Optimal control of hybrid dynamical systems with the maximum principle: Application to a non linear chemical process

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Abstract:
Chemical products manufacturing must respect sequences which lead them from an initial phase to a final one. In each phase the dynamic evolutions in the process are continuous. This paper presents a new method that minimizes the overall operating time to get the desired products, respecting the constraints on the continuous variables. It is based on the Pontryagin's maximum principle extended to discrete controlled hybrid dynamical systems. It is illustrated on a non linear chemical process.

Keywords:
hybrid dynamical systems, nonlinear optimal control, Pontryagin's maximum principle, chemical processes

1. INTRODUCTION

Chemical processes include manufacturing phases like, filling or emptying a reactor, heating or mixing a product. They may operate in multiple distinct phases (modes) that can be executed in parallel or in sequence. To achieve the different phases, resources as valves, pipes, reactors, heaters are needed. They have characteristics of different nature: actuators admit a logic control (open, close, heat, cool, …) and sensors give a continuous information (flow rate, heating power, temperature, ...). The model which is needed is then hybrid in the sense of including discrete and continuous variables. The sequences of phases are represented by discrete or Boolean variables, and the dynamic evolution of levels, concentrations or temperatures in the equipment are represented by differential and/or algebraic equations.
This paper presents a method which minimizes the overall time duration for the system to reach a final hybrid region (a hybrid region is made of a region of the continuous state space and a discrete phase) from an initial hybrid region, respecting the constraints on the continuous variables and the allowed discrete control sequences. The chosen approach in this paper is to determine all the controllable manufacturing sequences with a systematic controllability method [1] [2], and then to minimize the processing time of the sequences which may lead to the absolute minimum time duration whatever the sequence is. Usually, an experienced chemist engineer could often tell which sequence to choose.
Section 2 presents the hybrid system model. Section 3 gives a chemical process example to illustrate the method. The next section presents the time optimal control synthesis method. It is based on the Pontryagin's Maximum Principle (PMP) which is adapted to Hybrid Dynamical Systems (HDS) with no discontinuity on the state vector and with a discrete control. First, it is proven that the PMP can be applied to such HDS. Then, the necessary conditions to transform the optimal control problem into an algebraic and differential equations system are presented. In section 5, this method is applied to the chemical process example presented in section 3.

2. MODELING WITH HYBRID AUTOMATA

The hybrid process is modeled by a hybrid automata [3] [4]. As well as in the Branicky unified model [5], autonomous and controlled jumps (continuous variable discontinuity) and autonomous and controlled switching (vector field discontinuity) may be represented.
A hybrid automata HA is defined by a 8-tuple HA=(X, Q, μ_1, μ_2, Σ, μ_3, Q_0, Q_f):

- X is a vector subspace $X \subseteq \mathbb{R}^n$ which represents the state-space of the system. x is the continuous state vector of the system denoted by: $x=[x_1 \dots x_n]^T \in X$.
- Q is the possible discrete phases set (also called modes, locations or discrete states) of the hybrid process: $Q = \{l_j, j \in \{1, ..., m\}\}$. Then, the hybrid state of the system is given by the couple $(x,l) \in X \times Q$.
- μ_1 is the set of m vector fields associated with each phase l_j. The dynamics of the state vector x are denoted by: $\mu_1 = \{\mu_1(l_j), j \in \{1, ..., m\}\}$, that is: $\forall l_j \in Q, \dot{x} = \mu_1(l_j)(x)$. The function $\mu_1(l_j)$ is supposed to be locally Lipschitz with respect to x.
- μ_2 is the set of constraints for each phase: $\mu_2 = \{\mu_2(l_j) / j \in \{1,...,m\}\}$. $\mu_2(l_j)$ represents the constraints for the phase l_j. It is a manifold described by c_j linear inequalities: $\forall k \in \{1,...,c_j\}$, $C_k^T x \leq d_k$ with C_k a n-length vector and d_k a constant. The constraints $\mu_2(l_j)$

can not be violated, which means that the phase l_j is left as soon as an inequality of $\mu_2(l_j)$ is going to be false.

