Modelling, Reachability and Sub-Optimal control of a class of sequencing batch reactor

D. Mazouni, J. Harmand, A. Rappaport and H. Hammouri

Environmental and Biotechnological Laboratory of INRA, France

Overview

- Biological reations Modelling
  - Biological Carbon and nitrogen removal
  - Mass balance model
  - Model Simplification
- Accessibility and reachability
  - Dynamic bihaveour
  - Target and accessibility
  - Switching number
- Suboptimal control
  - Optimisation objectives
  - PMP principle
  - Reaction time duration
  - Switching parametrisation
- Conclusion and perspectives

The European Commission
Community Research
Confirming the International Role of Community Research

Biological Reaction Modelling

Carbon and nitrogen removal

- Two Biological phenomena are taken into account:
  - Carbon removal
  - Nitrogen removal (Nitrification and Denitrification)
- Two modes of treatment are needed :
  - aerobic for Carbon removal and Nitrification
  - anoxic for denitrification
- Three substrates and two biomasses are available
  - S1: Carbon
  - S2: Nitrogen Ammonium
  - S3: Nitrates and Nitrites
  - X1: Heterotrophic Bacteria
  - X2: Autotrophic Bacteria

Biological reactions

- Three reactions:

$$S_1 \xrightarrow{O2 \quad \varphi 1} X_1$$

$$S_2 \xrightarrow{O2 \quad \varphi 2} X_2 + S_3$$

$$S_1 + S_3 \xrightarrow{\varphi 3} X_1$$

- Growth rates:

$$\varphi_1 = \mu_1 (S_1) X_1$$

$$\varphi_2 = \mu_2 (S_2) X_2$$

$$\varphi_3 = \mu_3 (S_1, S_3) X_1$$

$$\mu_i (S \neq 0) > 0, \qquad \mu_i (0) = 0, \qquad X_i (0) \neq 0$$

Mass Balance Model for batch reactor

- Aerobic model

$$\frac{dX_1}{dt} = \mu_1(S_1)X_1$$

$$\frac{dX_2}{dt} = \mu_2(S_2)X_2$$

$$\frac{dS_1}{dt} = -K_{11}\mu_1(S_1)X_1$$

$$\frac{dS_2}{dt} = -K_{22}\mu_2(S_2)X_2$$

$$\frac{dS_3}{dt} = K_{32}\mu_2(S_2)X_1$$

- Anoxic model

$$\frac{dX_1}{dt} = \mu_3(S_1,S_3)X_1$$

$$\frac{dX_2}{dt} = 0$$

$$\frac{dS_1}{dt} = -K_{11}\mu_3(S_1,S_3)X_1$$

$$\frac{dS_2}{dt} = 0$$

$$\frac{dS_3}{dt} = -K_{33}\mu_3(S_1,S_3)X_1$$

Model simplification -1-

Control $u \in \{0,\ 1\}$

For aerobic mode $u = 1$ For anoxic mode $u = 0$

$$\frac{d}{dt}\begin{bmatrix} X_1 \\ S_1 \\ X_2 \\ S_2 \\ S_3 \end{bmatrix} = \left[\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -K_{11} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -K_{33} \end{bmatrix} + \begin{bmatrix} 1 & 0 & 1 \\ -K_{11} & 0 & -K_{11} \\ 0 & 1 & 0 \\ 0 & -K_{22} & 0 \\ 0 & K_{32} & K_{33} \end{bmatrix} u\right] \begin{bmatrix} \mu_1(S_1)X_1 \\ \mu_2(S_2)X_2 \\ \mu_3(S_1, S_3)X_1 \end{bmatrix}$$

