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Modelling and control of mass balance systems

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MODELLING AND CONTROL OF MASS BALANCE SYSTEMS

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1. Mass Balance Systems
2. Positivity condition
3. Law of mass conservation
4. Representations : Hamiltonian, Compartmental, stoichiometric
5. Examples
6. Open loop stability
7. Inflow controlled systems
8. A robust control design problem
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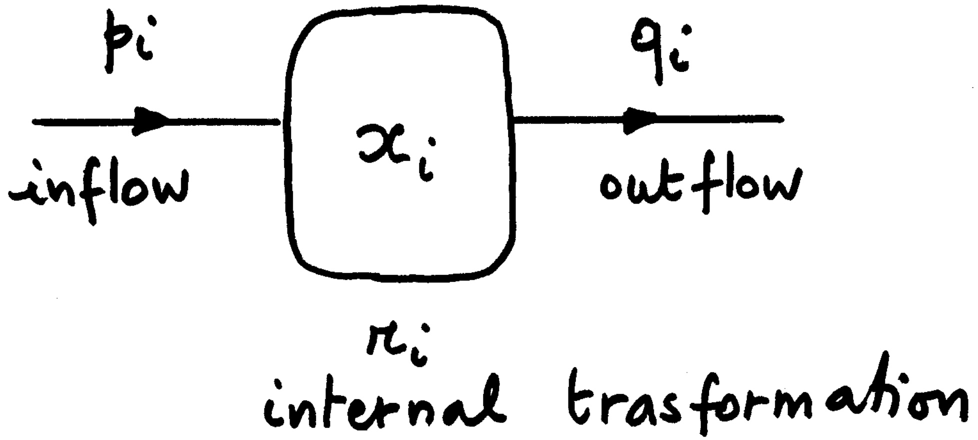
Mass balance systems

state variable $\quad x_i$ = amount of material



$\boxed{i = 1, \dots, n}$

mass balance $\quad \dot{x}_i = r_i - q_i + p_i$

$$\boxed{\text{mass balance equations}} \equiv \boxed{\text{state space model}} \equiv \boxed{\text{natural behav. model}}$$

$$\dot{x} = r(x,u) - q(x,u) + p(x,u)$$

	transformations	outflows	inflows
Physical	grinding	withdrawal	raw material
Chemical	reaction	excretion	reactants, nutrient
Biological	predation	mortality	immigration, birth

$$\dot{x} = r(x,u) - q(x,u) + p(x,u)$$

<u>control</u>
<u>input</u> $u(t)$ = manipulation of the rates by an external operator

$$u(t) \geq 0$$

Physical meaning $\Longrightarrow$

- <u>Positivity conditions</u>
- <u>Law of mass conservation</u>

$$\dot{x} = r(x,u) - q(x,u) + p(x,u)$$

Positivity condition

$$\boxed{\left.\begin{array}{l} x(0) \geq 0 \\ u(t) \geq 0 \quad \forall t \end{array}\right\} \Rightarrow \quad x(t) \geq 0 \quad \forall t}$$

1) $\left.\begin{array}{l} r(x,u) \\ q(x,u) \\ p(x,u) \end{array}\right\} : R_+^n \times R_+^m \longrightarrow R_+^n$, differentiable

(non negative orthant)

2) If $x_i = 0$, then $r_i(x,u) \geq 0$

3) If $x_i = 0$, then $q_i(x,u) = 0$

$$\dot{x} = r(x,u) - q(x,u) + p(x,u)$$

Law of mass conservation

Total mass in the system : $M(x) = \sum_{i=1}^{n} x_i$

Closed system = no inflows/outflows

$$\dot{x} = r(x,u)$$

$\boxed{\text{Mass Conservation}} \Longrightarrow \frac{dM(x)}{dt} = 0 \Longrightarrow \boxed{\sum_{i=1}^{n} r_i(x,u) = 0}$

$$\dot{x} = r(x,u)\left(-q(x,u) + p(x,u)\right)$$

Mass conservation condition

$$\sum_{i=1}^{n} r_i(x,u) = 0 \quad \Longrightarrow \quad \boxed{r_i(x,u) = \sum_{j\neq i} r_{ji}(x,u) - \sum_{j\neq i} r_{ij}(x,u)}$$

r_{ij} : non negative and differentiable

$$\Downarrow$$

Total mass

$$M(x) = \sum_{i=1}^{n} x_i \quad \Longrightarrow \quad \boxed{r(x,u) = F(x,u)\frac{\partial M}{\partial x}}$$

