Control of bioprocesses : some introductory concepts

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Content

- Adaptive linearizing control : basic concepts
- Control of fed-batch processes : a specific issue

Adaptive linearizing control is equivalent to PI control

Output dynamics : $$\frac{dy}{dt} = \frac{q}{V}(\alpha x_{in} - y) - \beta Q + \gamma r(x)$$

with q : control input

α, β, γ : nonlinear combination of yield coefficients

Desired closed loop dynamics : $$\frac{dy}{dt} = \lambda(y^* - y), \quad \lambda > 0$$

→ Control law (with *r, a, b* and *g* unknown) :

$$q = \frac{V}{\hat{\alpha} x_{in} - y}\left[\lambda(y^* - y) + \hat{\beta} Q - \widehat{\gamma r}\right]$$

Application : wastewater treatment by anaerobic digestion

- Biological wastewater treatment + CH_4 production

- Complex process simple reaction network :

organic matter

1) acidogenesis : $S_1 \longrightarrow X_1 + S_2 + CO_2$

2) methanization : $S_2 \longrightarrow X_2 + CH_4 + CO_2$

volatile fatty acids

- Process : CSTR (60 litres)

- Measurements : COD (= $S_1 + S_2$) + CH_4 gaseous outflow rate

- COD regulation (wastewater treatment objective)

Dynamical model (mass balance)

$$\frac{dX_1}{dt} = \mu_1 X_1 - D X_1$$

$$\frac{dS_1}{dt} = -k_1 \mu_1 X_1 + D S_{in} - D S_1$$

} acidogenesis

$$\frac{dX_2}{dt} = \mu_2 X_2 - D X_2$$

$$\frac{dS_2}{dt} = k_3 \mu_1 X_1 - k_2 \mu_2 X_2 - D S_2$$

$$\frac{dP_1}{dt} = k_4 \mu_2 X_2 - D P_1 - Q_1$$

} methanisation

$$\frac{dP_2}{dt} = k_5 \mu_1 X_1 + k_6 \mu_2 X_2 - D P_2 - Q_2$$

CO_2

Model reduction

- CH_4 and CO_2 are low solubility products :

$$
\begin{aligned}
Q_1 &= k_4 \mu_2 X_2 \\
Q_2 &= k_5 \mu_1 X_1 + k_6 \mu_2 X_2
\end{aligned}
$$

--> dynamical mass balance of S :

$$
\frac{dS}{dt} = D(S_{in} - S) + \frac{k_3 - k_1}{k_5} Q_2 - \left(\frac{k_6 (k_3 - k_1}{k_1 k_5} + \frac{k_2}{k_1} \right) Q_1
$$

- Assume Q_2 proportional to Q_1 ($Q_2 = \alpha Q_1$) :

$$
\frac{dS}{dt} = D(S_{in} - S) - \beta Q_1
$$

- Alternative : CH_4 is a low solubility product and the methanization is a fast reaction :

$$
\begin{aligned}
Q_1 &= k_4 \mu_2 X_2 \\
DS_{in} &= k_1 \mu_1 X_1
\end{aligned}
$$

--> dynamical mass balance of S :

