Optimal Control of Nonlinear Chemical Processes Using the Variational Iteration Method

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Abstract: In this paper, a design approach of an optimal control of nonlinear chemical processes is proposed. The idea consists in adopting the variational iteration method to solve the non-linear Hamilton equations derived from the minimum principle theory. These equations constitute a two-point boundary value problem with a coupled nature of solutions. Thus, by considering the correction functionals of the Hamilton equations, the Lagrange multipliers are easily identified and practical iteration formulas are derived. Based on this formulas, an algorithm is developed to determine iteratively the solutions of the Hamilton equations with a desired accuracy. Once the solutions are obtained, the optimal control law can be easily deduced. The design approach is illustrated by two examples from chemical engineering. Copyright© 2012 IFAC.

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1. INTRODUCTION

Non-linear optimal control plays an important part in chemical engineering and has received a considerable amount of attention from the control theory community (Ray, 1989; Bequette, 1991; Gupta, 1995). The non-linear nature of many chemical systems and the increasing importance of optimal control has led to the development of various numerical methods for computation of optimal control law that allow to optimize a given performance index (Sargent, 2006; Betts, 2009).

Several methods are available in the literature to solve optimal control problems. On one side, analytical theories, even if problems are in general solved numerically, include Variational Calculus (Van Brunt, 2004), Hamilton-Jacobi and Pontryagin’s principle of minimum or maximum (Pontryagin, 1964; Sewell, 1987; Corriou, 2004) for systems described by continuous state-space models and dynamic Programming based on Bellman’s principle of optimality (Bellman, 1957; Kirk, 1970) for systems described by discrete state-space models. Note that only fairly simple optimal problems can be solved analytically for instance when the performance index is quadratic and the dynamic system is linear (Naidu, 2003). On the other side, numerical methods (Betts, 2009) can be grouped into two categories: indirect and direct methods (Sargent, 2000). In the very common case of numerical methods, the solution of the optimal control problem is carried out by solving a non-linear programming problem (direct methods) or a non-linear two-point boundary value problem (indirect methods) which is difficult to achieve, and generally a computationally expensive and time-consuming numerical method is necessary (Bryson, 1999; Betts, 2009).

One of the most useful optimal control method is Pontryagin’s minimum principle (Pontryagin, 1964; Sewell, 1987). It consists in solving a two-boundary problem given by Hamilton equations with boundary conditions. However, in general, it is impossible to solve these equations analytically and the numerical solution is difficult to achieve due to the coupled nature of the solutions (Naidu, 2003). The problem becomes very difficult when these equations are highly non-linear as in the case of chemical systems. To overcome these difficulties, a design approach based on the variational iteration method is proposed in this work.

Non-linear differential equations can be solved easily and with high accuracy by means of the variational iteration method proposed by He (1999). Thus, good approximate solutions can be achieved by using practical iterative formulas derived from the correction functionals. This efficient mathematical tool is adopted to solve iteratively and more accurately the Hamilton equations that constitute necessary conditions to find an optimal control based on the minimum principle, thus achieving a global absolute optimum of the performance index. Thus, an algorithm is developed and applied to determine the optimal control of chemical reactors.

In the rest of the work, Section 2 is devoted to the variational iteration method. The minimum principle is introduced in Section 3. The proposed algorithm to solve non-linear optimal control problems is outlined in Section 4. Section 5 deals with the optimal control of a continuous-
stirred tank reactor and of a batch reactor by the proposed algorithm, followed by a conclusion in Section 6.

2. VARIATIONAL ITERATION METHOD

The variational iteration method that was recently developed is used to solve both ordinary and partial differential equations (He, 1999). This method provides the solution of the differential equations in terms of a fast convergent infinite series that may yield the exact solution in many cases. Consider the ordinary differential equation

$\mathcal{L} y(t) + N y(t) = g(t)$

where $\mathcal{L}$ and $N$ are linear and non-linear differential operators respectively, and $g(t)$ is an inhomogeneous term. In the variational iteration method, a correction functional is defined (He, 1999) for equation (1) under the form

$y^{(N+1)}(t) = y^{(N)}(t) + \int_0^t \lambda(\xi)[\mathcal{L}y^{(N)}(\xi) + Ny^{(N)}(\xi) - g(\xi)] d\xi$

where $\lambda(\xi)$ is a general Lagrange multiplier which can be identified using the stationary conditions, the superscript $N$ indicates the $N$th approximation and $y^{(N)}$ is considered as a restricted variation meaning that $\delta y^{(N)} = 0$.