Hamiltonian representation

antisymmetric $F(x,u) = -F^T(x,u)$

$$f_{ij}(x,u) = r_{ji}(x,u) - r_{ij}(x,u)$$

$$\dot{x} = r(x,u) - q(x,u) + p(x,u)$$

Another structural property

Positivity condition $\Longrightarrow$ $\boxed{r(x,u) - q(x,u) = G(x,u)\,x}$

$$\boxed{\begin{aligned} q_i(x,u) &= x_i\, \tilde{q}_i(x,u) \\ r_{ij}(x,u) &= x_i\, \tilde{r}_{ij}(x,u) \end{aligned}}$$

$$g_{ii}(x,u) = -\tilde{q}_i(x,u) - \sum_{j \neq i} \tilde{r}_{ij}(x,u) \leq 0$$

$$g_{ij}(x,u) = \tilde{r}_{ji}(x,u) \geq 0$$

$G(x,u)$ is a <u>compartmental</u> matrix

- Metzler matrix ($g_{ij} \geq 0 \quad \forall j \neq i$)
- $g_{ii} \leq 0$
- diagonally dominant

$$\dot{x} = r(x,u) - q(x,u) + p(x,u)$$

$\boxed{\text{Mass conservation}}$ $\Longrightarrow$ $$r(x,u) - q(x,u) \equiv \big[\underbrace{\underbrace{F(x,u)}_{\substack{\text{antisymmetric} \\ F(x,u) = -F^T(x,u)}} - \underbrace{D(x,u)}_{\substack{\text{diagonal} \\ \text{(dissipation)}}}}_{\text{Hamiltonian Representation}}\big]\frac{\partial M}{\partial x}$$

Total mass $M(x) = \sum_i x_i$

$\boxed{\text{Positivity}}$ $\Longrightarrow$ $$r(x,u) - q(x,u) \equiv \underbrace{G(x,u)}_{\text{compartmental matrix}}\, x$$

- Metzler $g_{ij} \geq 0 \quad \forall j \neq i$
- $g_{ii} \leq 0$
- diagonally dominant

$$\dot{x} = r(x,u)\left(-q(x,u) + p(x,u)\right)$$

Stoichiometric representation

$$r_i(x,u) = \sum_{j=1}^{s} c_{ij}\, \underbrace{\rho_j(x,u)}_{\text{positive and differentiable}} \qquad s < n$$

$$\boxed{r(x,u) = C\rho(x,u)}$$

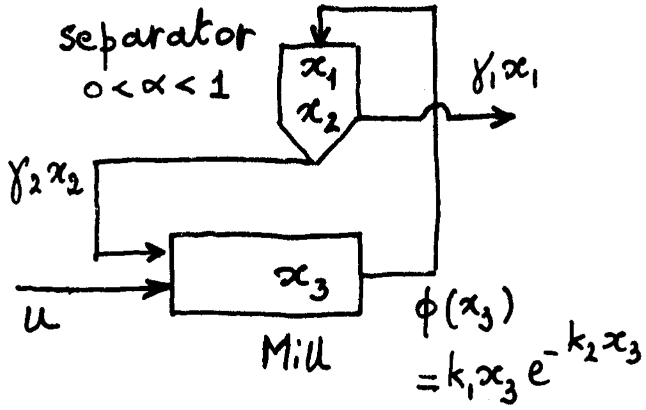
$C = [c_{ij}]$ = stoichiometric matrix

$\rho(x,u) = (\rho_1(x,u), \ldots, \rho_s(x,u))$

Property :

$$\sum_{i=1}^{n} c_{ij} = 0 \quad \Longrightarrow \quad \sum_i r_i(x,u) = 0 \quad \text{Mass conservation}$$

Example 1. A grinding process



$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix} = \underbrace{\begin{pmatrix} (1-\alpha)\,\phi(x_3) \\ \alpha\,\phi(x_3) - \gamma_2 x_2 \\ \gamma_2 x_2 - \phi(x_3) \end{pmatrix}}_{r(x,u)} - \underbrace{\begin{pmatrix} \gamma_1 x_1 \\ 0 \\ 0 \end{pmatrix}}_{q(x,u)} + \underbrace{\begin{pmatrix} 0 \\ 0 \\ u \end{pmatrix}}_{p(x,u)}$$

