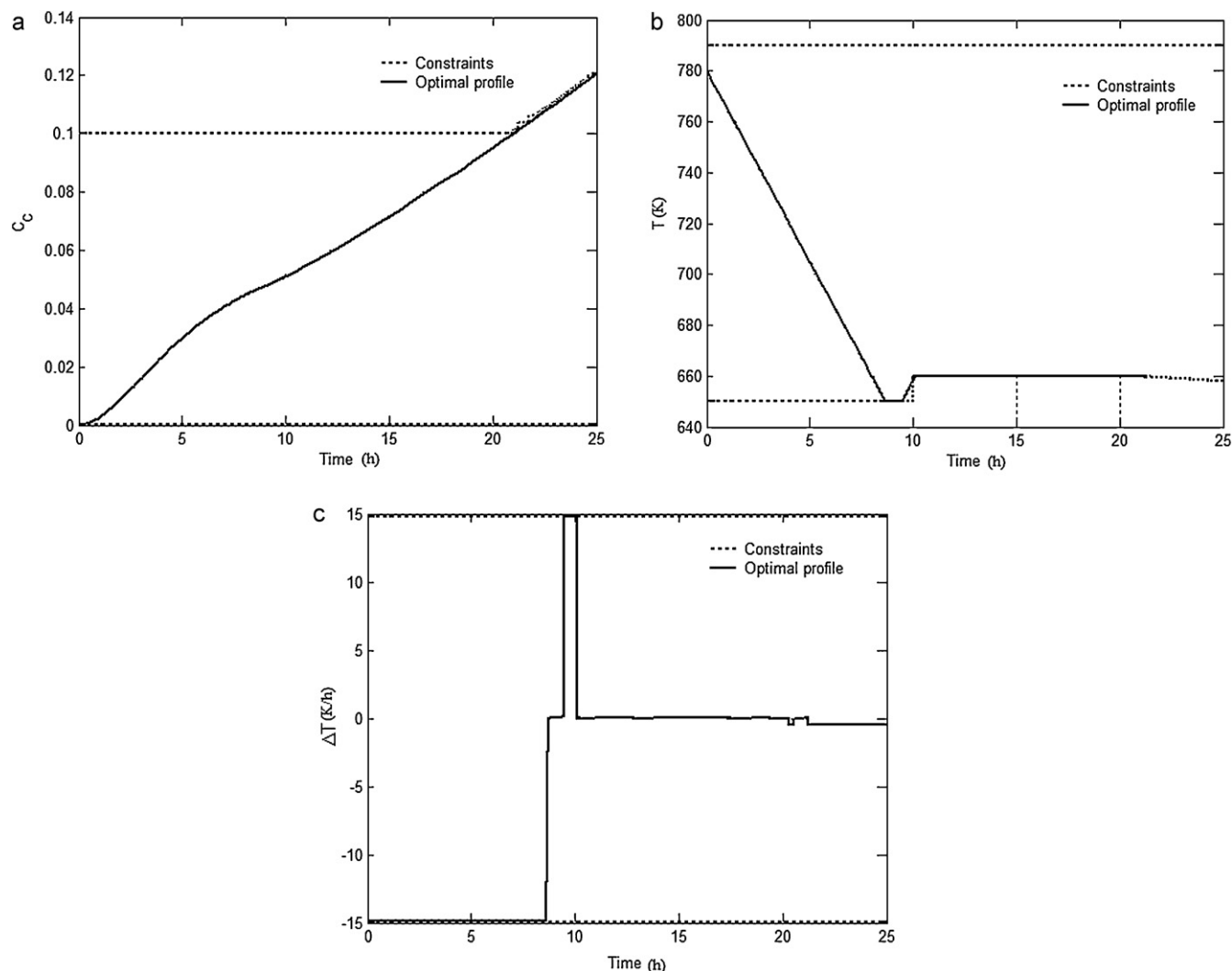


Fig. 10. Solution of the relaxed problem – intermediate infeasibility case. Trajectories of (a) C_C , (b) T , and (c) ΔT .

strained. There are no bounds on concentrations of reactants and products. The optimizer found a feasible solution at the lower temperature and maximum duty bounds, as shown in Fig. 12. Note also that the maximum concentration of component B in the reaction was 1.65 mol/L.

4.2.2. Infeasible problem

Now consider the case in which an upper bound of 1.3 mol/L is set on the on the maximum allowed concentration of the undesirable by-product B, and a maximum duty of the cooling jacket is defined as 136 kJ/h. In the optimization problem, this causes the maximum concentration of B and the maximum reaction duty Q constraints to compete against each other, since they cannot be satisfied simultaneously. Furthermore, the reaction temperature range during the system operation was reduced. In this case, we have imposed the constraints to the original problem as $0.0 \leq C_B(t) \leq 1.3$ mol/L, $50 \leq Q(t) \leq 136$ kJ/h, and $30.0 \leq T(t) \leq 40.0$ °C. These changes make the problem infeasible due to the conflict in constraint specifications (Fig. 13).

The optimizer tries to set the concentration of B to its maximum allowed value, thus violating the maximum cooler duty and reaching the lower bound of the reaction temperature. In this configuration, it is not possible to find any feasible solution and the optimizer fails. The solution for this problem is the relaxation of constraints related to the maximum duty,

minimum reaction temperature, and maximum concentration of B.

4.2.3. Relaxed problem

Applying the proposed methodology, we reformulated the problem to a multi-objective dynamic optimization problem, with the following competing objectives: maximization of C_B at final time and minimization of relaxations of constraints related to C_B , Q and T . We formulated the multi-objective problem in the same way as described before. Results are shown in Fig. 14. Note that the constraints C_B and T do not need to be relaxed. The values of standard deviation for the relaxed constraints were $\sigma_{C_B} = 0.01$, $\sigma_T = 0.1$ °C and $\sigma_Q = 1$ kJ/h. The optimizer minimizes the constraint relaxations to obtain a feasible solution through an algorithmic way without using any heuristics.

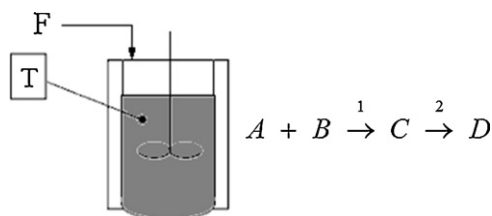


Fig. 11. Scheme and reactions of a semi-batch reactor.