By imposing the variation and by considering the restricted variation, equation (2) is reduced to

$\delta y^{(N+1)}(t) = \delta y^{(N)}(t) + \delta \left( \int_0^t \lambda(\xi) \mathcal{L}y^{(N)}(\xi) d\xi \right) \bigg|_{\xi=t}^{\xi=0} - \int_0^t \lambda(\xi) \left( \int_0^\xi \mathcal{L}y^{(N)}(\eta) d\eta \right) d\xi$

Then, by imposing the stationary conditions for (3), the optimal value of the Lagrange multiplier $\lambda(\xi)$ can be easily identified (He, 1999). Once $\lambda(\xi)$ is obtained, the solution of equation (1) can be readily derived by calculating the successive approximations $y^{(N)}(t)$ ($N = 1, \ldots, +\infty$) using formula (2). Note that the approximate solution $y^{(N)}(t)$ of the exact solution $y(t)$ can be achieved using any selected function $y^{(0)}(t)$ (He, 1999). Consequently, the approximate solution is given as the limit $y(t) = \lim_{N \to \infty} y^{(N)}(t)$.

Practically, especially for non-linear equations, it is difficult to calculate this limit. Consequently, an accurate solution can be obtained by considering a large value for $N$. This value depends on the domain $[0, t]$ where a good approximation of the solution is desired. The variational iteration method constitutes an efficient tool and an interesting alternative approach, which allows us to solve both linear and non-linear ordinary differential equations with high accuracy (Ganji et al., 2007). In the following, the variational iteration method will be used to solve a non-linear optimal control problem via the minimum principle.

3. MINIMUM PRINCIPLE

A non-linear optimal control problem is stated as follows. Find the optimal control law $u(t) : [0, t_f] \subset \mathbb{R} \to \mathbb{R}$ to minimize the performance index

$J = \psi[x(t_f), t_f] + \int_0^{t_f} \phi(x(t), u(t), t) dt$ (4)

subject to: $\dot{x}(t) = f(x(t), u(t), t)$ (5)

$x(0) = x_0$ (6)

and terminal constraints

$l(x(t_f), t_f) = 0$ (7)

where $x(t) \in \mathbb{R}^n$ is the state vector ($n$ is the system order), $u(t) \in \mathbb{R}$ is the control variable, $t_f$ is the fixed final time, $\psi : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ a terminal cost function. $\phi : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ is the functional. $l : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ and $f : \mathbb{R}^n \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}^n$ are smooth vector fields, $x(0)$ the known initial state. The final state $x(t_f)$ can be fixed or free.

It must be noted that no finite, infinite or integral constraints are present in the formulation of this problem except (7). When constraints are present, in general, the solution is constituted of several arcs. On one or several arcs, some of the constraints are satisfied whereas, on other arcs denoted as singular arcs, no constraint is satisfied. This latter corresponds exactly to the problem which is considered in the following. Thus, it is assumed that no constraint exists in the present problem.

The Hamiltonian $H(x, p(t), u(t), t)$ is defined as $H(x(t), p(t), u(t), t) = \phi(x(t), u(t), t) + p^T(t) f(x(t), u(t), t)$ (8) where $p(t)$ is the costate vector.

The following Hamilton equations are necessary conditions

$\dot{x}(t) = \partial H(x(t), p(t), u(t), t) / \partial u(t)$ (9)

$p(t) = -\partial H(x(t), p(t), u(t), t) / \partial x(t)$ (10)

The first equation (9) is the model (5) whereas the second equation is called the costate or adjoint equation, $p$ being the costate or adjoint vector. They constitute a two-point boundary value problem with (6) and the transversality equation at $t_f$, written as

$\left[ \frac{\partial \phi}{\partial t_f} + H(t_f) \right] \delta t_f + \left[ \frac{\partial \phi}{\partial x_f} - p(t_f) \right]^T \delta x_f + \frac{\partial \phi}{\partial u_f} \delta u_f = 0$

with:

$\langle \partial l / \partial t_f \rangle \delta t_f + \langle \partial l / \partial x_f \rangle \delta x_f = 0$ (11)