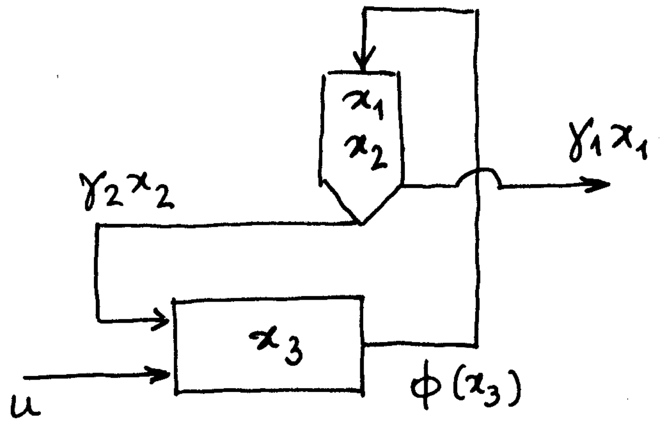
$$F(x,u) = \begin{pmatrix} 0 & 0 & (1-\alpha)\,\phi(x_3) \\ 0 & 0 & -\gamma_2 x_2 + \alpha\,\phi(x_3) \\ -(1-\alpha)\,\phi(x_3) & \gamma_2 x_2 - \alpha\phi(x_3) & 0 \end{pmatrix}$$

Hamiltonian

$$G(x,u) = \begin{pmatrix} -\gamma_1 & 0 & (1-\alpha)k_1 e^{-k_2 x_3} \\ 0 & -\gamma_2 & \alpha k_1 e^{-k_2 x_3} \\ 0 & \gamma_2 & -k_1 e^{-k_2 x_3} \end{pmatrix}$$

antisymmetric

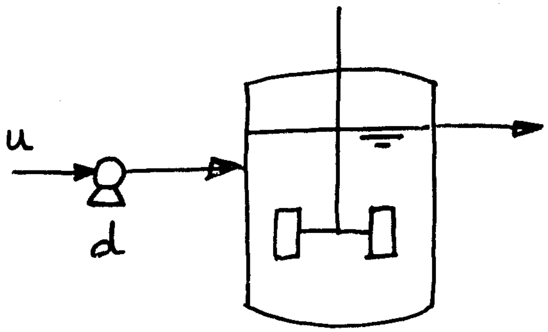
compartmental



$$\begin{pmatrix}\dot x_1\\ \dot x_2\\ \dot x_3\end{pmatrix} = \underbrace{\begin{pmatrix}1-\alpha & 0\\ +\alpha & -1\\ -1 & +1\end{pmatrix}}_{\text{stoichiometric matrix}} \underbrace{\begin{pmatrix}\phi(x_3)\\ \gamma_2 x_2\end{pmatrix}}_{\rho(x)} - \begin{pmatrix}\gamma_1 x_1\\ 0\\ 0\end{pmatrix} + \begin{pmatrix}0\\ 0\\ u\end{pmatrix}$$

$$\sum_i c_{ij} = 0 \quad !$$

Example 2. A depollution process



x_1 = biomass
x_2 = degraded org. matter
x_3 = organic pollutant
u = influent pollut. conc.
d = volumetric flow rate

Hydrolysis: $X_3 \xrightarrow[X_1]{} X_2$

Bact. Growth: $X_2 \xrightarrow[X_1]{} X_1$

(mass action kinetics)

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix} = \underbrace{\begin{pmatrix} \mu_1 x_1 x_2 \\ -\mu_1 x_1 x_2 + \mu_2 x_1 x_3 \\ -\mu_2 x_1 x_3 \end{pmatrix}}_{r(x,u)} - \underbrace{\begin{pmatrix} d x_1 \\ d x_2 \\ d x_3 \end{pmatrix}}_{q(x,u)} + \underbrace{\begin{pmatrix} 0 \\ 0 \\ du \end{pmatrix}}_{p(x,u)}$$

$$\underset{\text{Hamiltonian}}{F(x,u)} = \begin{pmatrix} 0 & \mu_1 x_1 x_2 & 0 \\ -\mu_1 x_1 x_2 & 0 & \mu_2 x_1 x_3 \\ 0 & -\mu_2 x_1 x_3 & 0 \end{pmatrix}$$

antisymmetric

$$\underset{\text{stoichiometric}}{\begin{pmatrix} 1 & 0 \\ -1 & +1 \\ 0 & -1 \end{pmatrix}} \begin{pmatrix} \mu_1 x_1 x_2 \\ \mu_2 x_1 x_3 \end{pmatrix}$$