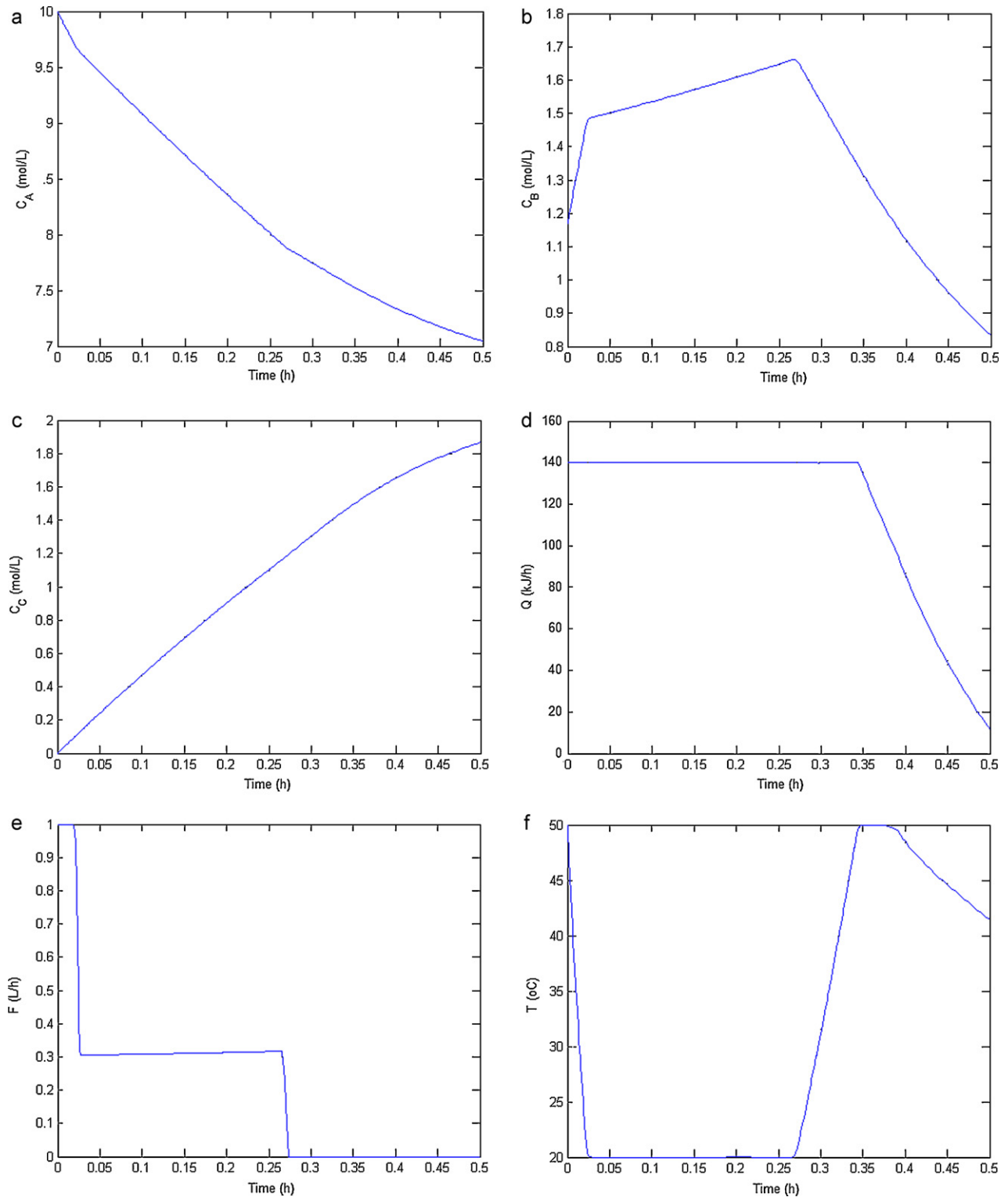


Fig. 12. Optimal solution of original problem. Trajectories of (a) C_A , (b) C_B , (c) C_C , (d) Q , (e) F and (f) T .

4.2.4. Solving conflicts on constraint specifications

4.2.4.1. Infeasible problem. Consider the same problem where the maximum concentration of undesirable by-product B is restricted to 1.2 mol/L, the maximum reaction heat rate is increased to 160 kJ/h, and the operating range of the reaction temperature is expanded ($30.0 \leq T(t) \leq 60.0$ °C). This problem becomes infeasible because C_B is very restrictive, causing conflict and competition between the constraints as shown in Fig. 15. Note the violation of

constraint C_B , as well as control profiles that are completely different from the original case. The optimizer could not find any optimal solution for this problem.

4.2.4.2. Relaxed problem. Similar to the previous case, after applying the relaxation strategy, the optimizer finds a solution relaxing only the constraint C_B while keeping the bounds of Q and T in their original positions, as shown in Fig. 16.

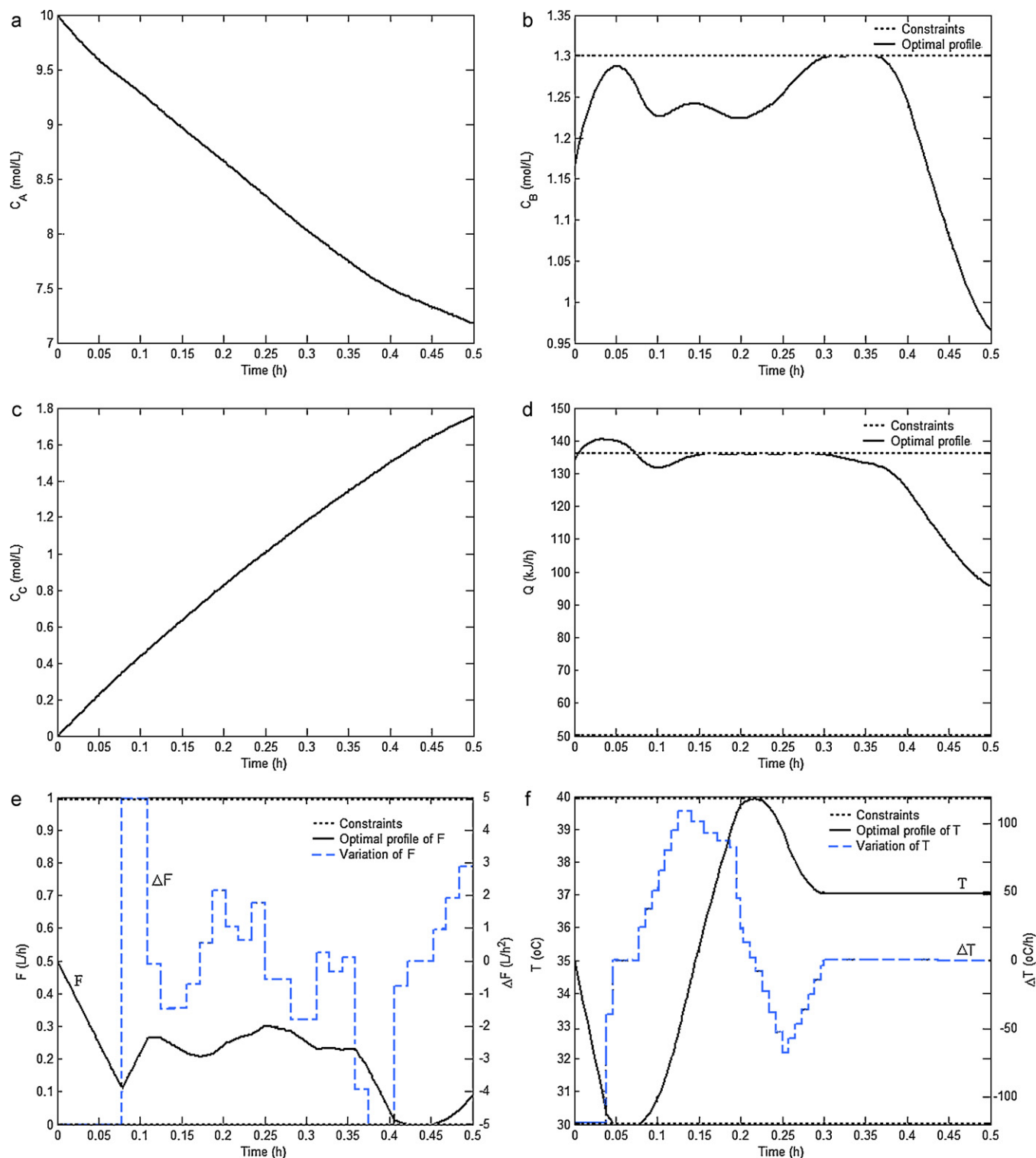


Fig. 13. Best result of the infeasible problem. Trajectories of (a) C_A (a), (b) C_B , (c) C_C , (d) Q , (e) F , ΔF , (f) T and ΔT .