- Σ is the events set. $\Sigma = \{\delta_{jk},\ j\in\{1,\dots,m\},\ k\in\{1,\dots,m\}/j\neq k\}$. Each event δ_{jk} defines the discrete transition $tr_{jk}\in Q^2$ from the location l_j to the location l_k. A discrete transition tr_{jk} can be either autonomous or controlled. If the constraints $\mu_2(l_j)$ are going to be violated then the event δ_{jk} is generated by the plant, δ_{jk} is uncontrolled and the transition is autonomous, else, δ_{jk} is generated by the control, δ_{jk} is controlled and the transition is controlled.
- μ_3 is a set of functions associated to the event δ_{jk}:

$$\mu_3 = \left\{\begin{matrix}\mu_3(l_j,\delta_{jk},l_k)\,/ \\ j\in\{1,\dots,m\}, k\in\{1,\dots,m\}, j\neq k, \delta_{jk} \text{ is defined}\end{matrix}\right\}$$

  It defines real valued variables jumps (or discontinuities) when an event occurs. if δ_{jk} exists, then the phase transition from l_j to l_k is defined and:

$$\mu_3(l_j,\delta_{jk},l_k):\mathbb{R}\rightarrow\mathbb{R}/\quad x(t^+) = \mu_3(l_j,\delta_{jk},l_k)\left(x(t^-)\right)$$

  if δ_{jk} does not exist, neither the phase transition from l_j to l_k, nor $\mu_3(l_j,\delta_{jk},l_k)$ are defined.
- Q_0, and Q_f are the sets of initial and final locations.

In order to simplify the hybrid automata graphical representation:

- $\mu_1(l_j)$ is not represented inside a phase if the vector field $\mu_1(l_j)(x) = \dot{x} = 0$.
- If $\mu_2(l_j)$ is not represented inside a phase, it is equal to the global constraint GC, which are defined separately.
- Initial and final phases are represented by double circles.

3. ILLUSTRATION ON A CHEMICAL PROCESS

The chemical process sketched on figure 1 will be modeled. It is a continuous stirred tank reactor (i.e. the liquid properties are homogenous everywhere inside the reactor) adapted from [6]. The aim of the system is to supply a consumer with a product at a flow rate F, having a concentration C and a temperature T, knowing that the incoming products have two different qualities.

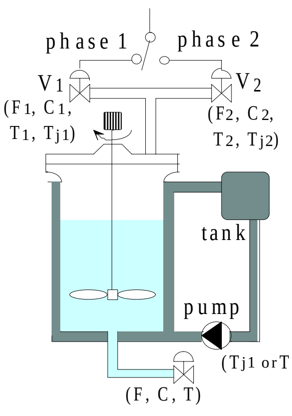

Figure 1. *process example*

The reactor may be either filled by valve V_1 and coupled to a heating system which supplies T_{j1} (defining a first dynamic phase), or filled by valve V_2 and heated at temperature T_{j2} (defining a second dynamic phase). The heating system is realized by a jacket (index j) which surrounds the reactor, a tank and a pump. In this jacket, a liquid circulates at a given temperature T_{ji}, $i\in\{1,2\}$.

The reactor characteristics are given next: maximum capacity: V_M=10 m^3, thermal exchange area: A=28.2 m^2, thermal exchange coefficient: U=72.09 $J.(s.m^2.K)^{-1}$. The liquid supplied at the output has the following properties: molecular weight: w_m=0.01802 $kg.mol^{-1}$, density: d=1000 $kg.m^3$, heat capacity: C_p=33.7 $J.(K.mol)^{-1}$. In the first dynamic phase, the incoming liquid has the following properties: concentration: C_1=100 $mol.m^{-3}$, flow rate: $F_1=5\times10^{-4}$ $m^3.s^{-1}$, temperature: T_1=308 K, temperature in jacket: T_{j1}=308 K. In the second dynamic phase, the incoming liquid has the next properties: concentration: C_2=5000 $mol.m^{-3}$, flow rate: $F_2=8\times10^{-4}$ $m^3.s^{-1}$, temperature: T_2=324 K, temperature in jacket: T_{j2}=324 K. Finally, the consumer needs a product at a fixed flow rate $F = 7\times10^{-4}$ $m^3.s^{-1}$.