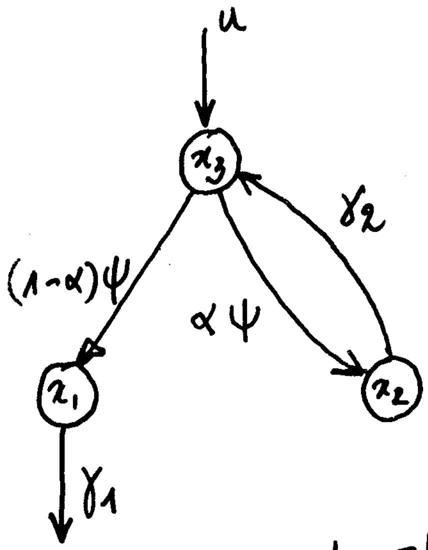
$$G(x,u) = \begin{pmatrix} -d & \mu_1 x_1 & 0 \\ 0 & -d-\mu_1 x_1 & \mu_2 x_1 \\ 0 & 0 & -d-\mu_2 x_1 \end{pmatrix}$$

compartmental

Why compartmental ?

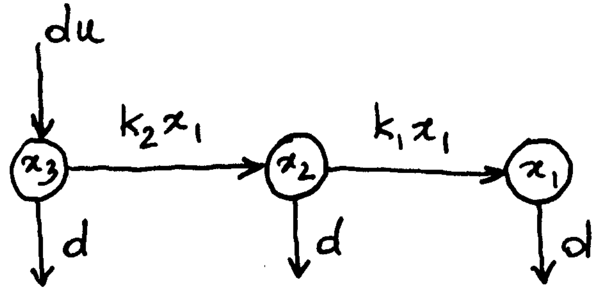
Network of conceptual reservoirs called <u>compartments</u>

Labels of arcs = entries of $G(x)$



$$\psi = k_1 e^{-k_2 x_3}$$

Grinding process



Depollution process.

$$\dot{x} = r(x,u) - q(x,u) + p(x,u)$$

Special case : linear inflows/outflows

$$\underset{\text{outflows}}{q(x,u)} = \begin{pmatrix} a_1 x_1 \\ a_2 x_2 \\ \vdots \\ a_n x_n \end{pmatrix} \qquad \underset{\text{inflows}}{p(x,u)} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ u \end{pmatrix}$$

single input

$$\dot{x} = r(x) - \underbrace{A}_{\mathrm{diag}\{a_i\}} x + \underbrace{b}_{\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}} u$$

$$\boxed{\text{o.k for both examples}}$$

Open loop stability $\quad u(t) = \bar{u}$ = constant > 0

- Equilibrium in the positive orthant $\bar{x}$?
- Globally asymptotically stable ?

1) State affine mass balance systems

$$\dot{x} = \underbrace{G(\bar{u})}_{\text{compartmental matrix}} x + b\bar{u}$$

$G(\bar{u})$ Hurwitz

(= fully "outflow connected")

$\Rightarrow$ single GAS equilibrium

$$\dot{x} = r(x) - Ax + bu$$

2) Conservative Lotka-Volterra systems

$$\dot{x}_i = \left(-a_i + \sum_j p_{ij}\, x_j\right) x_i \qquad i = 1, \dots, n-1$$

$$\dot{x}_n = \left(-a_n + \sum_j p_{nj}\, x_j\right) x_n + \bar{u}$$

$$r(x) = F(x)\frac{\partial M}{\partial x} \qquad \text{Hamiltonian representation}$$

$$\downarrow$$

$$f_{ij}(x) = p_{ij}\, x_i x_j \qquad P = [p_{ij}] \text{ antisymmetric}$$

Lyapunov function $\quad V(x) = \sum_i x_i - \bar{x}_i \ln x_i$

$$\dot{V}(x) = \underbrace{(x-\bar{x})^T P (x-\bar{x})}_{=0} - \frac{\bar{u}\,\bar{x}_n}{x_n}\left(1 - \frac{x_n}{\bar{x}_n}\right)^2$$