$$
\frac{dS}{dt} = D(S_{in} - S) - \frac{k_1 k_2}{k_3 k_4} Q_1
$$

Application : anaerobic digestion

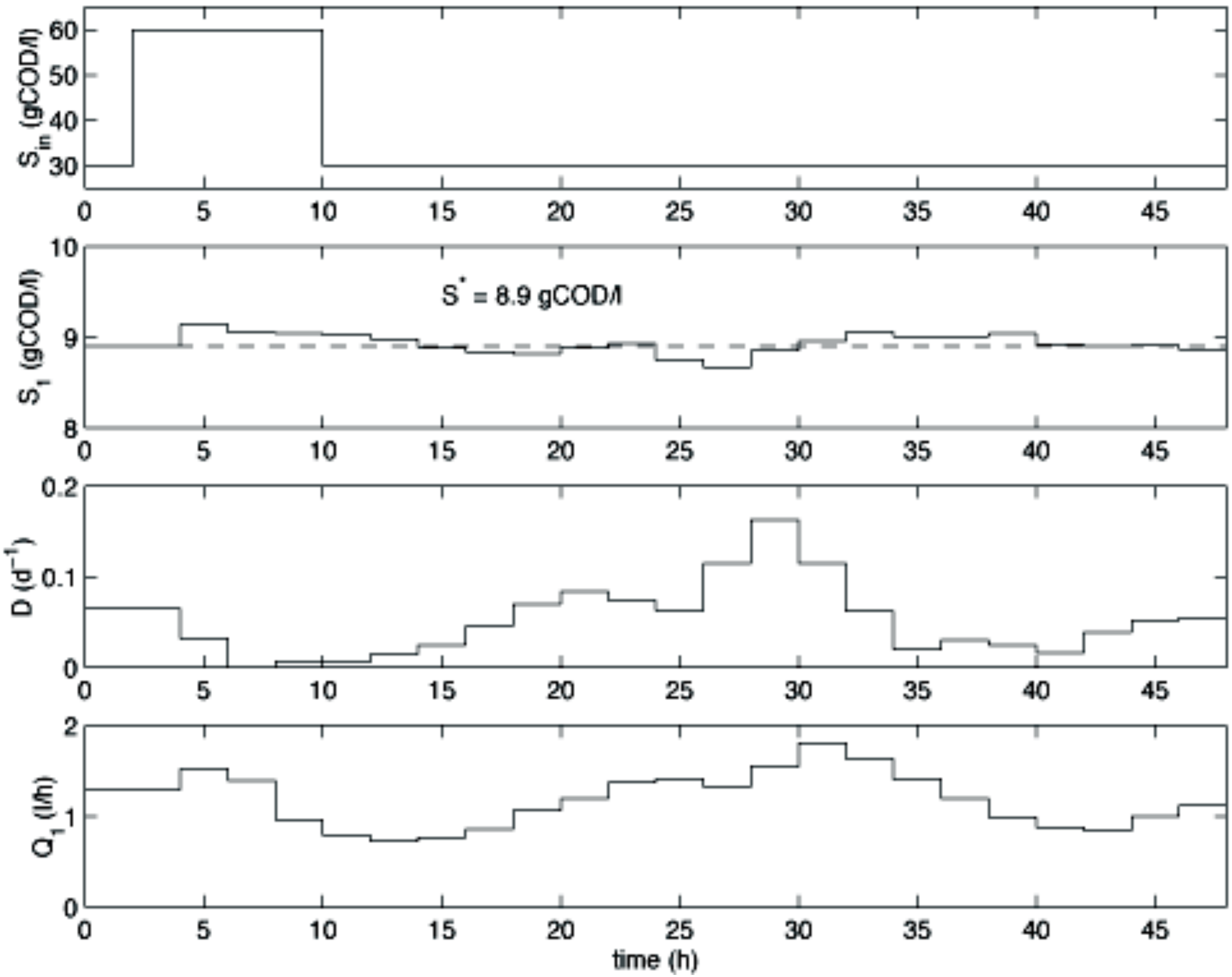
Mass balance equation of S : $\dfrac{dS}{dt} = \dfrac{q}{V}(S_{in} - S) - \beta Q$

Control law (« Lyapunov design ») :

$$
\begin{aligned}
q &= \frac{V}{S_{in} - y}\left[\lambda(S^* - S) + \hat{\beta}Q\right] \\
\frac{d\hat{\beta}}{dt} &= \delta(S^* - S), \quad \delta > 0
\end{aligned}
$$

Or by integrating the parameter adaptation equation :

$$
q = \frac{V}{S_{in} - y}\left[\underbrace{\lambda(S^* - S)}_{\text{proportional action}} + \underbrace{\delta Q \int_0^t (S^* - S)d\tau}_{\text{integral action}}\right]
$$



S_in (gCOD/l)
S* = 8.9 gCOD/l
S_1 (gCOD/l)
D (d^-1)
Q_1 (l/h)
time (h)