4.3. Case 3 – dynamic optimization of a continuous reactor

Consider a system with output multiplicity on steady-state behavior, where a defined value of the manipulated variable (input) results in different values of the controlled variable (output). This system consists of a non-isothermal CSTR with two exothermic irreversible reactions in series. This reactor has a cooling jacket

where the water flow rate Q_C is the control variable of this system (Tlacuahuac, Moreno, & Biegler, 2008), as shown in Fig. 17. This process has a complex nonlinear behavior, as shown by the bifurcation diagrams of Fig. 18. Table 1 shows the definition of the dimensionless variables and parameters of the CSTR. Fig. 18c is the main diagram, representing the reaction temperature (x_3) versus cooling water flow (q_C).

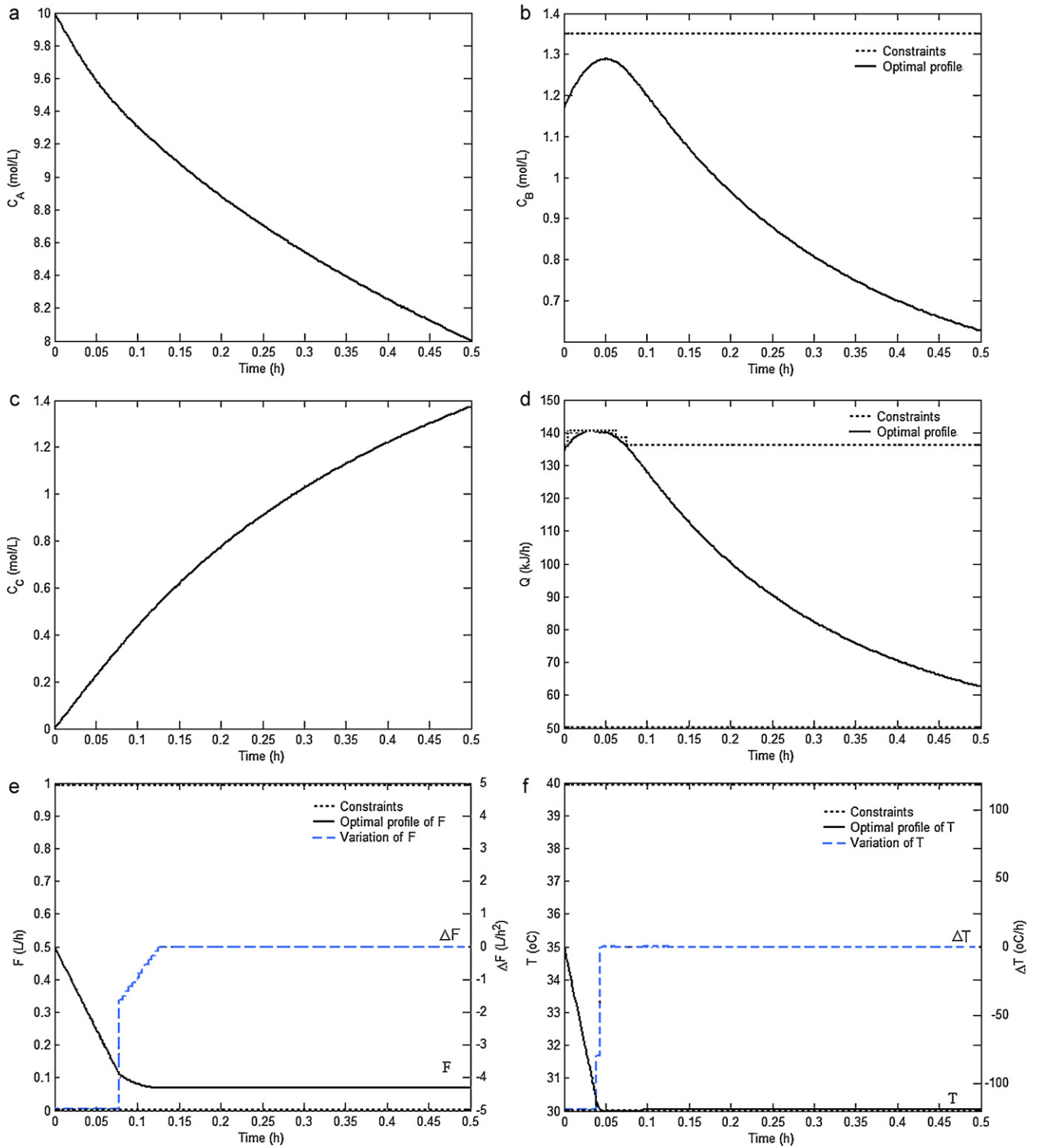


Fig. 14. The relaxed problem solution. Trajectories of (a) C_A , (b) C_B , (c) C_C , (d) Q , (e) F and ΔF , (f) T and ΔT .

Table 1

Dimensionless variables and parameters of the CSTR.

$x_1 = C_A/C_{A0}$	$x_2 = C_B/C_{A0}$	$\delta_1 = V/V_c$	$\delta_2 = \rho C_p / \rho_c c_{pc}$
$x_3 = \Gamma(T - T_{j0})/T_{j0}$	$x_4 = \Gamma(T_c - T_{j0})/T_{j0}$	$S = k_2(T_{i0})/k_1(T_{j0})$	$\phi = (V/Q_0)k_1(T_{j0})$
$\Gamma = E_1/RT_{j0}$	$\tau = (Q_0/V)t$	$\alpha = -\Delta H_B / -\Delta H_A$	$\beta = -\Delta H_A C_{A0} \Gamma / \rho C_p T_{j0}$
$q = Q/Q_0$	$q_c = Q_c/Q_0$	$x_{1f} = C_{Af}/C_{A0}$	$x_{2f} = C_{Bf}/C_{A0}$
$\psi = E_2/E_1$	$\delta = UA/\rho C_p Q_0$	$x_{3f} = \Gamma(T_f - T_{j0})/T_{j0}$	$x_{4f} = \Gamma(T_{cf} - T_{j0})/T_{j0}$
	$\eta(x_3) = e^{[\psi x_3 / (1+x_3/\Gamma)]}$	$\eta_2(x_3) = e^{[\psi x_3 / (1+x_3/\Gamma)]}$	