$\Longrightarrow$ single GAS equilibrium

$$\dot{x} = r(x) - Ax + bu$$

3) Simplified Rosenbrock's Theorem (Automatica 1962)

- $\left(\frac{\partial r}{\partial x} - A\right)$ is a compartmental matrix in the pos. orthant.
- bounded state
- Lyapunov function $V = \sum_i |\dot{x}_i|$

4) Gouzé's Theorem (ECC 97)

- Hamiltonian viewpoint $r_i(x) = \sum_j [r_{ji} - r_{ij}]$ $\quad r_{ij}(\underline{\underline{x_i}})$
- $[r_{ij}(x_i) - r_{ij}(\bar{x}_i)](x_i - \bar{x}_i) \geq 0 \quad \forall x_i \geq 0$
- Lyapunov function $V = \sum_i |x_i - \bar{x}_i|$

$\Longrightarrow$ single GAS equilibrium

$$\dot{x} = r(x) - Ax + B\bar{u}$$

Open loop stability analysis : $u(t) = \bar{u} = \text{constant} > 0$

- Single equilibrium, globally asymptotically stable in the positive orthant $\bar{x} > 0$?

• Lotka-Volterra conservative systems	Hamiltonian matrix $F(x)$ bilinear	$V = \sum_i (x_i - \bar{x}_i \ln x_i)$
• Rosenbrock (1962)	$(\frac{\partial r}{\partial x} - A)$ Jacobian compartmental matrix	$V = \sum_i \lvert \dot{x}_i \rvert$
• Gouzé (ECC 97)	$r_{ij}(x_i)$ non monotonic	$V = \sum_i \lvert x_i - \bar{x}_i \rvert$

System without inflows

$$\dot{x} = r(x) - Ax + \cancel{bu}$$

Assumption $\quad r(x) - Ax = G(x)\,x$

$\downarrow$

The compartmental matrix $G(x)$ is "fully outflow connected"

$\Rightarrow$ $x = 0$ is the single GAS equilibrium of the unforced system $\dot{x} = r(x) - Ax$

Lyap. f.

$\uparrow$

Physical meaning: without inflows, the total mass $M(x)$ decreases $\longrightarrow 0$ = dissipativity = natural wash-out

$\boxed{\text{o.k. for both examples}}$

$$\dot{x} = r(x) - Ax + bu$$

Bounded input / Bounded state

State bounded $\Longleftrightarrow$ Total mass bounded

$0 \leq u(t) \leq u^{max}$

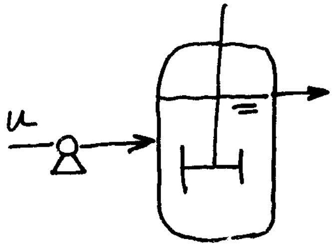
$$\frac{dM}{dt} = -\sum_i a_i x_i + \left(\sum_i b_i\right) u$$

- if $a_i > 0 \quad \forall i$

- then
  1) bounded state
  2) simplex $\Delta = \left\{ x \in R^n_+ : M(x) \leq \dfrac{(\sum_i b_i) u^{max}}{\min_i (a_i)} \right\}$ invariant

Open loop stability : Multiple equilibria.