The continuous state vector has 3 components: x_1 is the liquid output concentration C, x_2 is the liquid output temperature T and x_3 is the liquid volume V inside the reactor. The differential non linear equations in dynamic phases $\mu_1(l_i)$ $i\in\{1,2\}$ are given below:

$$\dot{x}_1 = \frac{F_i}{x_3}(C_i - x_1) \tag{1}$$

$$\dot{x}_2 = \frac{F_i}{x_3}(T_i - x_2) + \frac{UAw_m}{dC_p x_3}(T_{ji} - x_2) \tag{2}$$

$$\dot{x}_3 = F_i - F \tag{3}$$

The system must be driven from an initial phase l_0, where the continuous region is reduced to a single point x_0 (2500 $mol.m^{-3}$, 303 K, 10 m^3) and dynamics are null (i.e. $\mu_1(l_0)$: $\dot{x}$=0), to the desired final phase (where dynamics are also null) with the constraints $\mu_2(l_3)$: $2200\le x_1\le 2300$, $311\le x_2\le 315$, $0\le x_3\le 10$. The global constraints are GC: $2000\le x_1\le 2500$, $303\le x_2\le 323$, $0\le x_3\le 10$.

The process model is sketched on figure 2.

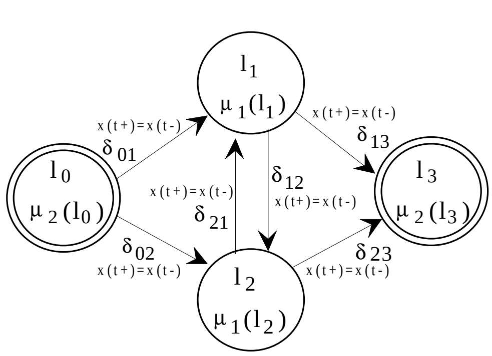

Figure 2. *process model*

4. TIME OPTIMAL CONTROL FOR HYBRID SYSTEMS: THE MAXIMUM PRINCIPLE

4.1. Basic concepts

The process can be driven to its final phase by switching from one of its dynamic phase to the other and letting evolve the time in each dynamic phase until the state vector value is acceptable for the final desired hybrid region. The controllable sequences to be optimized are determined with the controllability method presented in [1] and [2]. This method is based on the computation of geometrical sets in the state-space. These calculated sequences are hybrid : they are composed of a sequence of phases which respects the constraints on the continuous state variables.

In this paper, it is proposed to calculate time durations for these sequences which minimize the overall time duration. The chosen approach to solve this problem is an extension of the Pontryagin's Maximum Principle (PMP), usually used for continuous systems, to Hybrid Dynamical Systems (HDS). The PMP is applicable to any system having a piecewise continuous control [7]. First, it will be verified that the considered HDS fit this assumption.

The studied class of HDS are systems which switch between m vector fields μ_1 over time on occurrence of a discrete control Σ. They are called Discrete Controlled HDS (DCHDS). They can also be described as follows:

$$\dot{x}(t) = f(x(t), u(t)) \qquad (4)$$

where:

- $x \in X \subset \mathbb{R}^n$ is the state vector,
- $u=[u_1 \ \ldots \ u_m]^T \in U \subset \{0, 1\}^m$ is the control vector such that $\forall t_a \le t < t_b$, $\exists i \in \{1,...,m\}$, such that $u_i=1$ and $\forall j \in \{1,...,m\}/j \neq i$, $u_j=0$. This means that the system is in the phase i from t_a to t_b.
- $f(x,u) = \sum_{k=1}^{m} u_j \otimes \mu_1(l_j)$ is a function vector of dimension n. The symbol $\otimes$ represents the Kronecker product.

As long as the system remains in the same phase i, u(t) is constant. Moreover, if the control sequence length is finite, the number of discontinuities of the control is countable and then, the control is piecewise constant. Thus, the PMP can be applied to DCHDS.

Now, let us describe how the PMP can be extended to such systems. First, the time minimization criterion is: $J = \int_{t_0}^{t_f} dt$ with the initial time t_0 and the final time t_f. Therefore, $\dot{x}_0 = f_0 = 1$. The Hamiltonian function is:

$$H(x,p,u) = \sum_{i=1}^{m} H_i u_i \qquad (5)$$

where $p \in \mathbb{R}^n$ is the adjoint vector defined by $\dot{p} = -\left(\frac{\partial f}{\partial x}\right)^T p$ and H_i is the Hamiltonian of phase l_i defined by the dynamic $\mu_1(l_i)$:

$$H_i(x,p) = p_0 f_0 + \sum_{j=1}^{n} p_j \mu_1(l_i)(x_j) \qquad (6)$$

The Hamiltonian system is:

$$\dot{x} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial x} \qquad (7)$$