Model simplification -2-

$$\dot{S}_1 + K_{11}\dot{X}_1 = 0 \qquad S_1 + K_{11}X_1 = S_1(0) + K_{11}X_1(0) = M_1$$

$$\dot{S}_2 + K_{22}\dot{X}_2 = 0 \qquad S_2 + K_{22}X_2 = S_2(0) + K_{22}X_2(0) = M_2$$

$$X_1 = \frac{S_1 - M_1}{K_{11}}, \quad X_2 = \frac{S_2 - M_2}{K_{22}}$$

$$\frac{d}{dt}\begin{bmatrix} S_1 \\ S_2 \\ S_3 \end{bmatrix} = \left[\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{K_{33}}{K_{11}} \end{bmatrix} + \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & \frac{K_{32}}{K_{22}} & -\frac{K_{33}}{K_{11}} \end{bmatrix} u \right] \begin{bmatrix} \mu_1(S_1)(S_1 - M_1) \\ \mu_2(S_2)(S_2 - M_2) \\ \mu_3(S_1, S_3)(S_1 - M_1) \end{bmatrix}$$

$$\dot{z}(t) = f(z(t)) + g(z(t))u(t)$$

Accessibility and reachability

Dynamic behavior -1-

In aerobic

$$\dot{S}_3 + \frac{K_{32}}{K_{22}}\dot{S}_2 = 0 \qquad S_3 - S_3(0) + \frac{K_{32}}{K_{22}}(S_2 - S_2(0)) = 0$$

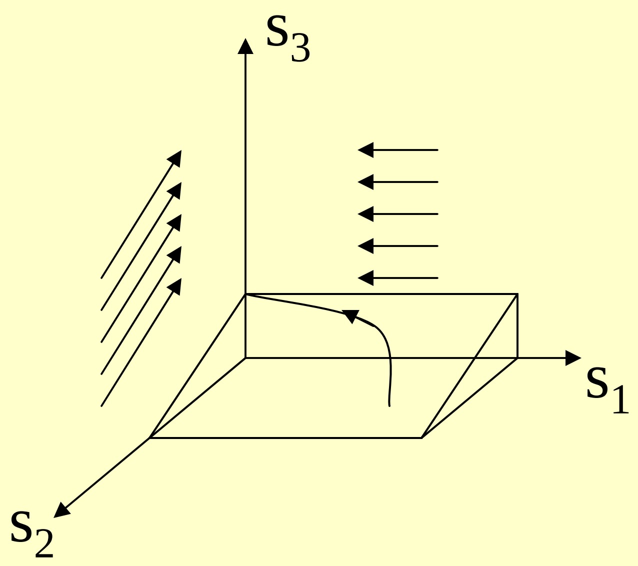
$$\dot{S}_1 = \mu_1(S_1)\left(S_1 - M_1\right) \qquad S_1(t) > 0$$

In anoxic

$$\dot{S}_3 - \frac{K_{33}}{K_{11}}\dot{S}_1 = 0 \qquad S_3 - S_3(0) - \frac{K_{33}}{K_{11}}(S_1 - S_1(0)) = 0$$