Case study #2 : control of volatile fatty acids S_2

- Objective : to prevent the process from instability

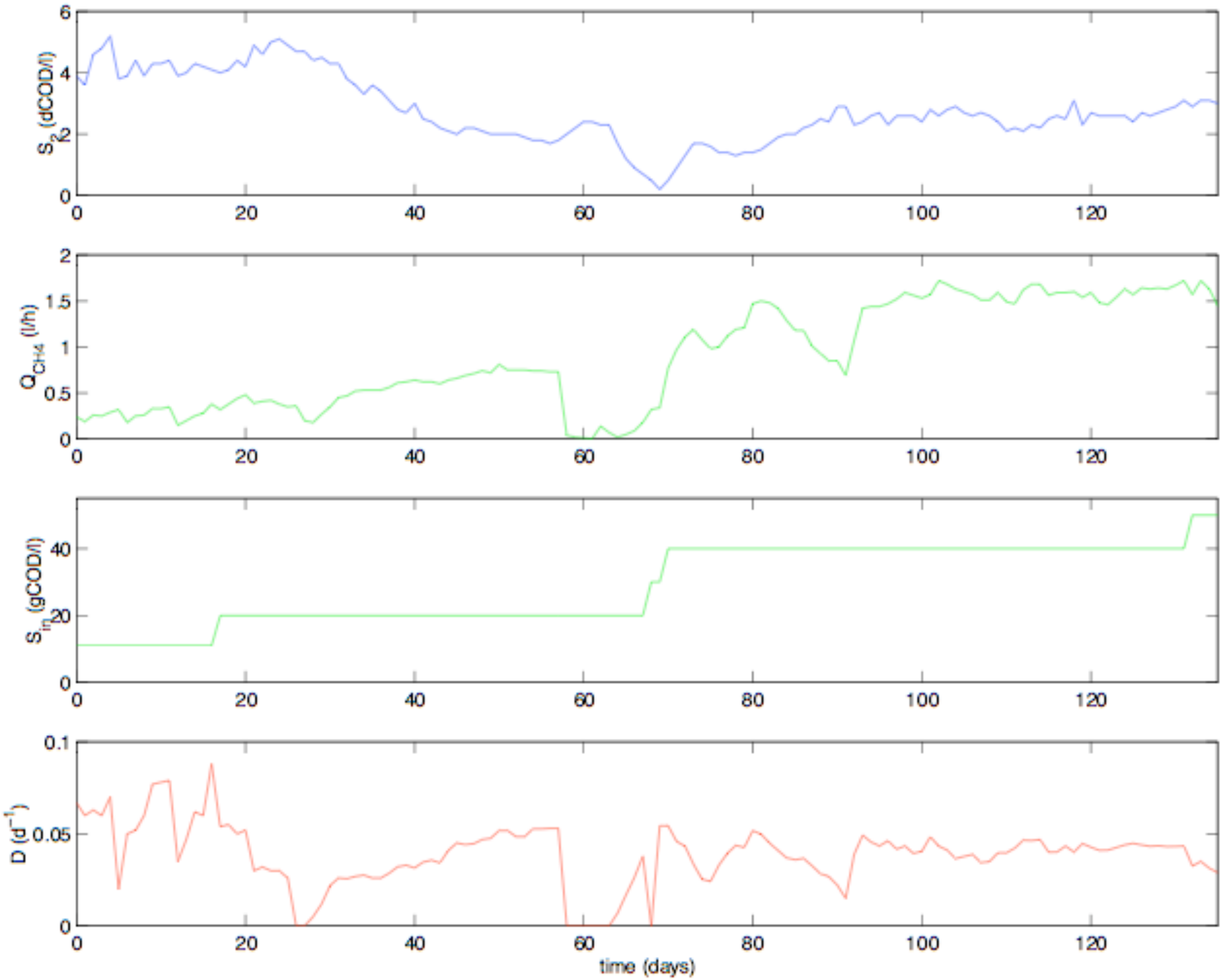
- Assumption : methanization is the limiting step
  (S_2 may accumulate)

- Model reduction : CH_4 is a low solubility product and the acidogenesis is a fast reaction :

$$
\begin{aligned}
Q_1 &= k_4 \mu_2 X_2 \\
D S_{in} &= k_1 \mu_1 X_1
\end{aligned}
$$