The PMP defines necessary conditions for optimality which must be verified by the optimal control u_o [7] [8]:

$$p_0=-1 \qquad (8)$$

$$H(x,p,u_o) = \sup_{u \in U} \sum_{i=1}^{m} H_i u_i \qquad (9)$$

Moreover, if the final instant t_f is not fixed:

$$H(x,p,u_o) = 0 \qquad (10)$$

The state vector optimal trajectory reaches the final manifold $\mu_2(l_f)$ on k_f boundaries (with $1 \le k_f \le \min(n,c_f)$). They are noted $\mu_{2k}(l_f)$. If the trajectory x(t) is optimal, then the transversality conditions on the adjoint vector [7] [8] are verified:

$$p(t_f) = \left[\frac{\partial \mu_{2k}(l_f)}{\partial x}\right]^T \pi_{f|t=t_f} \qquad (11)$$

where π_f is a k_f length vector.

The previous conditions (equations 8 to 11) are due to the classical form of the PMP, i.e. when it is applied to continuous systems. The extension of the PMP to DCHDS leads to new necessary conditions which are now presented. but first, it is recalled that the discrete transition tr_{ij} can be either controlled or autonomous when the DCHDS switches from the dynamics $\mu_1(l_i)$ to the dynamics $\mu_1(l_j)$ at time τ.

4.2. Equations issued of discrete transitions

If a controlled transition occurs, new equations are issued of equation (9). The Hamiltonian function H_i at the phase l_i and the Hamiltonian function H_j at the phase l_j respect the following conditions:

$\sup_{u \in U} H = H_i > H_j$ at t=τ-dt and $H_i < H_j = \sup_{u \in U} H$ at t=τ+dt

$$\text{Then, } \sup_{u \in U} H = H_i = H_j \text{ at } t=\tau \qquad (12)$$

Then transversality conditions at the switching time τ imply:

$$p(\tau+dt)=p(\tau-dt) \qquad (13)$$

In phase l_i, if the manifold $\mu_2(l_i)$ get violated at time $t=\tau$, δ_{ij} must occur. The transition from the phase l_i to the phase l_j happens when the optimal trajectory of the state vector reaches k_i boundaries of this manifold. These k_i equalities are noted $\mu_{2k}(l_i)$. The next equations can be written:

$$H_j = H_i + \left[\frac{\partial \mu_{2k}(l_i)}{\partial t}\right]^T \pi_{i|t=\tau} \qquad (14)$$

$$p(\tau + dt) = p(\tau - dt) - \left[\frac{\partial \mu_{2k}(l_i)}{\partial x}\right]^T \pi_{i|t=\tau} \qquad (15)$$

where π_i is a k_i length vector. As the equation (11), the equations (13) and (15) are transversality conditions. The last four equations (12 to 15) are obtained by using the principle that the optimal problem can be cut in two separate optimal problems op_1 (for $0<t<\tau$ with the terminal condition $x(\tau)_{op1}=x(\tau)_{op2}$) and op_2 (for $\tau<t<t_f$). It uses the dynamic programming principle, where the Bellman function is verified [9]. Mathematical rigorous demonstration can be found in [10] and [11]. The transition function μ_3 can be introduced in these last equations in order to deal with systems having sate vector discontinuities.

In this section, we have seen how an optimal control problem for DCHDS can be translated into an system of algebraic and differential equations. The number of equations N_{eq} in this system depends of the state variables number n, the number of dynamic phases p (i.e. phases the dynamic of which is not null) and the number of autonomous transitions c. The complexity, the calculation of which can be found in [12], is:

$$N_{eq} = 2np+n+c+p \qquad (16)$$

5. CONTROL SYNTHESIS FOR THE EXAMPLE

An optimal control for the process modeled in section 3 will be calculated. Two cases are considered. First, the solution to the optimal problem when the constraints of the dynamic phases are neglected, is calculated. This solution is used to calculate the optimal problem solution when the constraints are respected.