$$\dot{S}_2 = 0 \qquad S_2(t) = S_2(0)$$

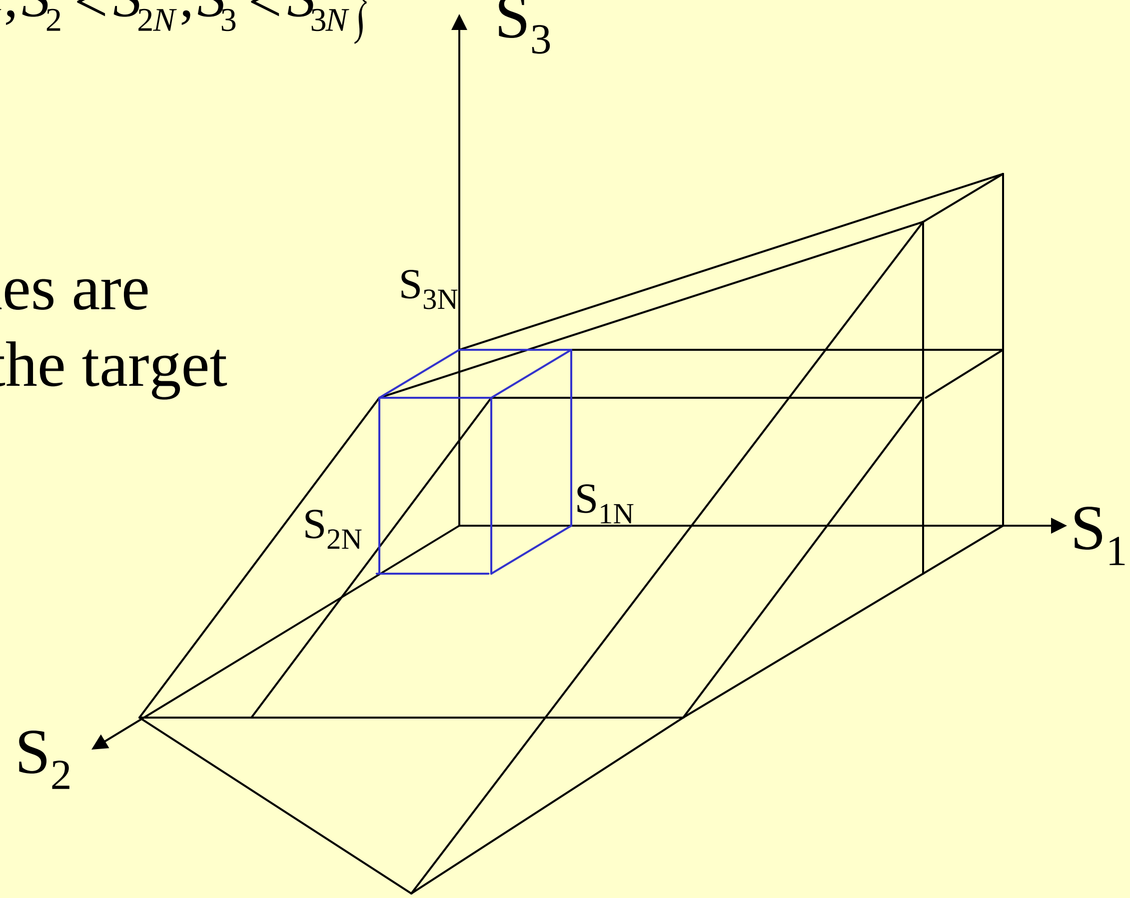
Dynamic behavior -2-



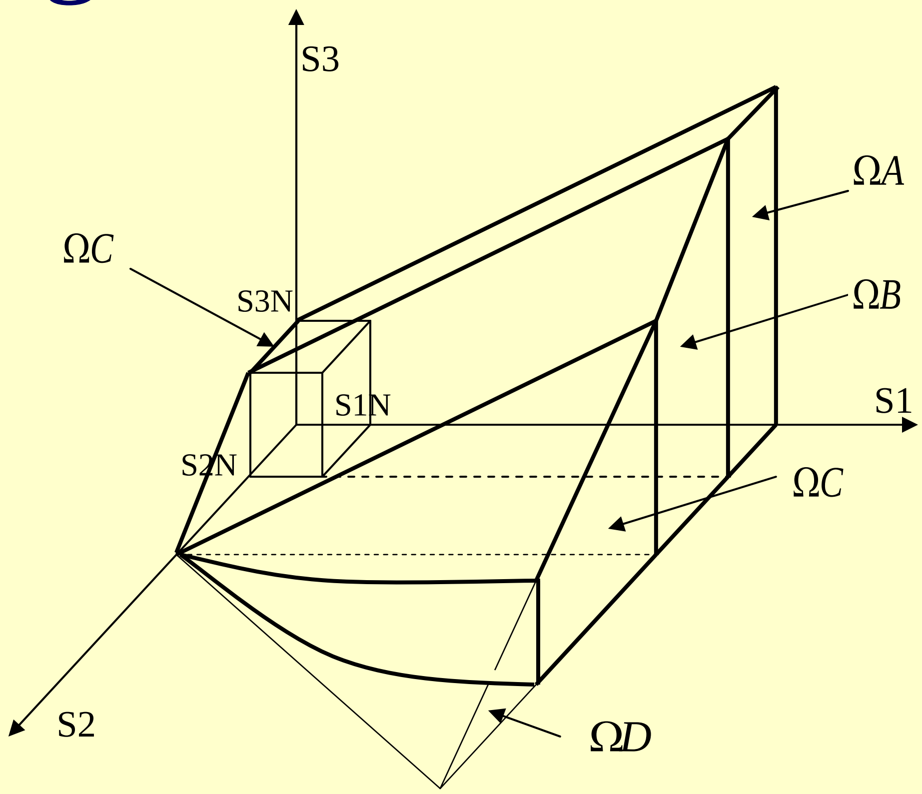
Target and Reachability

$$C=\left\{\left(S_1,S_2,S_3\right)\in R^3 / S_1<S_{1N},S_2<S_{2N},S_3<S_{3N}\right\}$$

At most two switches are necessary to reach the target



Target and Reachability

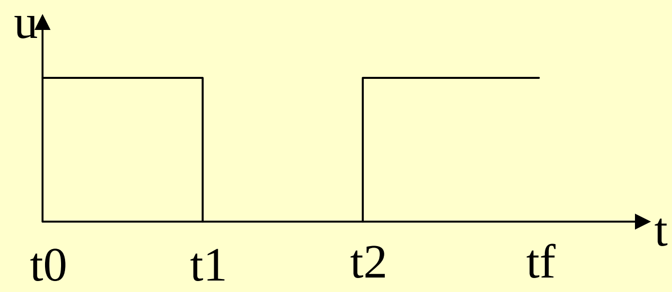


Optimisation Objectives

Reach the target C from the initial conditions in minimum time.

Use the minimum number of switches

Find t1 and t2 to minimize the total time