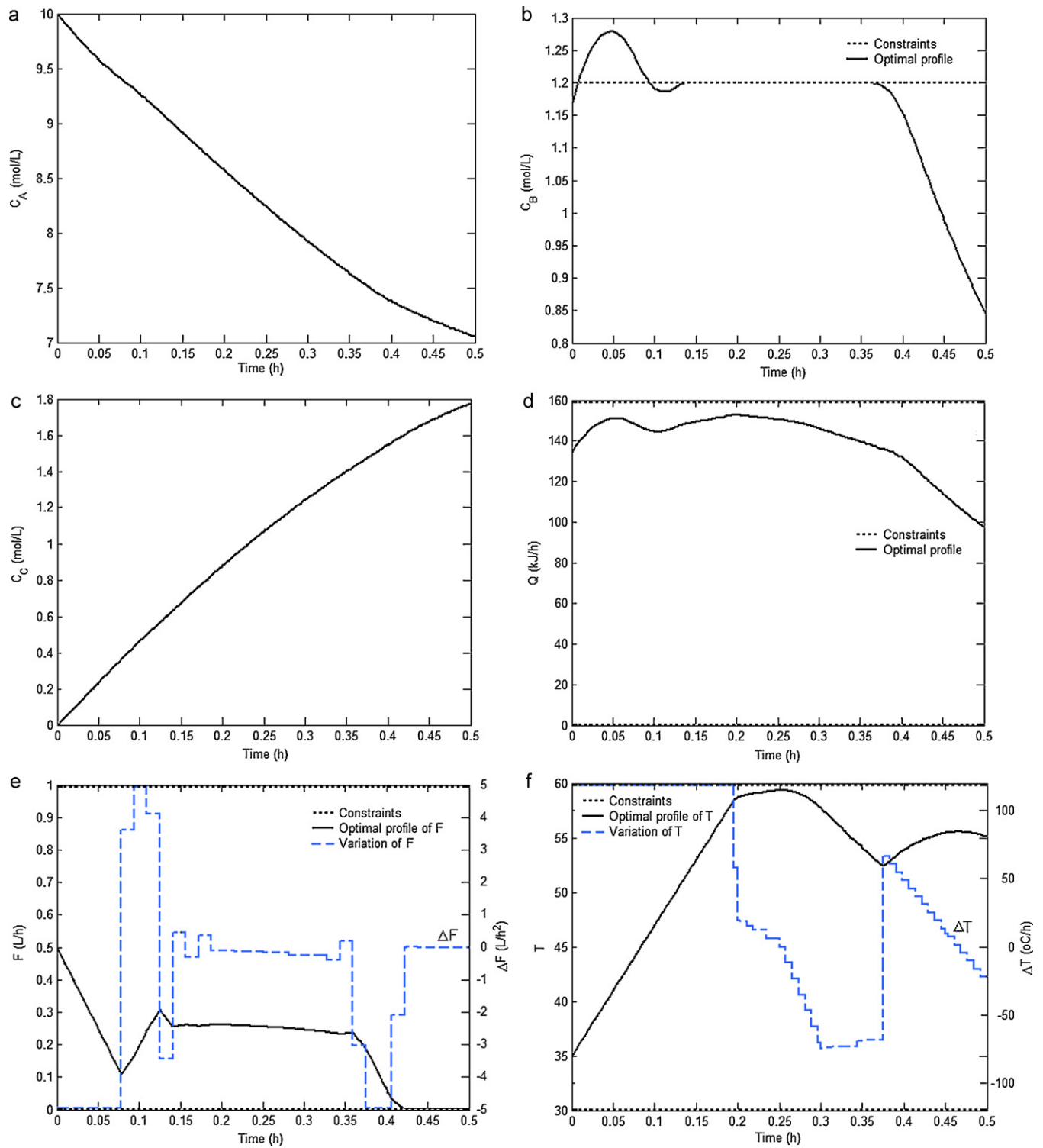


Fig. 15. Best result of the infeasible problem – conflict on specifications. Trajectories of (a) C_A , (b) C_B , (c) C_C , (d) Q , (e) F and ΔF , and (f) T and ΔT .

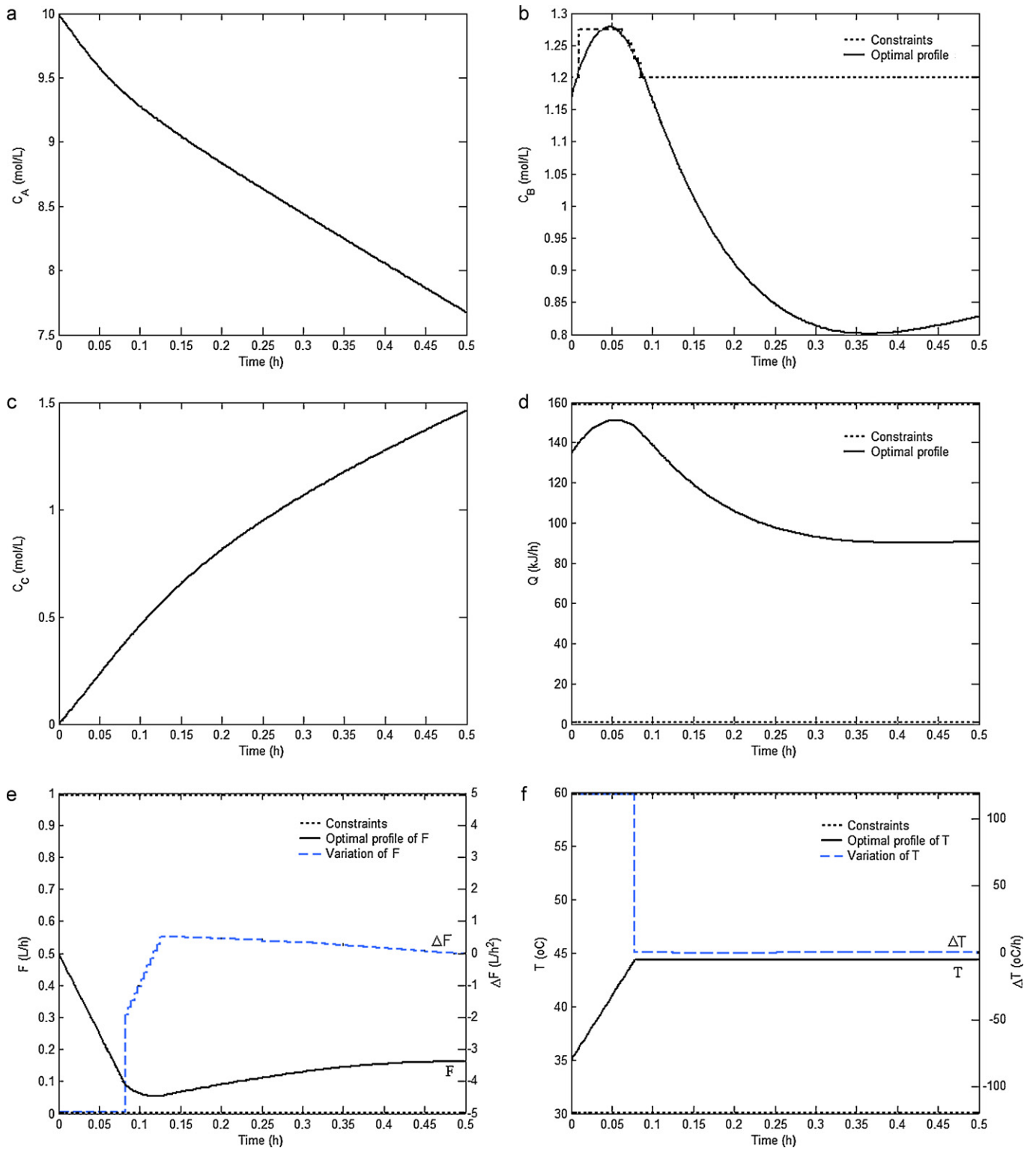


Fig. 16. Solution of the relaxed problem – conflict on specifications. Trajectories of (a) C_A , (b) C_B , (c) C_C , (d) Q , (e) F and ΔF , and (f) T and ΔT .