5.1. Some preliminaries

The controllability method gives the shortest discrete controllable sequence $seq=[l_0, l_1, l_2, l_1, l_3]$ taking into account the loop l_2-l_1 in the model (cf. fig 2.). It is decided that the optimal control in the constrained case will be calculated for the shortest controllable sequence seq.
The shape of all the continuous state variables possible trajectories in the constrained case was graphically sketched by the controllability method. After some observations on the process evolution behavior, it can be concluded that the final point x_f of the optimal trajectory is equal to $x_f=(2300, 311, x_{f3})$ with $0 \le x_{f3} \le 10$.
Because we are interested mainly by the dynamic phases, the dynamic sequences dynseq is defined: $dynseq=[l_1\ l_2\ l_1]$. The state vector and the adjoint vector will be noted x_{si} and p_{si} where $i \in \{1,...,|dynseq|\}$ is the position number of the phase in the dynamic sequence. For example, x_{s3} for dynseq denotes the state vector x in the third phase of dynseq, i.e. in the phase l_1. The time t_{si} denotes the remaining time in the i^{th} phase of the considered dynamic sequence.

5.2. The unconstrained optimal problem

The sequence seq is composed of p=3 dynamic phases, c=0 autonomous transitions (unconstrained case) and there are n=3 state variables. Therefore, the equation (16) states that the system of algebraic and non linear differential equations in the unconstrained case is made of 24 equations. They are established as follows:

Phase l_1: At time t=0, the process is in dynamic phase l_1. Equations (6) and (8) lead to: $H_1=-1+p_{s1}^T \mu_1(l_1)$. By equation (10), $H_1=0$ whatever t and at t=0, x_0 is fixed, so a first equation (eq1) is obtained:

$$H_1=-1+p_{s1}(0)^T \mu_1(l_1)(x_{s1}(0))=0$$

During the phase l_1, the dynamic is $\mu_1(l_1)$. Therefore, three differential equations (eq2 to eq4) must be taken into account: $\dot{x}_{s1}=\mu_1(l_1)$. With equation (7), three differential equations (eq5 to eq7) identify the adjoint vector: $\dot{p}_{s1} = -\left(\frac{\partial H_1}{\partial x}\right)^T$.

Switch from the phase l_1 to the phase l_2: At time $t=t_{s1}$, the process switches from l_1 to l_2. It is a controlled event because, in this part, the constraints on the state vector in the dynamic phases are neglected. Because the state vector x has no discontinuities when a transition occurs: $x_{s2}(0) = x_{s1}(t_{s1})$. The equation (13) leads to and $p_{s2}(0) = p_{s1}(t_{s1})$. From equations (6) and (8): $H_2=-1+p_{s2}^T \mu_1(l_2)$. From equation (12), a new equation is found (eq8):

$$H_2(x_{s1}(t_{s1}),p_{s1}(t_{s1}))-H_1(x_{s1}(t_{s1}),p_{s1}(t_{s1}))=0$$

Phase l_2: the state and the adjoint vector dynamics in phase l_2 gives six new differential equations (eq9 to eq14): $\dot{x}_{s2}=\mu_1(l_2)(x)$ and $\dot{p}_{s2} = -\left(\frac{\partial H_2}{\partial x}\right)^T$.

Switch from the phase l_2 to the phase l_1: At time $t=t_{s2}$, one equation (eq15) is established:

$$H_1(x_{s2}(t_{s2}),p_{s2}(t_{s2}))-H_2(x_{s2}(t_{s2}),p_{s2}(t_{s2}))=0$$

Phase l_2: the state and the adjoint vector dynamics in phase l_2 gives six new differential equations (eq16 to eq21).

At the final time $t=t_f=t_{s1}+t_{s2}+t_{s3}$, the continuous state variables reach k_f boundaries of the final constraint region $\mu_2(l_3)$. It is recalled that the optimal trajectory ends on the following straight line x_f= (2300, 311, x_3). Therefore, $k_f=2$ and two new equations are defined (eq22, eq23). By equation (11), it is deduced $p_{s2}(t_{s2})=[\pi_{f1}\ \pi_{f2}\ 0]^T$. Only the third equation (eq24) is interesting.