Sub-Optimal Control

PMP principle for minimal time control

Let Consider $z = [S_1 \quad S_2 \quad S_3] \quad u \in [0 \quad 1]$

Minimizing $J = \int dt$ for $\dfrac{dz(t)}{dt} = f(z(t)) + g(z(t))u(t)$

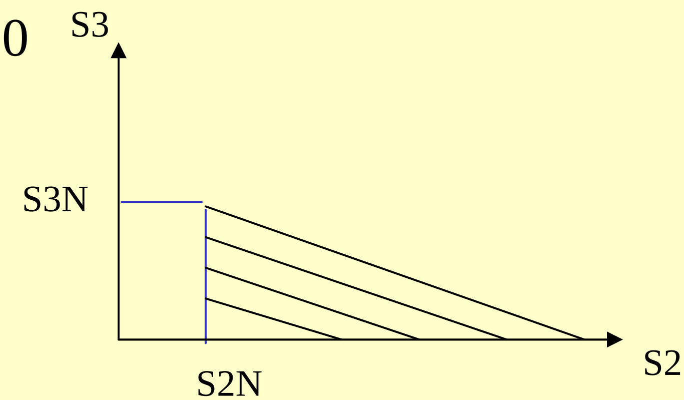
Hamiltonian $H(z(t),u(t)) = \lambda(t)\big(f(z(t)) + g(z(t)u(t)\big) + \lambda_0$

$$\frac{d\lambda(t)}{dt} = -\frac{\partial H(t)}{\partial Z}$$

Optimal control $u^* = \begin{cases} u_{\min} & if \quad \lambda(t)g(t) > 0 \\ u_S & if \quad \lambda(t)g(t) = 0 \\ u_{\max} & if \quad \lambda(t)g(t) < 0 \end{cases}$