According to Pontryagin’s minimum principle, if $u^*(t)$ is a solution of the optimal control problem (4–7), then

$u^*(t) = \arg \min_u H(x(t), p(t), u(t), t)$ (12)

Consequently, in the absence of constraints,

$\partial H(x(t), p(t), u(t), t) / \partial u(t) = 0 \Rightarrow u^*(t) = \Phi(x(t), p(t), t)$ (13)

which is referred as weak Pontryagin’s minimum principle. The solution of the optimal control problem exists if

$\partial^2 H(x(t), p(t), u(t), t) / \partial u^2(t) > 0$ (14)

where $u(t)$, $p(t)$, and $x(t)$ satisfy the Hamilton conditions (9) and (10). For singular arcs, the generalized Legendre-Clebsch condition (Bryson, 1999) holds

$-\left(1/k\right)^2 [d/dt]^{2k} H_u \geq 0$, $k = 0, 1, \ldots$ (15)

The optimal value of the Hamiltonian is

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\[ H^*(x(t), p(t), t) = H(x(t), p(t), u(t), t)|_{u(t)=\Phi(x(t), p(t), t)} \]

The solution of equations (9-10), with boundary conditions (6) and (7) or (11), gives the optimal trajectories \( x^*(t) \) and \( p^*(t) \). Then, by substituting these trajectories in the optimal control law (13), the open-loop optimal control \( u^*(t) \) results.

The solution of Hamilton equations (9) and (10) requires \( 2n \) boundary conditions. The first \( n \) boundary conditions are related to the initial state \( x(0) \), which is always known, and the \( n \) other boundary conditions are related to the final state. Thus, when the final time \( t_f \) is fixed, if the final state \( x(t_f) \) is specified, consequently the \( n \) other boundary conditions are

\[ x(t_f) = x_f \] \hspace{1cm} (16)

but if the final state \( x(t_f) \) is free, the remaining \( n \) boundary conditions are given by the transversality equation (11) at \( t_f \) yielding the terminal constraint on the costate variable \( p(t_f) \) as

\[ p(t_f) = \frac{\partial \psi(x(t_f), t_f)}{\partial x(t_f)} \] \hspace{1cm} (17)

Note that the analytical solution of the Hamilton equations (9) and (10) can be obtained only for some special types of optimal control. The numerical solution of this two-point boundary value problem is difficult because of the coupled nature of the solutions \( x(t) \) and \( p(t) \) (Naidu, 2003), that is, the state \( x(t) \) has to be solved by forward integration of (5) starting from its initial condition \( x(0) \) and the costate \( p(t) \) has to be solved by backward integration of (10) starting from its final condition \( p(t_f) \) since its initial condition \( p(0) \) is unknown. When \( p(0) \) is used for forward integration of (10), this corresponds to the shooting method.

In this work, the variational iteration method will be adopted to solve the two-point boundary value problem defined by Hamilton equations (9) and (10), which allows us to obtain the optimal control law \( u^*(t) \).

\[ p^{(N+1)}(t) = p^{(N)}(t) - \int_0^t \lambda_p(\xi) \nabla x(\xi) H^* \left( x^{(N)}(\xi), p^{(N)}(\xi), \xi \right) \, d\xi \] \hspace{1cm} (19)

where \( \lambda_p(\xi) \) and \( \lambda_x(\xi) \) are the column vectors of Lagrange multipliers, and \( \otimes \) is the Hadamard product (element by element product).

Having identified the Lagrange multipliers vectors \( \lambda_x(\xi) \) and \( \lambda_p(\xi) \), the successive approximations \( x^{(N+1)}(t) \) and \( p^{(N+1)}(t) \) of the exact solutions \( x(t) \) and \( p(t) \) will be readily obtained by using any selected functions \( x^{(0)}(t) \) and \( p^{(0)}(t) \) for initialization. Thus, in order to simplify the calculations, it is proposed to take

\[ x^{(0)}(t) = x(0) \] \hspace{2cm} and \hspace{2cm} \[ p^{(0)}(t) = p(0) \] \hspace{1cm} (20)

since the initial state \( x(0) \) is always known. With respect to the choice of \( p^{(0)}(t) \), the initial costate vector \( p(0) \) is an unknown vector denoted in the following as \( \theta \) of dimension \( n \). Nevertheless, using the correction functionals (18) and (19), the solution \( x^{(N)}(t) \) and \( p^{(N)}(t) \) can be carried out by considering \( p(0) \) as a vector of unknown constants. The real value of \( p(0) \) will be determined after a convergence process based on the satisfaction of either the boundary condition (16) or (17).