This system, composed of 24 equations, has also 24 unknown variables : the vector $p_{s1}(0)$, time t_{s1}, vectors $p_{s1}(t_{s1})$ and $x_{s1}(t_{s1})$, time t_{s2}, vectors $p_{s2}(t_{s2})$ and $x_{s2}(t_{s2})$, time t_{s3}, vectors $p_{s3}(t_{s3})$ and $x_{s3}(t_{s3})$. The system of equations is solved using a numerical optimization method with matlab. The result is:

t=0 $\quad x(0)=\begin{bmatrix}2500\\303\\10\end{bmatrix} \quad p(0)=\begin{bmatrix}-7.13\\427\\-969\end{bmatrix}$

$t=t_{s1}$=5434s $\quad x(t_{s1})=\begin{bmatrix}1900\\306\\8.91\end{bmatrix} \quad p(t_{s1})=\begin{bmatrix}-9.50\\1063\\-241\end{bmatrix}$

$t=t_{s2}$=1552s $\quad x(t_{s2})=\begin{bmatrix}2300\\311\\9.07\end{bmatrix} \quad p(t_{s2})=\begin{bmatrix}-10.9\\1473\\0\end{bmatrix}$

$t=t_{s3}$=0s $\quad x(t_{s3})=x(t_{s2}) \quad p(t_{s3})=p(t_{s2})$

The optimal trajectories are presented figures 3 to 5 at the end of the paper. $t_{s3}=0$ means that the shortest sequence, if the constraints are not respected, is $[l_0, l_1, l_2, l_3]$ and this sequence leads to the optimal control. Then, it is not necessary to try longer sequences because the remaining times in the phases before l_3 would be always null.

5.3. The constrained optimal problem

It must be determined if the events δ_{12} and δ_{21} which lead to dynseq$_c$ are controlled or not. The resulting equations of the system would not be the same.

In the unconstrained case, the optimal trajectory of the state variables respects the dynamic phases constraints everywhere except around the first transition from l_1 to l_2, where the concentration is below the allowed minimum: 2000 mol.m^{-3} (c.f. figures 3 and 5). Therefore, in the constrained case, the process must switch from $\mu_1(l_1)$ to $\mu_1(l_2)$ when x_1=2000. It defines an autonomous transition on the occurrence of δ_{12}.

The shape of all the continuous state variables possible trajectories (sketched with the controllability method) show that, if the first switch occurs on the constraints limit, the second does not. So, event δ_{21} is controlled.

The system of algebraic and differential non linear equations is established by the same method as in the unconstrained case. Equations due to the autonomous transition are substituted to the equation eq8 of the previous system of equations. At time $t=t_{s1}$, x_1=2000. It defines and gives an equation to introduce in the system. Equation (15) gives the three next equations: $p_{s2}(0)=p_{s1}(t_1)-[\pi_{11}\ 0\ 0]^T$, and equation (14) gives a new equation: $H_2 = H_1 + \left(\frac{\partial \mu_{2k}(l_1)}{\partial t}\right)^T \pi_1\big|_{t=\tau}$.

The sequence seq is composed of p=3 dynamic phases, c=1 autonomous transitions and n=3 because there are 3 state variables. Therefore, there are 25 algebraic and non linear differential equations in the constrained case. There are also 25 unknown variables: the vector $p_{s1}(0)$, time t_{s1}, vectors $p_{s1}(t_{s1})$ and $x_{s1}(t_{s1})$, the shifting value π_{11} on the adjoint vector at time $t=t_{s1}$, time t_{s2}, vectors $p_{s2}(t_{s2})$ and $x_{s2}(t_{s2})$, time t_{s3}, vectors $p_{s3}(t_{s3})$ and $x_{s3}(t_{s3})$. The solution is calculated with the same algorithm than before. The resulting values are:

t=0 $\quad x(0)=\begin{bmatrix}2500\\303\\10\end{bmatrix} \quad p(0)=\begin{bmatrix}-6.54\\494\\-883\end{bmatrix}$

$t=t_{s1}$=4460s $\quad x(t_1)=\begin{bmatrix}2000\\305.6\\9.11\end{bmatrix} \quad p(t_1)=\begin{bmatrix}-8.26\\1037\\-307\end{bmatrix} \quad \pi_{11}=3.59$

$t=t_{s2}$=2033s $\quad x(t_2)=\begin{bmatrix}2486\\312\\9.31\end{bmatrix} \quad p(t_2)=\begin{bmatrix}-14.1\\1572\\-127\end{bmatrix}$

$t=t_{s3}$=1484s $\quad x(t_3)=\begin{bmatrix}2300\\311\\9.01\end{bmatrix} \quad p(t_3)=\begin{bmatrix}-15.3\\2033\\0\end{bmatrix}$

The optimal trajectories are presented figures 3 to 5 at the end of the paper. The shifting value π_{11} is noted pi on the figure 4. The calculation of optimal control for a longer controllable sequence have been realized. As it could be guessed, the remaining times in the dynamic phases just before l_3 are null.