--> dynamical mass balance of S_2 :

$$
\frac{dS_2}{dt} = D\left(\frac{k_3}{k_1} S_{in} - S_2\right) - \frac{k_2}{k_4} Q_1
$$


S_2 (dCOD/l)
Q_{CH4} (l/h)
S_{in} (gCOD/l)
D (d^{-1})
time (days)

Control of fed-batch processes : a specific issue

- Fed-batch processes : limited time operation

- Typical objective : to optimize the production over the process operation duration

- Example : yeast growth
  - Optimal control : « exponential » growth
  - Practical issue : how to incorporate this specific feature in a simple (e.g. PI) controller?

Case study : fedbatch reactor with a simple growth reaction and Haldane kinetics

- System dynamics :

$$\begin{aligned} \frac{dS}{dt} &= \frac{q}{V}(S_{in} - S) - k_1 \mu X \\ \frac{dX}{dt} &= \mu X - \frac{q}{V} X \\ \frac{dV}{dt} &= q \\ \mu &= \frac{\mu_0 S}{K_S + S + \frac{S^2}{K_I}} \end{aligned}$$

- Process operation objective : to maximize the total production of biomass VX

--> Optimal control : to find $u(t)$ that maximizes $J = V(t_f)X(t_f)$

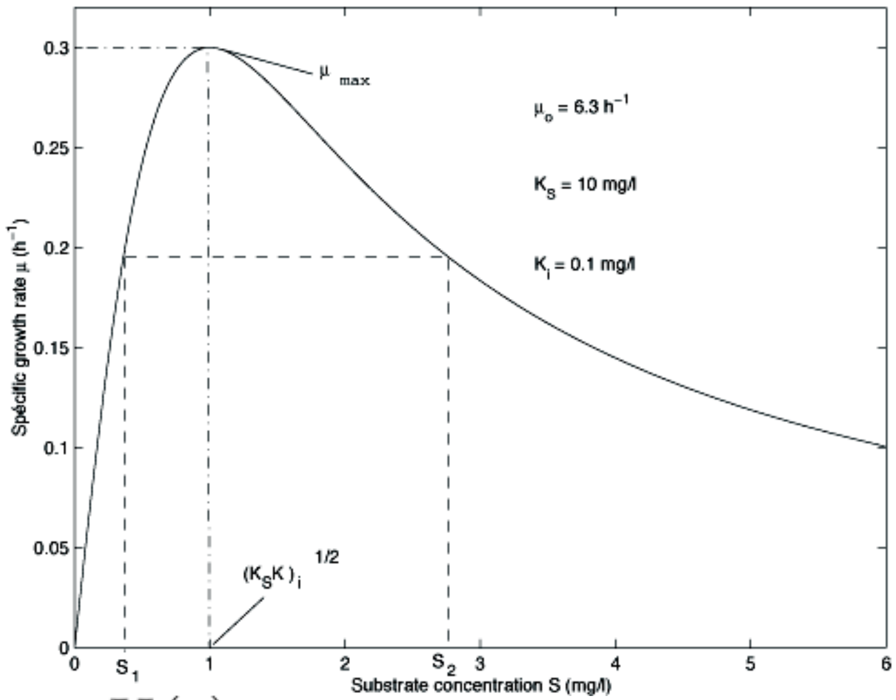
Optimal control

- Consider : $u(t) = S_{in}(t)$

- Pontryagin Maximum Principle

singular arc if $$\frac{\partial \mu}{\partial S} = 0$$

i.e. if $$S_{sing} = \sqrt{K_S K_I}$$

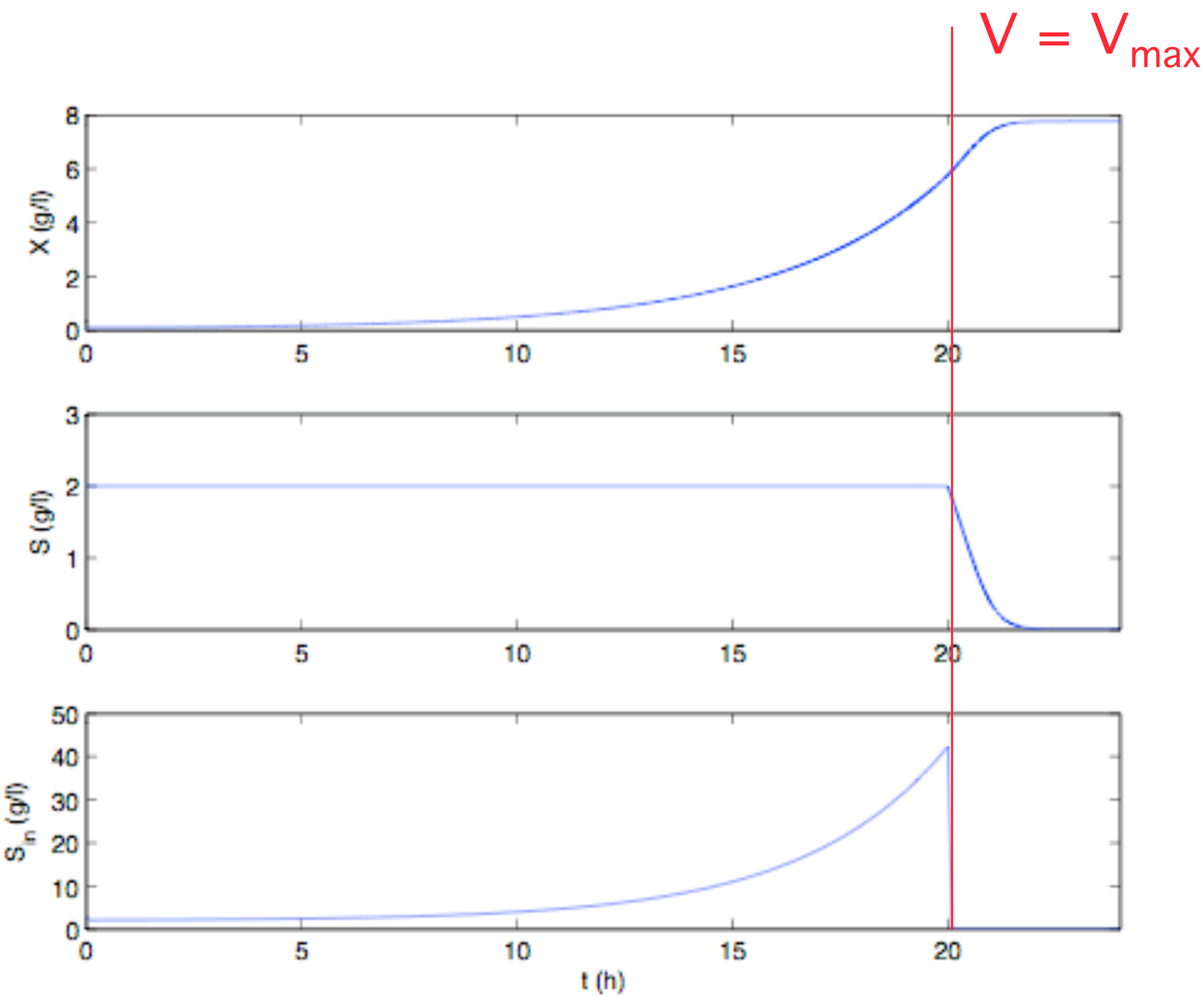


- If $S(0) = S_{sing}$:

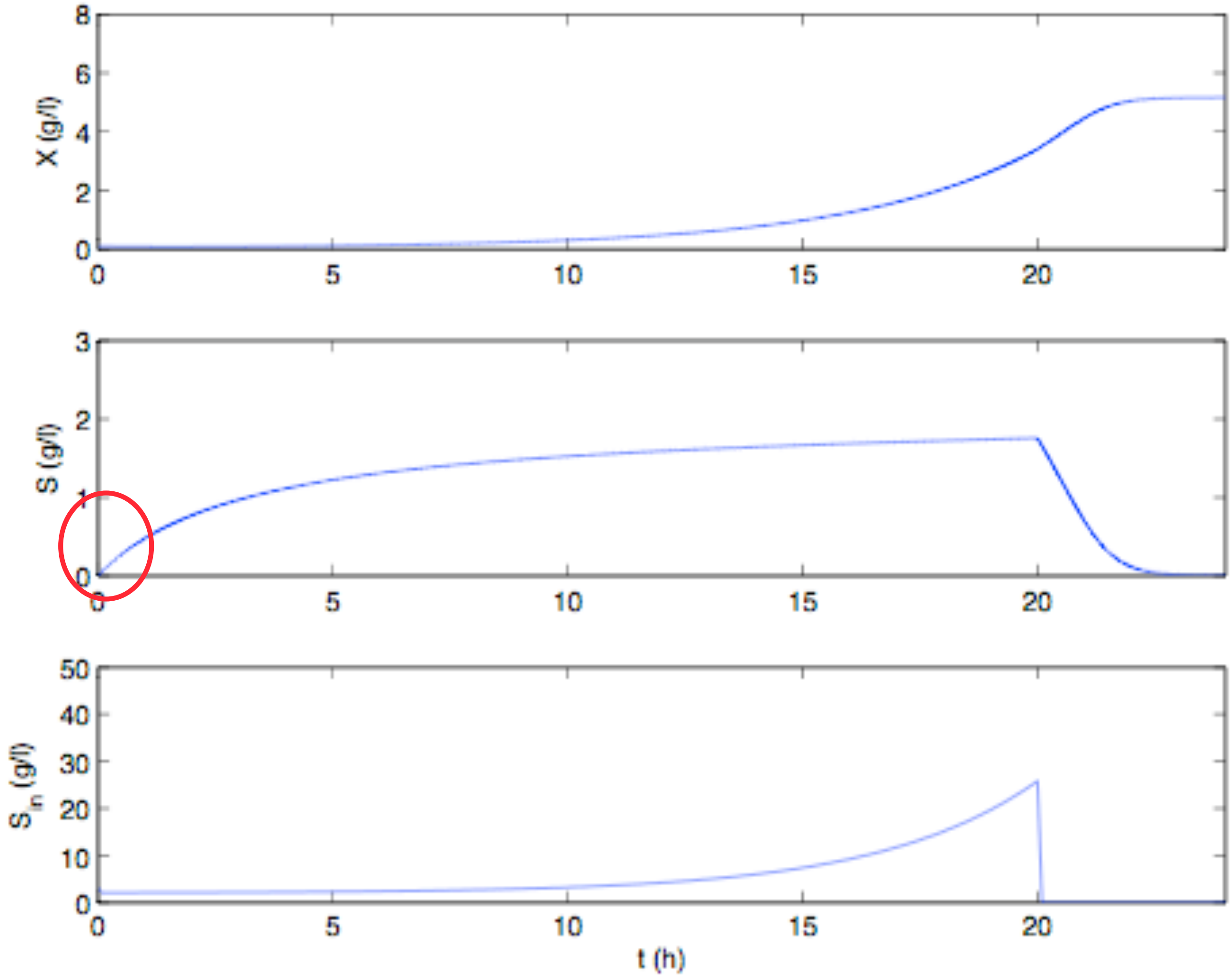
$$S_{in,opt} = \sqrt{K_S K_I} + \frac{V(t)}{q} k_1 \frac{\mu_0 X(t)}{1 + 2\sqrt{\frac{K_S}{K_I}}}$$

and : $$V(t)X(t) = V(0)X(0)e^{\mu_{max} t} \text{ with } \mu_{max} = \frac{\mu_0}{1 + 2\sqrt{\frac{K_S}{K_I}}}$$