Consequently, the approximate solutions are given by

\[ x(t) = \lim_{N \to \infty} x^{(N)}(t) \] \hspace{1cm} and \hspace{1cm} \[ p(t) = \lim_{N \to \infty} p^{(N)}(t) \] \hspace{1cm} (21)

and according to (13), the optimal control law is

\[ u^*(t) = \Phi(x^{(N)}(t), p^{(N)}(t), t) \] \hspace{1cm} (22)

Notice that, by using the variational iteration method, the shooting method is easily computed using recursive formulas and gives fast convergent successive approximations of the exact solution if this latter exists. If the exact solution is not available, the method provides an approximate solution of high accuracy by performing only few iterations. He (1999) states that the more accurate the identification of the multiplier, the faster the approximations converge to its exact solution. For instance, for linear problems, as the Lagrange multiplier can be exactly identified, the exact solution can be obtained by only one iteration (He, 1999). The convergence of the variational iteration method was thoroughly investigated in the literature (Tatari and Dehghan, 2007; Odibat, 2010). Consequently, if the exact solutions \( x(t) \) and \( p(t) \) exist, the series (18) and (19) converge toward these solutions. In this case, the optimal control law is given by (13). If the exact solutions cannot be achieved, approximate solutions \( x^{(N)}(t) \) and \( p^{(N)}(t) \) with high accuracy can be obtained by considering an appropriate value of \( N \) denoted by \( N^* \). The value \( N^* \) is taken as the smallest value of \( N \) above which the convergence of the approximate solutions is achieved.

The variational iteration method is an effective and reliable method to solve linear and nonlinear differential equations even with symbolic variables. The method gives fast convergent successive approximations of the exact solution if such a solution exists, or an approximate solution with an acceptable accuracy even if few iterations are used (He, 1999; Ganji et al., 2007). Compared to numerical methods, the variational iteration method provides analytic and numerical solutions without linearization or discretization, and the obtained result is not affected by rounding error. Thus, the variational iteration method represents an alternative and efficient method to obtain the optimal control law by solving Hamilton equations.

Our concern will be focused on solving Hamilton equations, using variational iteration method, thus correction functionals for the Hamilton equations (9) and (10) are

\[ x^{(N+1)}(t) = x^{(N)}(t) + \int_0^t \lambda_x(\xi) \nabla x(\xi) H^* \left( x^{(N)}(\xi), p^{(N)}(\xi), \xi \right) \, d\xi \] \hspace{1cm} (18)

where \( \lambda_p(\xi) \) and \( \lambda_x(\xi) \) are the column vectors of Lagrange multipliers, and \( \otimes \) is the Hadamard product (element by element product).

The optimal control law results as

\[ u^*(t) \approx u^{(N^*)}(t) = \Phi \left( x^{(N^*)}(t), p^{(N^*)}(t), t \right) \] \hspace{1cm} (23)
For the choice of \( N^* \), it is proposed to evaluate the performance index (4), at each iteration \( N \), by considering the approximate solutions \( x^{(N)}(t) \) and \( u^{(N)}(t) \), i.e.

\[
J^{(N)} = \psi \left( x^{(N)}(t_f), t_f \right) + \int_0^{t_f} \phi \left( x^{(N)}(t), u^{(N)}(t), t \right) \, dt
\]

and after the iteration \( N = N^* \) the variational iteration method converges to an approximate solution, and the performance index (24) will also converge toward a given limit for any value of \( N \geq N^* \).