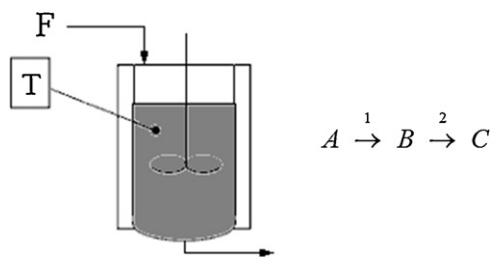


Fig. 17. Scheme and reactions of a continuous reactor.

The mathematical model that describes this process is the following:

$$\begin{aligned} \frac{dC_A}{dt} &= \frac{Q}{V}(C_{Af} - C_A) - k_1(T)C_A \\ \frac{dC_B}{dt} &= \frac{Q}{V}(C_{Bf} - C_B) - k_2(T)C_B + k_1(T)C_A \\ \frac{dT}{dt} &= \frac{Q}{V}(T_f - T) + k_1(T)C_A \frac{(-\Delta H_A)}{\rho C_p} \\ &\quad + k_2(T)C_B \frac{(-\Delta H_B)}{\rho C_p} - \frac{UA}{\rho C_p V}(T - T_c) \\ \frac{dT_c}{dt} &= \frac{Q_c}{V_c}(T_{cf} - T_c) + \frac{UA}{\rho_c C_{pc} V_c}(T - T_c) \end{aligned} \quad (12)$$

where the kinetic constants are: $k_1(T) = k_{01} e^{(-E_1/RT)}$ and $k_2(T) = k_{02} e^{(-E_2/RT)}$. Rewriting the model in a dimensionless form results in:

$$\begin{aligned} \frac{dx_1}{d\tau} &= q(x_{1f} - x_1) - \phi\eta(x_3)x_1 \\ \frac{dx_2}{d\tau} &= q(x_{2f} - x_2) - \phi S\eta_2(x_3)x_2 + \phi\eta(x_3)x_1 \\ \frac{dx_3}{d\tau} &= q(x_{3f} - x_3) + \delta(x_4 - x_3) + \beta\phi[\eta(x_3)x_1 + \alpha S\eta_2(x_3)x_2] \\ \frac{dx_4}{d\tau} &= \delta_1[q_c(x_{4f} - x_4) + \delta\delta_2(x_3 - x_4)] \end{aligned} \quad (13)$$

where x_1 is the dimensionless concentration of reactant A, x_2 is the dimensionless concentration of reactant B, x_3 is the dimensionless reactor temperature, x_4 is the dimensionless cooling jacket temperature. Table 1 shows the definition of the dimensionless variables and model parameters and Table 2 shows the values of the parameters used in this case.

Eq. (14) represents the dynamic optimization problem for this process, which seeks to minimize the deviation of the state trajec-

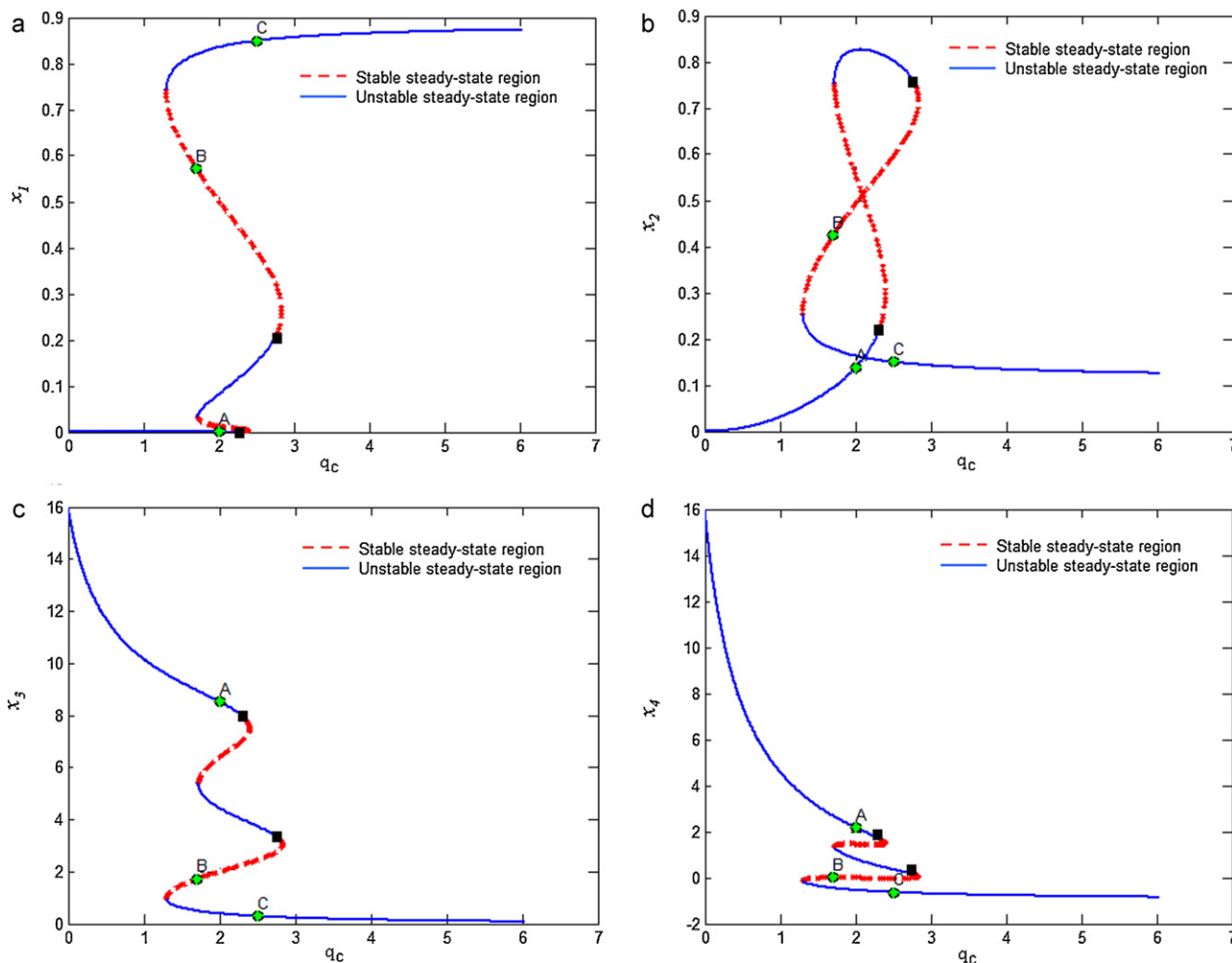


Fig. 18. Bifurcation diagrams of CSTR with two Hopf bifurcation points (■).