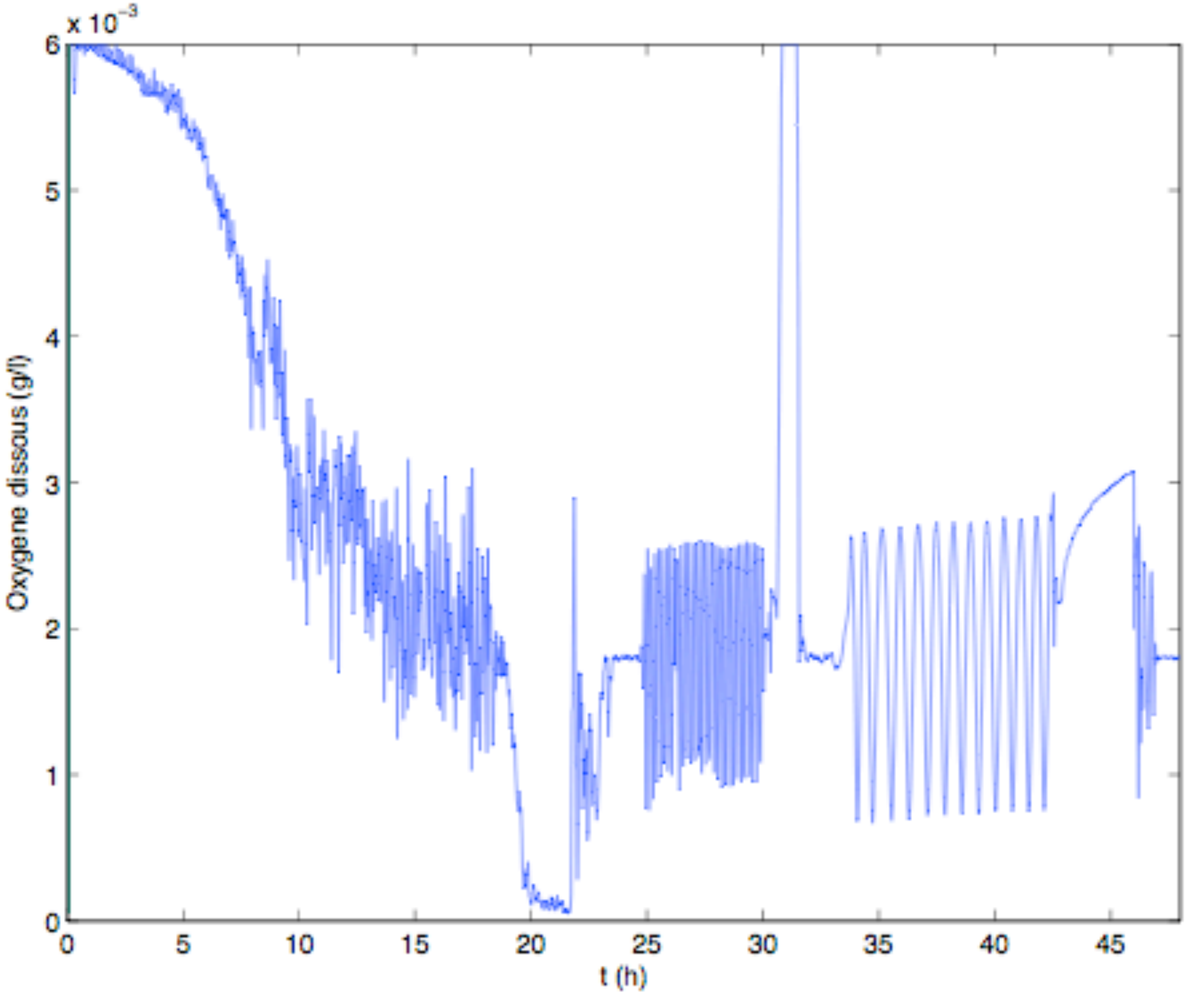
exponential growth



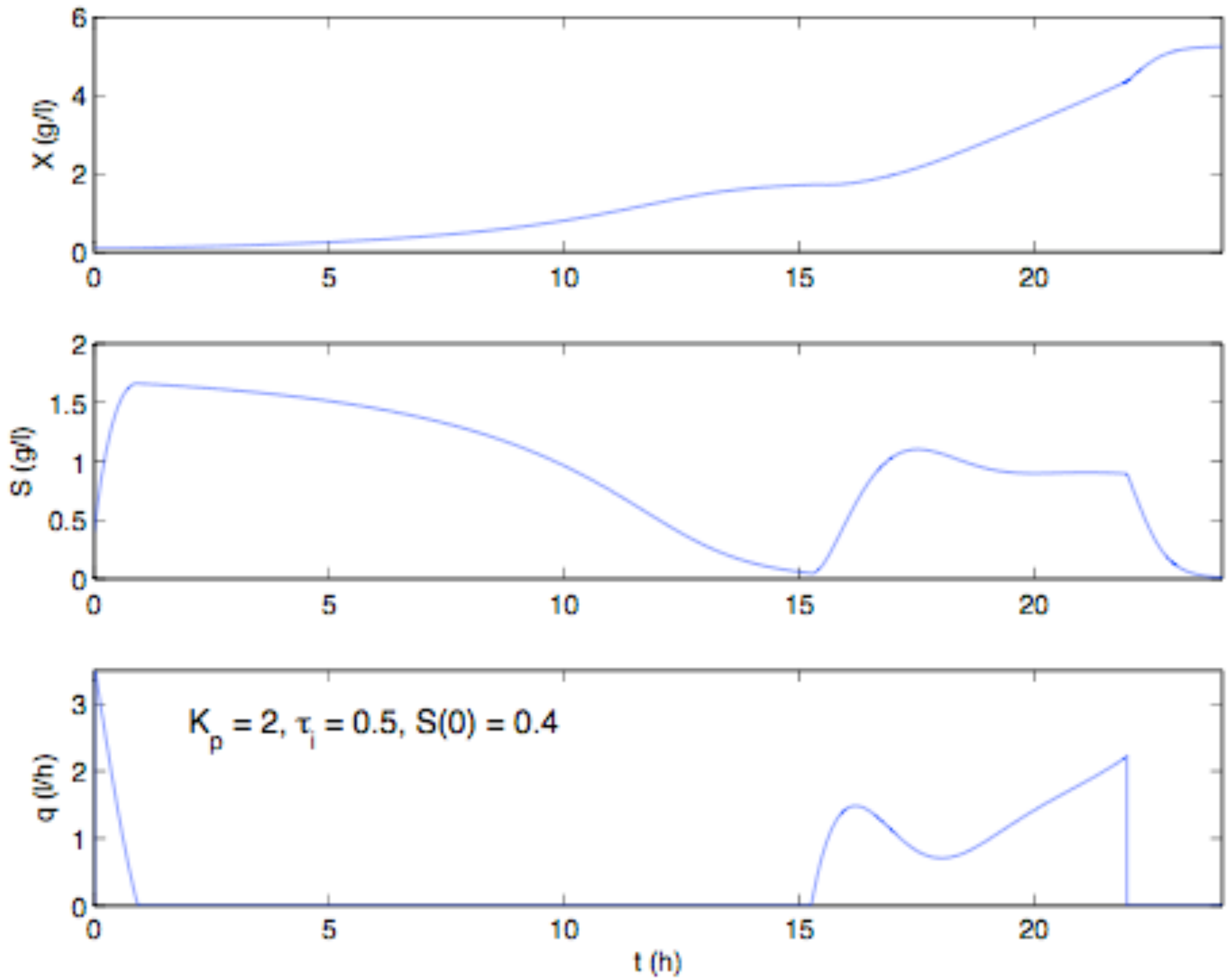
V = Vmax
X (g/l)
S (g/l)
Sin (g/l)
t (h)


X (g/l)
S (g/l)
S_{in} (g/l)
t (h)
0
5
10
15
20
0
2
4
6
8
0
1
2
3
0
10
20
30
40
50

Industrial application of a PI regulator for the control of oxygen in a fedbatch process



PI regulator : a numerical simulation



The proportional gain should contain an exponential term

Closed-loop dynamics of S with an exponential growth :

$$\frac{dS}{dt} = \frac{1}{V}\Big(-k_1\mu V(0)X(0)e^{\mu t} + K_P(S_{in}-S)(S^*-S)$$
$$K_I(S_{in}-S)\int_0^t (S^*-S)d\tau\Big)$$

--> $K_p = K_{p1}\, e^{\mu t}$

to “compensate” the exponential growth term

NB : no exponential term on the integral action

PI with exponential term