Consequently, all values \( N \geq N^* \) are appropriate, but to obtain a simple optimal control expression, one can simply take \( N = N^* \). This is explained by the fact that after the iteration \( N = N^* \), the contributions of the integral parts in the correction functionals (18) and (19) become negligible so that the solutions can be approximated as

\[
x(t) \approx x^{(N^*)}(t) \quad \text{and} \quad p(t) \approx p^{(N^*)}(t)
\]

Notice that, in the case where exact solutions exist, after the iteration \( N = N^* \), these contributions will be null, so that

\[
x^{(k)}(t) = x^{(k+1)}(t) \quad \text{and} \quad p^{(k)}(t) = p^{(k+1)}(t), \forall k \geq N^*
\]

The different steps of the proposed design approach, in the absence of constraints, can be summarized as:

- **Step 1.** Define the Hamiltonian \( H(x(t), p(t), u(t), t) \) according to (8).
- **Step 2.** Derive the Hamilton equations (9) and (10), and the boundary conditions.
- **Step 3.** Determine the expression of the optimal control law \( u^*(t) \) as explained by (13).
- **Step 4.** If possible, check the existence of the solution using one of the conditions (14).
- **Step 5.** Define \( H^*(x(t), p(t), t) \) and the Hamilton equations by substituting the obtained optimal control law \( u^*(t) \) respectively in (8) and (9-10).
- **Step 6.** Define the correction functionals (18) and (19).
- **Step 7.** Identify the Lagrange multipliers vectors \( \lambda_x(\xi) \) and \( \lambda_p(\xi) \).
- **Step 8.** Set \( N = 0 \), \( x^{(0)}(t) = x(0) \) and set \( p^{(0)}(t) = \theta \) where \( \theta \) is an unknown constant vector to be determined by an iterative procedure.
- **Step 9.** Calculate \( x^{(N+1)}(t) \) and \( p^{(N+1)}(t) \) using (18) and (19). The integral parts involved can be evaluated either analytically or numerically depending on the complexity of Hamilton equations (9) and (10).
- **Step 10.** Determine \( \theta = p^{(N)}(0) \) by imposing either the condition (16) or (17) depending on the nature of final state \( x(t_f) \), which can be fixed or free. If there is no solution for \( \theta \), go to step 9, else go to step 11.
- **Step 11.** Evaluate the performance index \( J^{(N)} \) given by (24).
- **Step 12.** If \( |J^{(N)} - J^{(N-1)}| \geq \epsilon \) (where \( \epsilon > 0 \) is a desired threshold), set \( N = N + 1 \) and go to step 9, else go to Step 13.
- **Step 13.** Set \( N^* = N \) and deduce the open-loop optimal control law as in (23). ■

Note that, in the case of multiple solutions of \( \theta \) at step 10, at step 11 the performance index \( J^{(N)} \) will be evaluated for all possible solutions, and the solution that provides the optimal performance index will be kept for further calculations in the following steps.

## 5. APPLICATION EXAMPLES

### 5.1 Optimal control of temperature of a CSTR

Consider the temperature control problem by cooling-rate manipulation of a continuous-stirred tank reactor (CSTR). The optimal control problem of the temperature is formulated as follows (Ray, 1989)

\[
\min J = \frac{1}{2} \int_0^{0.5} \left[ (x(t) - 1.3)^2 + \mu u^2(t) \right] \, dt, \quad \mu > 0
\]

subject to:

\[
\dot{x}(t) = 1 - x(t) + a e^{-\gamma/x(t)} - u(t) \quad (26)
\]

\[
x(0) = 1.5, \quad x(0.5) = 1.3 \quad (27)
\]

In the reactor model (26), the dimensionless variables are defined as

\[
x(t) = \frac{T - T_0}{T_e}, \quad t = \frac{t}{\tau}, \quad a = -\frac{\Delta H}{\rho c V}, \quad \gamma = \frac{Q}{\rho c V}.
\]

The integral parts involved can be evaluated either in (8) and (9-10), respectively in (8) and (9-10), \( \lambda_x(\xi) = \frac{\gamma}{x(\xi)} \), \( \lambda_p(\xi) = \frac{\gamma}{x(\xi)} \), which can be fixed or free. If there is no solution for \( \theta \), go to step 9, else go to step 11.