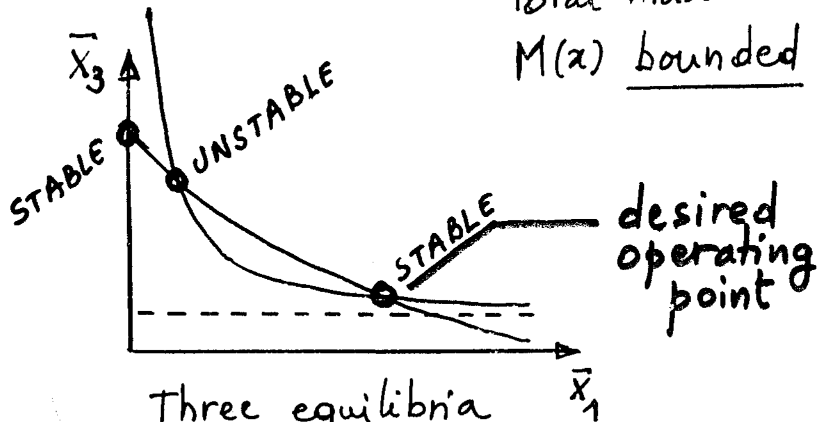
Depollution process BIBS



$$\dot{x}_1 = \mu_1 x_1 x_2 - d x_1$$

$$\dot{x}_2 = -\mu_1 x_1 x_2 + \mu_2 x_1 x_3 - d x_2$$

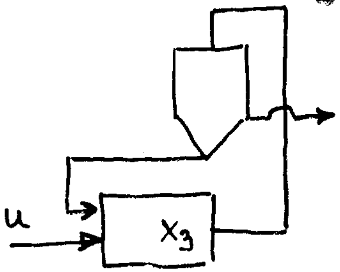
$$\dot{x}_3 = -\mu_2 x_1 x_3 - d x_3 + \bar{u}$$



Three equilibria

Total mass $M(x)$ bounded

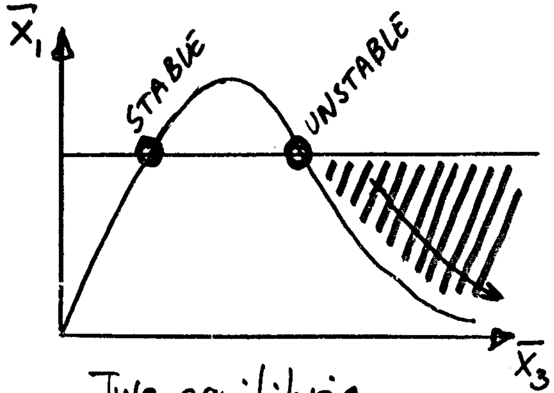
Grinding process BIUS



$$\dot{x}_1 = (1-\alpha)\,\phi(x_3) - \gamma_1 x_1$$

$$\dot{x}_2 = \alpha\,\phi(x_3) - \gamma_2 x_2$$

$$\dot{x}_3 = \gamma_2 x_2 - \phi(x_3) + \bar{u}$$



Two equilibria

$M(x)$ may be unbounded!

Plugging!

Grinding process : the instability set

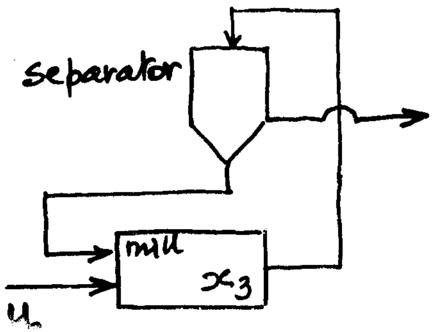
$$(1-\alpha)\,\phi(x_3) < \gamma_1 x_1 < \bar{u}$$

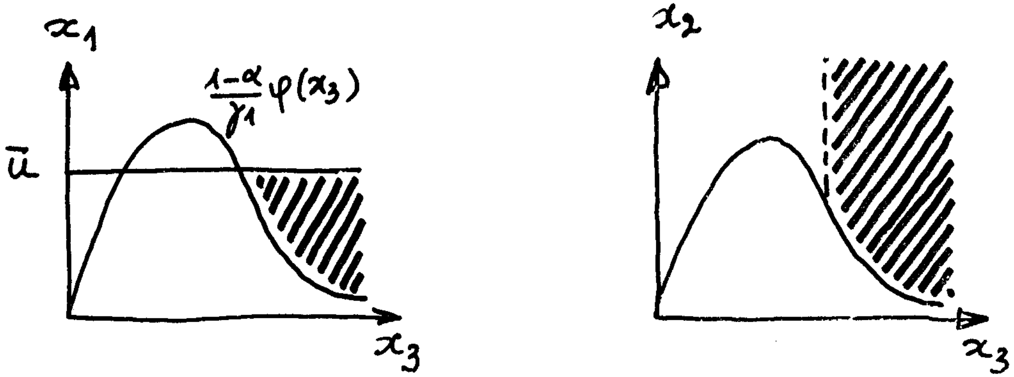
$$\alpha\,\phi(x_3) < \gamma_2 x_2$$

$$\partial\phi/\partial x_3 < 0$$

Example : Instability of industrial grinding process.