6. CONCLUSION

In this paper, we have presented how to synthesize the time optimal control for Discrete Controlled Hybrid Dynamical Systems (DCHDS).

The synthesis method does not impose a maximum number of continuous state variables. Nevertheless, the number of equations to solve increases rapidly, so only a numerical solution is calculated. But the possible non linearity of the dynamics introduces convergence and uniqueness of solution problems (local Vs global minimum). Therefore, the initial guess for the numerical solution calculation must be adequately chosen.

In addition to these numerical convergence problems, the existence and the uniqueness of an optimal solution is not systematic. The equations system, stated thanks to the PMP theory, gives necessary but no sufficient conditions. Moreover, the system of equations to be solved can be non linear. So the solution may be not unique. By now, it has only been proven that an optimal control exists and is unique for linear systems [7].

These last two points are classical problems of non linear control and more works to clarify it for DCHDS should be interesting to realize.

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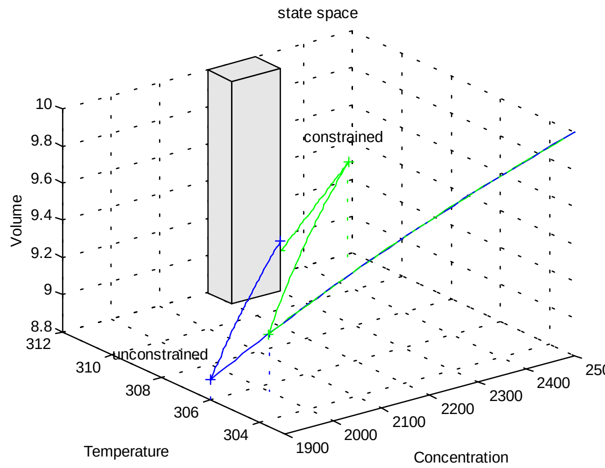

Figure 3. *the state space*

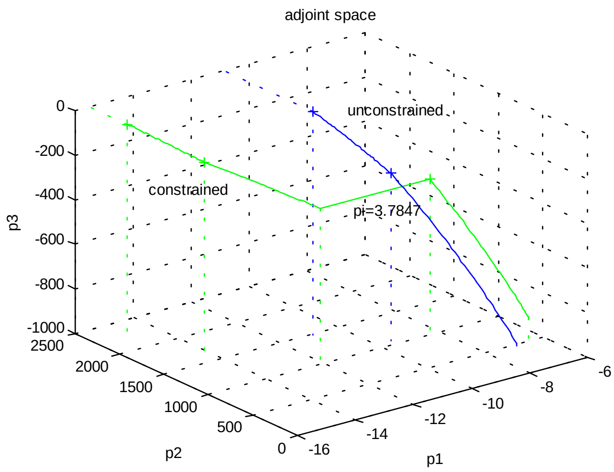

Figure 4. *the adjoint space*

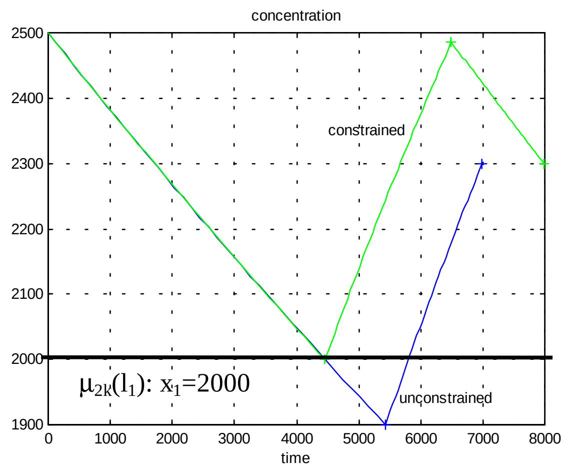

Figure 5. *concentration versus time*