**Thus,** the corresponding correction functionals are

\[
x^{(N+1)}(t) = x^{(N)}(t) + \int_0^t \lambda_x(\xi) \left[ \dot{x}(\xi) - 1 + x^{(N)}(\xi) \right] d\xi
\]

\[
- a e^{-\gamma/x^{(N)}(\xi)} + p^{(N)}(\xi)/\mu \right] d\xi
\]

\[
p^{(N+1)}(t) = p^{(N)}(t) + \int_0^t \lambda_p(\xi) \left[ \dot{p}(\xi) + \ddot{x}(\xi) - 1.3 \right] d\xi
\]

\[
- \ddot{p}(\xi) + a \gamma \dot{x}(\xi) e^{-\gamma/x^{(N)}(\xi)} / (\dot{x}(\xi))^2 \right] d\xi
\]

To show how to identify the Lagrange multipliers, let us consider the identification of \( \lambda_x(\xi) \). Considering that all variables are independent, by taking the variation with respect to the independent variable \( x^{(N)}(t) \), noticing that \( \dot{x}(\xi) \) and \( \ddot{x}(\xi) \) denote the restricted variations, i.e.

\[
\delta \dot{x}(\xi) = \delta x^{(N)}(t) + \int_0^t \lambda_x(\xi) \left[ \delta \dot{x}(\xi) + \delta \ddot{x}(\xi) + \delta \dot{x}(\xi) \right] d\xi
\]

\[
= \delta x^{(N)}(t) + \left[ \lambda_x(\xi) \delta x^{(N)}(\xi) \right]_{\xi = t}
\]

\[
- \int_0^t \left[ \lambda_x(\xi) + \lambda_x(\xi) \right] \delta x^{(N)}(\xi) d\xi
\]
As $\delta x(N)(0) = 0$, thus

$$\delta x(N+1)(t) = [1 + \lambda x(t)] \delta x(N)(t) - \int_0^t [\hat{\lambda}_x(\xi) + \lambda x(\xi)] \delta x(N)(\xi) \, d\xi$$  \hspace{1cm} (32)

Considering the requirement of stationary correction functional $\delta x(N+1)(t) = 0$, whatever the variations $\delta x(N)(t)$, the following stationary conditions result

$$\hat{\lambda}_x(\xi) + \lambda x(\xi) = 0, \quad \forall \xi \in [0, t]$$  \hspace{1cm} (33)

$$1 + \lambda x(0) = 0$$  \hspace{1cm} (34)

The solution of the ordinary differential equation (33) with the boundary condition (34) gives the following Lagrange multiplier $\lambda_x(\xi) = -e^{\xi-t}$. Following the same approach with respect to the variation $\delta p^{(N+1)}(t)$, the Lagrange multiplier $\lambda_p(\xi)$ can be easily identified as $\lambda_p(\xi) = -e^{t-\xi}$.

By starting with the initial state $x(t) = 1.5$ and the initial costate vector $p^0(t) = \theta$ with $\theta$ unknown, and by considering a threshold $\epsilon = 10^{-6}$, the proposed approach converges after 8 iterations ($N = N^* = 8$). Note that, the integral parts involved in the iteration formulas are evaluated numerically using Gauss-Legendre integration method (Corriou, 2010). The values of the normalized performance index and of the normalized initial costate vector $p(0)$ are shown in Figure 1. Figure 2 shows the calculated trajectories for $N = 5$ (before convergence) and for $N = N^* = 8$ (optimal trajectories).

5.2 Optimal control of a batch reactor

Consider a batch reactor in which the parallel reaction mechanism $A \xrightarrow{k_1} B, \quad A \xrightarrow{k_2} C$ occurs. Both reactions are first order and irreversible. The objective is to find the temperature time profile $T^*(t)$ that maximizes the yield of species $B$ at final time $t_f$. The mass balance relations for species, $A(x_1(t))$ and $B(x_2(t))$, in the batch reactor are

$$\dot{x}_1(t) = -(k_1(t) + k_2(t)) \, x_1(t)$$  \hspace{1cm} (35)

$$\dot{x}_2(t) = k_2(t) \, x_1(t)$$  \hspace{1cm} (36)

with $k_1 = k_{10} e^{-E_1/R T(t)} (i = 1, 2)$ with $k_{10} = 10^6 \text{s}^{-1}$, $k_{20} = 5.10^{11} \text{s}^{-1}$, $E_1 = 10^4 \text{cal/gmol}$ and $E_2 = 2.10^4 \text{cal/gmol}$ (England et al., 2005). It can be noticed that the numerical value (noted $v$) of $k_2$ is such that $v(k_2) = 0.5 v^2(k_1)$. The final time is $t_f = 1$. This optimal control problem has been studied by (Biegler, 1984; Logsdon and Biegler, 1989; England et al., 2005) by considering a constraint on the temperature $T(t)$. Here, the optimal control law design is achieved by assuming that the temperature is not constrained. The model can be simplified by assuming as manipulated variable $u(t) = k_1(t)$ which amounts to manipulate the temperature. Thus, the optimal control problem is given by

$$\min_J = -x_2(t_f)$$

$$u(t)$$

subject to : $\dot{x}_1(t) = -(u(t) + 0.5 u^2(t)) \, x_1(t)$

$$\dot{x}_2(t) = u(t) \, x_1(t)$$

$$x(0) = [1 \, 0]^T$$

(40)