Particular case: without switching

In aerobic $$S_3 - S_3(0) + \frac{K_{32}}{K_{22}}(S_2 - S_2(0)) = 0$$



All the trajectories in

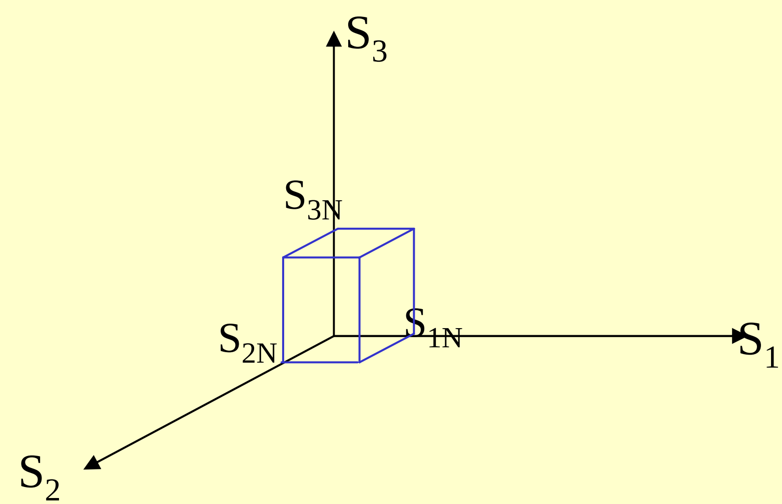
$$\Omega = \left\{ (S_1, S_2, S_3) \in R^{3+} \quad / S_3 < -\frac{K_{32}}{K_{22}} S_2 + S_{3N} \right\}$$

verify

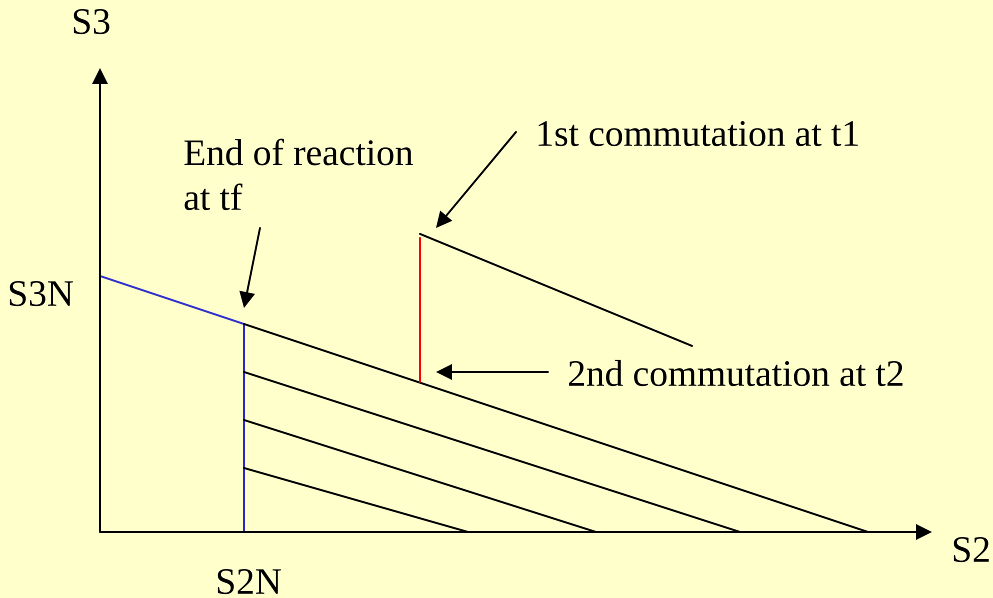
$$\lambda(t_f) = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \quad or \quad \begin{pmatrix} 0 & 1 & 0 \end{pmatrix}$$