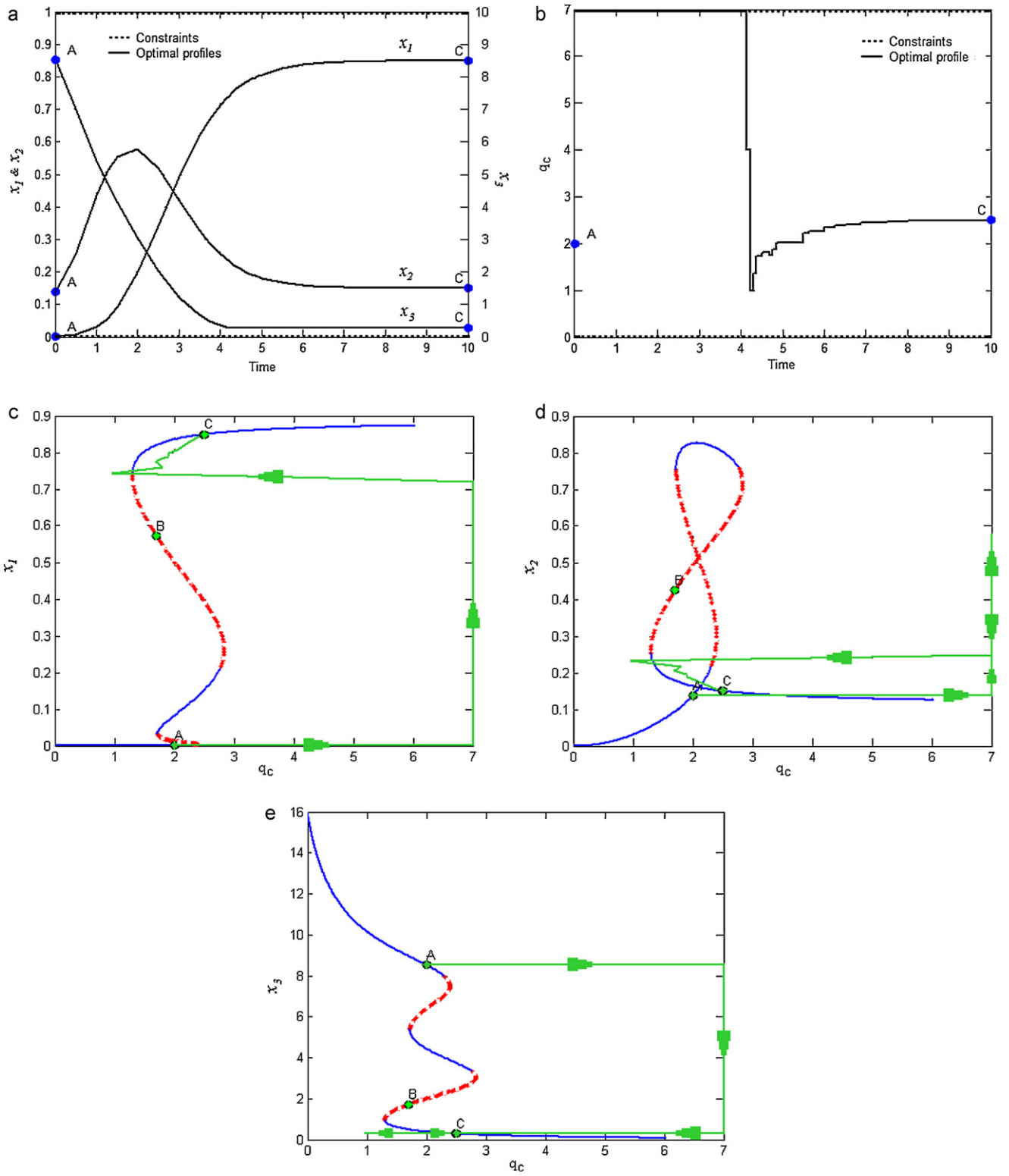


Fig. 19. The original problem solution. Trajectories of (a) x_1 , x_2 and x_3 , (b) q_c , (c, d, and e) bifurcation diagrams of the state variables for the A → C transition.

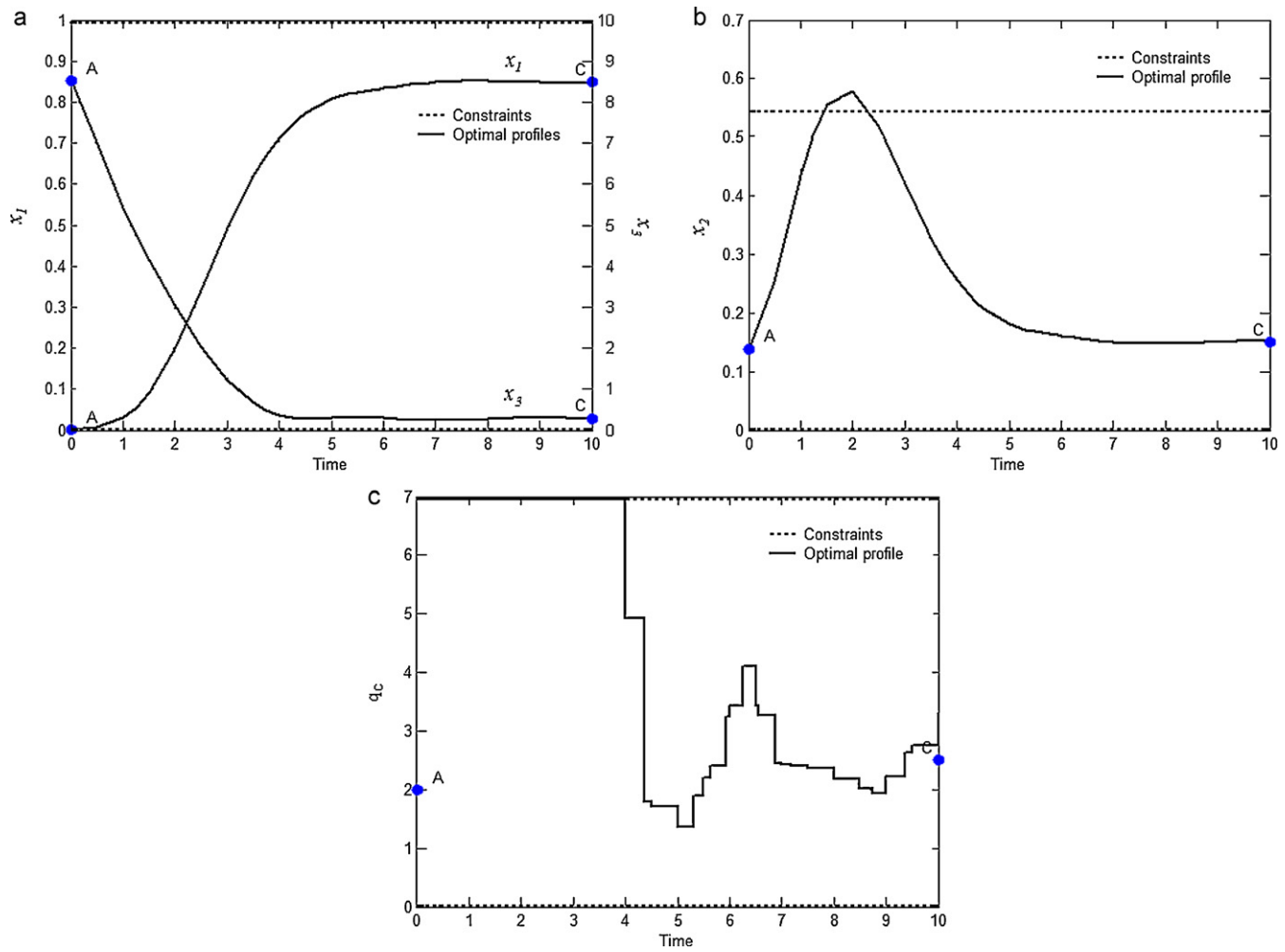


Fig. 20. Feasible solution to the problem – conflicting specifications. Trajectories of (a) x_1 and x_3 , (b) x_2 , (c) q_c .