Based on the minimum principle, the optimal control law expression is

$$u^*(t) = -1 + p_2(t)/p_1(t)$$  \hspace{1cm} (41)

$$\partial^2 H(x(t), p(t), t)/\partial u^2(t) = -p_1(t) x_1(t)$$  \hspace{1cm} (42)

Note that the condition of positivity of (42) should be verified at the end of iterations. For this problem, the criterion is resumed to the algebraic term so that, according to (17), $p(t_f) = [0, -1]^T$. The initial state $x(0)$ is given by (40).

The corresponding correction functionals are:

$$x_1^{(N+1)}(t) = x_1^{(N)}(t) - \int_0^t e^{(t-\xi)/2} \left[ x_1^{(N)}(\xi) - 0.5 x_1^{(N)}(\xi) + 0.5 x_1^{(N)}(\xi) \left( \tilde{p}_2^{(N)}(\xi)/\tilde{p}_1^{(N)}(\xi) \right)^2 \right] d\xi$$  \hspace{1cm} (43)

$$x_2^{(N+1)}(t) = x_2^{(N)}(t) - \int_0^t \left[ x_2^{(N)}(\xi) + x_1^{(N)}(\xi) - x_1^{(N)}(\xi) \left( \tilde{p}_2^{(N)}(\xi)/\tilde{p}_1^{(N)}(\xi) \right) \right] d\xi$$  \hspace{1cm} (44)

$$p_1^{(N+1)}(t) = p_1^{(N)}(t) + \int_0^t e^{(t-\xi)/2} \left[ p_1^{(N)}(\xi) + 0.5 p_1^{(N)}(\xi) - p_2^{(N)}(\xi) \left( 1 - 0.5 p_2^{(N)}(\xi)/p_1^{(N)}(\xi) \right) \right] d\xi$$  \hspace{1cm} (45)

$$p_2^{(N+1)}(t) = p_2^{(N)}(t) - \int_0^t \tilde{p}_1^{(N)}(\xi) d\xi$$  \hspace{1cm} (46)

Starting with the initial state $x(0) = x_0$ and the initial costate vector $p^0(t) = [\theta_1, \theta_2]^T$ with $\theta$ unknown, and considering a threshold $\epsilon = 10^{-6}$, the proposed approach converges after 16 iterations ($N = N^* = 16$). The values of
the performance index and of the initial costate vector \( p(0) \) are shown in Figure 3. The optimal value of the performance index optimal value is \( J^{(16)} = 0.57663881 \). Figure 4 shows the resulting optimal state and costate trajectories and the optimal control over the time. Note that, from Figure 4, it is apparent that \( p_1(t) < 0 \) and \( x_2(t) > 0, \forall t \in [0, 1] \), thus the condition of positivity of (42) holds, consequently the obtained control law ensures a maximum of the final concentration \( x_2(t_f) \).

6. CONCLUSION

In this work, a design approach of an optimal control for non-linear systems is developed. The different steps are given under the form of an algorithm, which is easy to implement as a symbolic and numerical computer program. The main idea consists to solve by forward integration the necessary conditions of optimality, i.e. Hamilton equations derived from the minimum principle iteratively using the corresponding correction functionals. Consequently, the optimal control law which provides a global absolute optimum of the cost function can be easily deduced. The proposed approach is applied to two problems of optimal control of chemical reactors and it is shown that an exact or an approximate analytical solution, as a function of the time variable, of the optimal control can be achieved using few iterations.

REFERENCES


Fig. 3. Evolution of the criterion \( J \) and the parameter vector \([\theta_1, \theta_2]\) for the batch reactor.


Fig. 4. Optimal trajectories for the batch reactor.