$$\lambda(t) g(t) < 0$$

So $u^* = 1$ for $(S_1, S_2, S_3) \in \Omega$



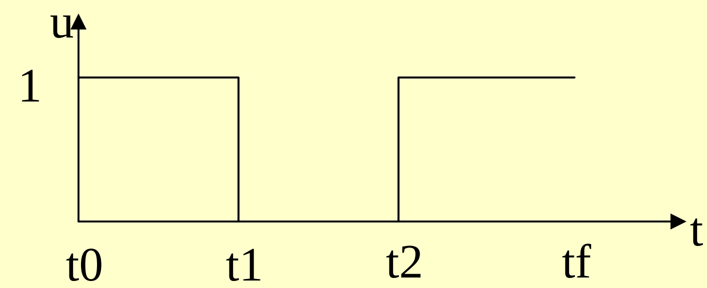
Switching Instants Parametrisation



- tf when trajectory reach the target
- t2 when the trajectory reach the switching surface
- t1 ?

Reaction time duration For general case

$$t = t_{aerobic} + t_{anoxic} + t_{aerobic}$$



$$t_{aerobic} = \int_{t0}^{t1} dt + \int_{t2}^{tf} dt = \max\left(\left(\int_{S1(t0)}^{S1(t1)} \frac{ds}{h_1^{ae}(s)} + \int_{S1(t2)}^{S1N} \frac{ds}{h_1^{ae}(s)}\right), \left(\int_{S2(t0)}^{S2(t1)} \frac{ds}{h_2^{ae}(s)} + \int_{S2(t2)}^{S2N} \frac{ds}{h_2^{ae}(s)}\right)\right)$$

$$t_{aerobic} = \int_{S2(t0)}^{S2(t1)} \frac{ds}{h_2^{ae}(s)} + \int_{S2(t2)}^{S2N} \frac{ds}{h_2^{ae}(s)} = \int_{S20}^{S2N} \frac{ds}{h_2^{ae}(s)}$$

Does not depend on u !

$$t_{anoxic} = \int_{t1}^{t2} dt$$

Anoxic phase duration

Let: $$l(t) \triangleq S_1(t_1) - S_1(t) = \frac{K_{11}}{K_{22}}\left(S_3(t_1) - S_3(t)\right) \qquad t \in [t_1,\ t_2]$$