Table 2
Values of variables and model parameters (Tlacuahuac et al., 2008).

x_{1f}	x_{2f}	x_{3f}	x_{4f}	q	α	β
1.0	0.0	0.0	-1.0	1.0	1.0	8.0
ϕ	S	ψ	δ	δ_1	δ_2	Γ
0.133	0.01	1.0	1.0	10.0	1.0	1000

trajectories from the desired values during the transitions between two steady states of the operating region.

$$\min_{z,u} \left\{ \text{ISE} = \int_0^{t_f} \|z(t) - \hat{z}\|^2 dt \right\}$$

s.t.

$$\frac{dz}{dt} = F(z, u, t), z(0) = z_0$$

$$z_L \leq z(t) \leq z_U, u_L \leq u(t) \leq u_U$$

(14)

where z is the state variable, u is the control variable, and \hat{z} is the set point of the state variable.

The case study of this kind of process usually consists on the transitions $A \rightarrow B$, $A \rightarrow C$, and $B \rightarrow C$ (Tlacuahuac et al., 2008). The focus in this work is the solution of the feasibility problem during the transition $A \rightarrow C$. Table 3 shows the operating points of these transitions.

We can write the multi-objective problem formulation that solves the optimization and feasibility problem for this system as follows:

$$\min_{\Delta\gamma, x_2, s_{x_2}} \gamma(t_f)$$

s.t.

$$\frac{dx_1}{dt} = q(x_{1f} - x_1) - \phi\eta(x_3)x_1$$

$$\frac{dx_2}{dt} = q(x_{2f} - x_2) - \phi S\eta_2(x_3)x_2 + \phi\eta(x_3)x_1$$

$$\frac{dx_3}{dt} = q(x_{3f} - x_3) + \delta(x_4 - x_3) + \beta\phi[\eta(x_3)x_1 + \alpha S\eta_2(x_3)x_2]$$

$$\frac{dx_4}{dt} = \delta_1[q_c(x_{4f} - x_4) + \delta\delta_2(x_3 - x_4)]$$

$$x(0) = \{A, B, \text{ or } C\}$$

$$\frac{d\gamma}{dt} = \Delta\gamma\gamma(0) = 0$$

$$\frac{d\text{ISE}}{dt} = (x_3 - x_3^{SP})^2 \text{ISE}(0) = 0$$

$$g_{x_2} = x_2 - s_{x_2}$$

$$\psi_{\text{ISE}}(t_f) = w^{\text{ISE}}\gamma(t_f) - \text{ISE}(t_f) + \text{ISE}_L, \psi_{\text{ISE}}(t_f) \geq 0$$

$$\psi_{x_2}(t) = \Delta\gamma(t) - \left(\frac{s_{x_2}(t)}{\sigma_{x_2}} \right)^2, \psi_{x_2}(t) \geq 0$$

$$0 \leq x_1 \leq 1$$

$$0 \leq x_3 \leq 10$$

$$0 \leq g_{x_2} \leq 0.55$$

$$0 \leq q_c \leq 7.0$$

$$-0.1 \leq s_{x_2} \leq 0.1$$

(15)

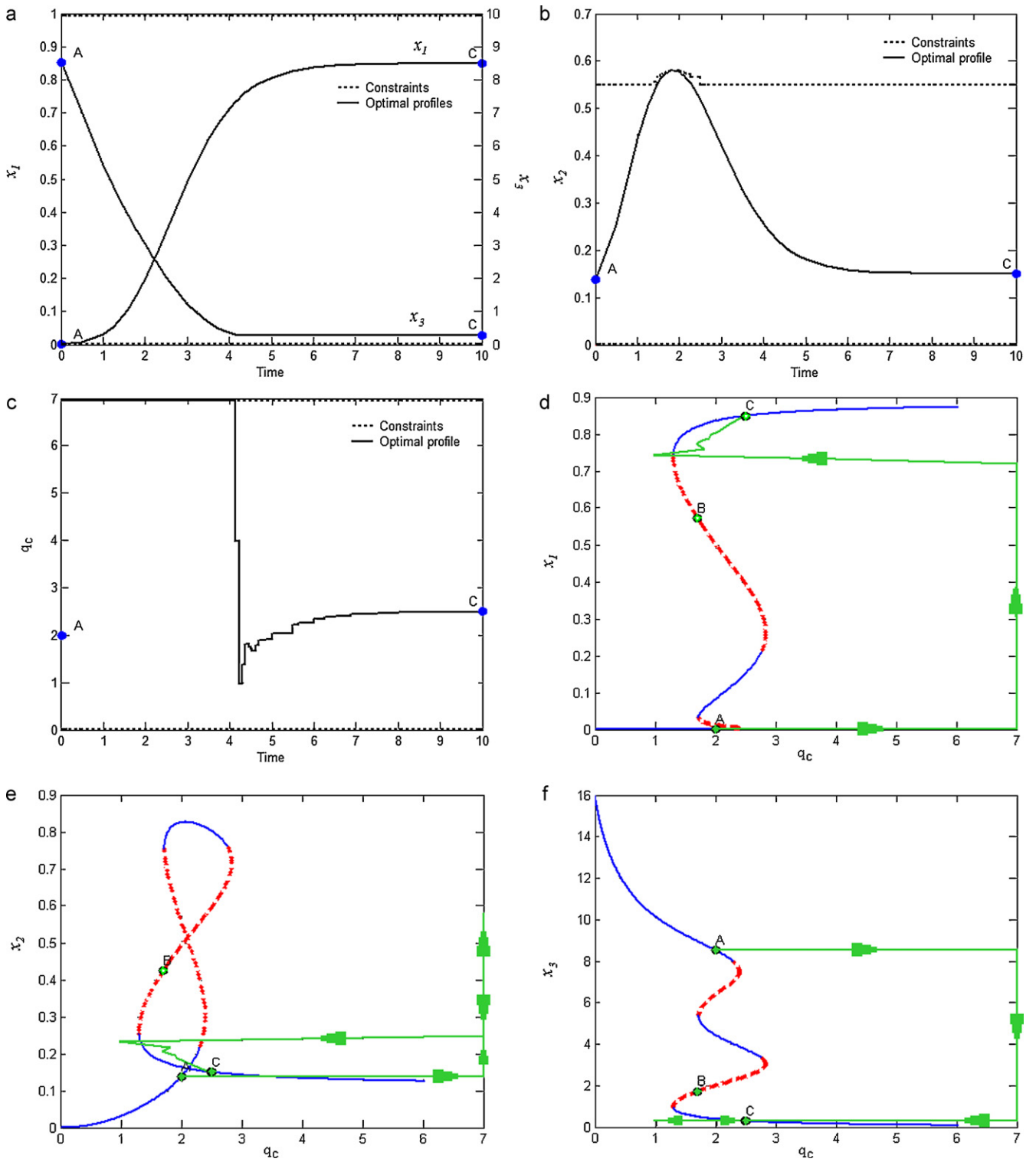


Fig. 21. The relaxed problem solution. Trajectories of (a) x_1 and x_3 , (b) x_2 , (c) q_c . (d, e, and f) bifurcation diagrams of the state variables for the A \rightarrow C transition.