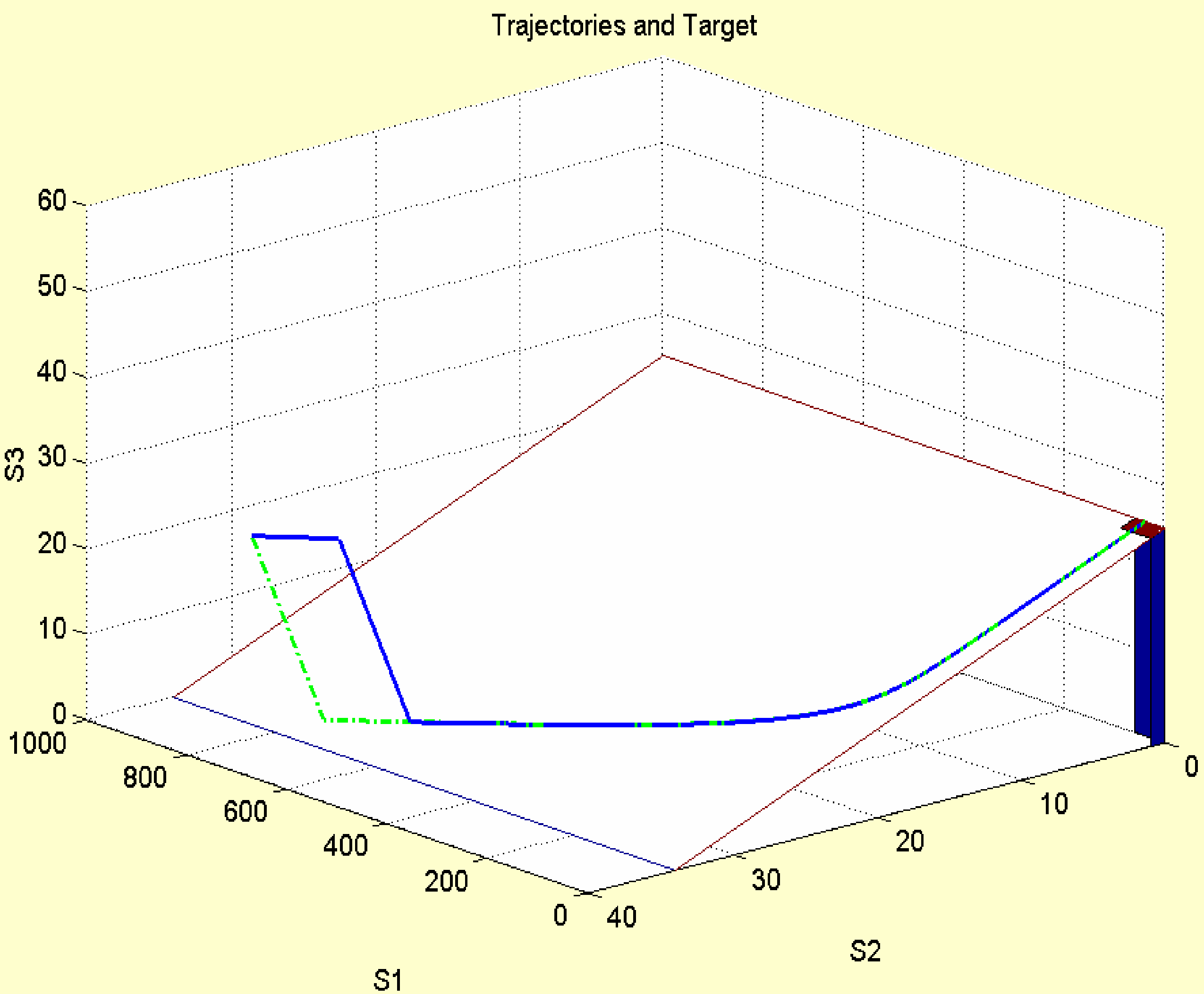
$$\Delta \triangleq l(t_2) = \frac{K_{11}}{K_{33}}\left(S_3(t_1) - S_3(t_2)\right) = \frac{K_{11}}{K_{33}}\left(S_{30} + \frac{K_{32}}{K_{éé}} S_{20} - S_{3N}\right)$$