Table 3
Nominal steady states.

	A	B	C
x_1	0.0016	0.5917	0.8495
x_2	0.1387	0.4249	0.1503
x_3	8.5188	1.7306	0.2871
x_4	2.1729	0.0013	-0.6323
Q_c	2.00	1.70	2.50

where ISE is the integral of the square errors (the deviation of the reactor temperature from its set point x_3^{SP}). The value of standard deviation for the relaxed constraint is $\sigma_{x_2} = 0.01$.

4.3.1. Original problem

In the $A \rightarrow C$ transition case, the problem demonstrated to be feasible as shown in Fig. 19. One can notice that there is an important overshoot in the trajectory of C_B (x_2). In addition, in the bifurcation diagrams the optimizer suggests that the cooling water flow rate goes straight to its maximum bound, cooling the reactor as fast as possible.

4.3.2. Infeasible problem

Now consider the case where an upper bound of 0.55 is defined for the concentration of B, and the maximum cooling water flow rate is restricted to 7.0, causing competition and conflicts between these constraints (Fig. 20).

4.3.3. Relaxed problem

In this case, we solved the multi-objective dynamic optimization problem as previously presented with the following competing goals: to minimize the ISE at final time while minimizing the relaxation of the constraint C_B . In Fig. 21, we can see that there was a minimal relaxation on C_B and the state trajectories and control profiles were kept close to the original problem. As in the previous example, the relaxation technique recovered the shape of the original feasible problem.

5. Conclusions

In this work, we proposed a method for solving infeasible dynamic optimization problems through a path constraint relaxation technique. We have applied the methodology in three examples of reaction systems to demonstrate the performance of the proposed method, exploring scenarios of initial and intermediate infeasibility, and situations with conflicting constraints. The case studies have shown the effectiveness of the approach for achieving feasible solution of optimal control problems when they are structurally infeasible. The success of this technique can provide more robustness to DRTO systems. We also observed that the proposed relaxation technique results in minimal movement of the constraints.

References

Biegler, L. T., & Zavala, V. M. (2008). Large-scale nonlinear programming using IPOPT: An integrating framework for enterprise-wide dynamic optimization. *Computers & Chemical Engineering*, 33(3), 575–582.

- Biegler, L. T. (2009). Technology advances for dynamic real-time optimization. *Computer Aided Chemical Engineering – 10th International Symposium on Process Systems Engineering: Part A*, 27, 1–6.
- Binder, T., Cruse, A., Villas, C., & Marquardt, W. (2000). Dynamic optimization using a wavelet based adaptive control vector parameterization strategy. *Computers and Chemical Engineering*, 24, 1201–1207.
- Camacho, E. F., & Bordons, C. (1999). *Model predictive control*. Berlin: Springer-Verlag, p. 196–199.
- Cervantes, A. M., Waechter, A., Tutuncu, R., & Biegler, L. T. (2000). A reduced space interior point strategy for optimization of differential algebraic systems. *Computers & Chemical Engineering*, 24, 39–51.
- Chinneck, J. W. (1994). MINOS: Infeasibility analysis using MINOS. *Computers and Operations Research*, 21, 1–9.
- Chinneck, J. W. (2004). The constraint consensus method for finding approximately feasible points in nonlinear programs. *INFORMS Journal on Computing*, 16(3), 255–265.
- Chinneck, J. W. (2008). Feasibility and infeasibility in optimization: algorithms and computational methods. *International Series in Operations Research and Management Sciences Springer*, 118, 97–129.
- Drud, A. (1994). CONOPT – A large-scale GRG-code. *INFORMS Journal on Computing*, 6(2), 207–216.
- Gill, P. E., Murray, W., & Saunders, M. A. (2005). SNOPT: An SQP algorithm for large-scale constrained optimization. *SIAM Review*, 47(1), 99–131.
- Greenberg, H. J. (1993). How to analyze the results of linear programs-part 3: Infeasibility diagnosis. *Interfaces*, 23(6), 120–139.
- Jacobson, D. H., & Lele, M. M. (1969). A transformation technique for optimal control problems with a state variable inequality constraint. *IEEE Transactions on Automatic Control*, AC-14, 457–464.
- Kadam, J. V., & Marquardt, W. (2007). *Integration of economical optimization and control for intentionally transient process operation. Assessment and future directions of nonlinear model predictive control*. Heidelberg, Berlin: Springer, p. 419–434.
- Lang, Y.-D., & Biegler, L. T. (2007). A software environment for simultaneous dynamic optimization. *Computers and Chemical Engineering*, 31(8), 931–942.
- Ray, W. H. (1981). *Advanced process control*. New York: McGraw-Hill.
- Schlegel, M., Marquardt, W., Ehrig, R., & Nowak, U. (2004). Sensitivity analysis of linearly-implicit differential-algebraic systems by one-step extrapolation. *Applied Numerical Mathematics*, 48, 83–102.
- Schlegel, M., & Marquardt, W. (2006). *Industrial & Engineering Chemistry Research*, 45(24), 8083–8094.
- Srinivasan, B., Palanki, S., & Bonvin, D. (2003). Dynamic optimization of batch processes I. Characterization of the nominal solution. *Computers and Chemical Engineering*, 27, 1–26.
- Tamiz, M., Mardle, S. J., & Jones, D. F. (1996). Detecting IIS in infeasible linear programmes using techniques from goal programming. *Computers and Operations Research*, 23, 113–119.
- Tlacuahuac, A. F., Moreno, S. T., & Biegler, L. T. (2008). Global optimization of highly nonlinear dynamic systems. *Industrial & Engineering Chemistry Research*, 47, 2643–2655.
- van Loon, J. (1981). Irreducibly inconsistent systems of linear inequalities. *European Journal of Operational Research*, 8, 283–288.
- Vassiliadis, V. S., Sargent, R. W. H., & Pantelides, C. C. (1994). Solution of a class of multistage dynamic optimization problems. 2. Problems with path constraints. *Industrial & Engineering Chemistry Research*, 33, 2123–2133.
- Yang, J. (2008). Infeasibility resolution based on goal programming. *Computers & Operations Research*, 35(5), 1483–1493.
- Wächter, A., & Biegler, L. T. (2006). On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. *Mathematical Programming*, 106(1), 25–57.