$$S_1(t) = S_1(t_1) - l(t)$$

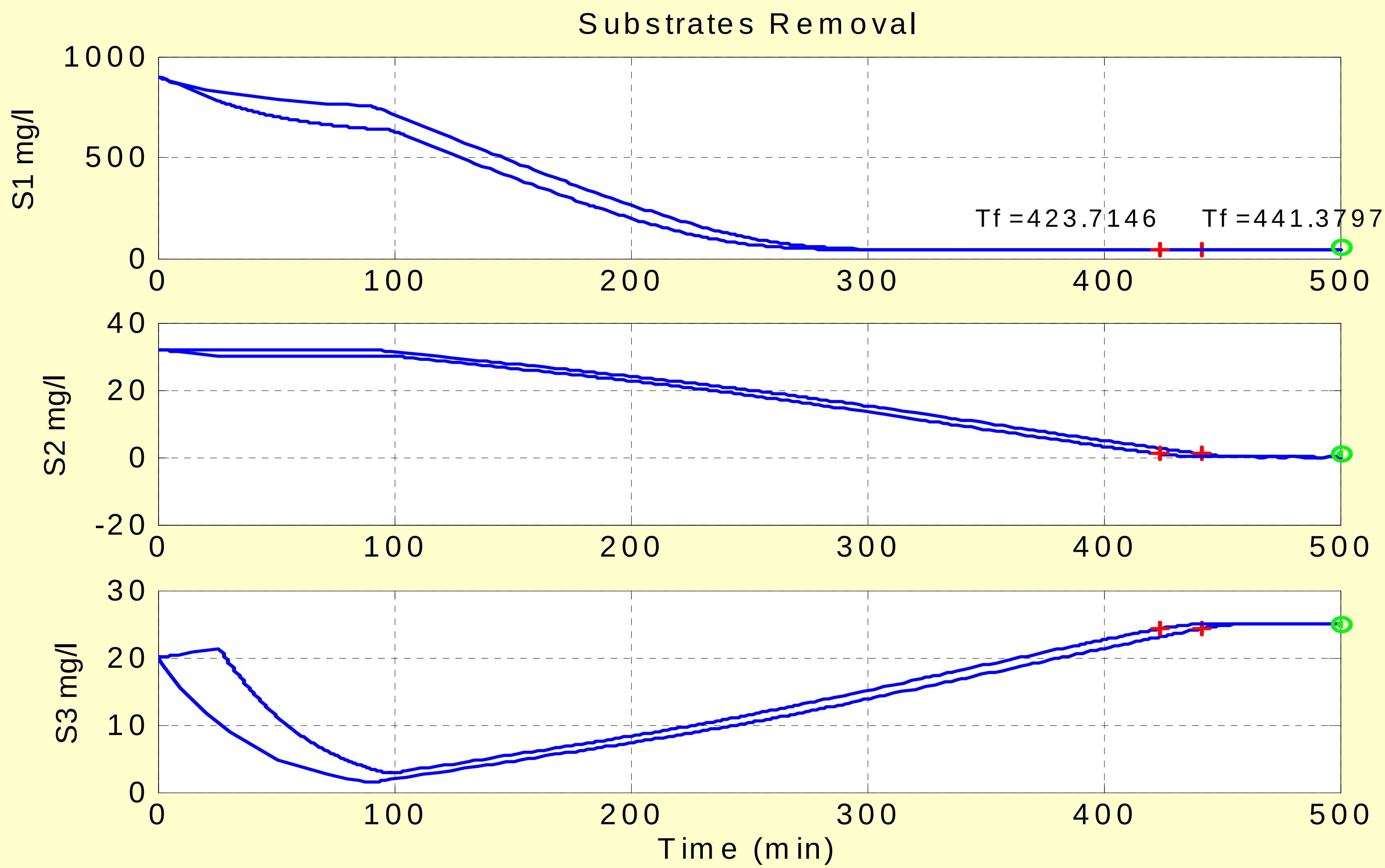
$$S_3(t) = S_3(t_1) - \frac{K_{33}}{K_{11}} l(t)$$

$$\frac{dl}{dt} = -\frac{dS_1}{dt} = -h_3^{ae}(S_1, S_3) = -h_3^{ae}\left(S_1(t_1) - l, S_3(t_1) - l\right)$$

$$t_{anoxic} = \int_{t1}^{t2} dt \qquad t_{anoxic} = -\int_0^{\Delta} \frac{dl}{h_3^{ae}\left(S_1(t_1) - l, S_3(t_1) - l\right)} = \int_0^{\Delta} L\left(S_1(t_1), S_3(t_1), l\right) dl$$



Trajectories and Target
S3
60
50
40
30
20
10
0
1000
800
600
400
200
0
S1
40
30
20
10
0
S2


Substrates Removal
1000
500
0
S1 mg/l
Tf =423.7146
Tf =441.3797
0
100
200
300
400
500
40
20
0
-20
S2 mg/l
30
20
10
0
S3 mg/l
Time (min)

Conclusion

- Model simplification for controlability and optimisation study
- Dynamic behavior and trajectory analyses
- Control and Time minimisation for batch reactor

Perspectives

- On line Application on real bio process