"Plugging Phenomenon"



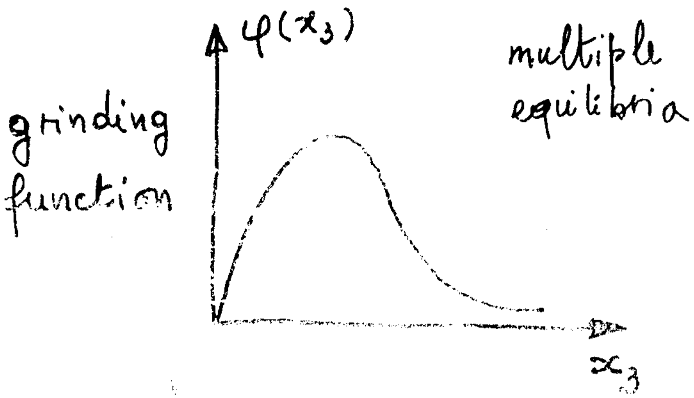


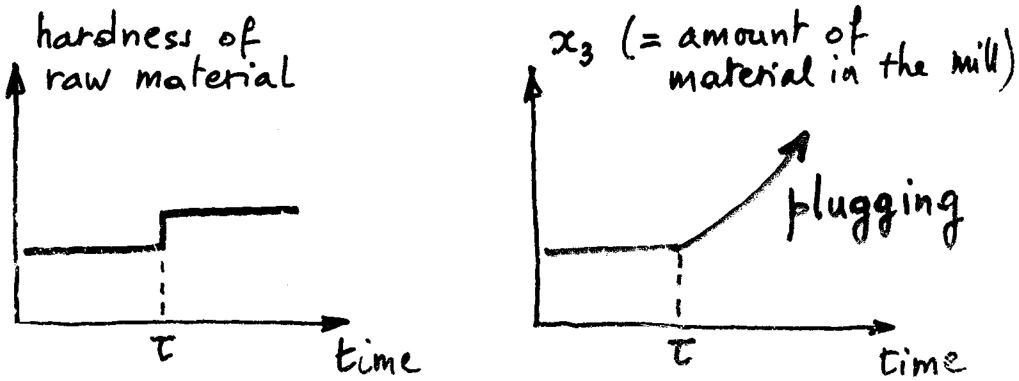
The instability invariant set

$$\dot{x}_1 = -\gamma_1 x_1 + (1-\alpha)\,\varphi(x_3)$$

$$\dot{x}_2 = -\gamma_2 x_2 + \alpha\,\varphi(x_3)$$

$$\dot{x}_3 = \gamma_2 x_2 - \varphi(x_3) + u$$





The unstable behaviour

Engineering problem

Intermittent disturbances } may induce **undesirable behaviour**

↓ ↓

Toxic matter in the depollution process	⇒	convergence to wash out equilibrium
Change of hardness of raw material in the grinding proc.	⇒	plugging = unbounded accumulation of material in the mill

$$\dot{x} = r(x) - Ax + bu$$

(multiple equilibria)

To prevent the process from undesirable behaviour

$\boxed{\rightarrow \text{Feedback control?}}$

- positive and bounded $0 \leq u \leq u_{max}$
- single GAS equilibrium (= the "good" operating point)
- robust against uncertainty $r(x)$

CASE I : BIUS Robust stabilisation of the total mass

CASE II : BIBS Output regulation of an initial compartment

$$\dot{x} = r(x) - Ax + bu$$

CASE I : BIUS systems

Problem : risk of unbounded accumulation of material in the system (Plugging)

Solution : stabilise (by state feedback) the total mass $M(x)$ at a set point M^*

Robust Control law

$$\tilde{u}(x) = \sum_i a_i x_i + \lambda \left[M^* - M(x) \right]$$

$$u(x) = \max\left(0, \tilde{u}(x)\right) \geq 0$$

system fully outflow connected $\Longrightarrow$ bounded state and $M(x) \longrightarrow M^*$

Application to the grinding process

$$\dot{x}_1 = (1-\alpha)\,\phi(x_3) - \gamma_1 x_1$$

$$\dot{x}_2 = \alpha\,\phi(x_3) - \gamma_2 x_2$$

$$\dot{x}_3 = \gamma_2 x_2 - \phi(x_3) + u$$

Control law

$$u(x) = \max\left[0,\ \lambda M^* + (\gamma_1 - \lambda)x_1 - \lambda x_2 - \lambda x_3\right]$$

Closed loop analysis

Closed loop system has a single GAS equilibrium in the positive orthant if:

$$\frac{\partial \phi}{\partial x_3} > - \frac{\gamma_1 \gamma_2}{\alpha \gamma_1 + (1-\alpha)\gamma_2}$$

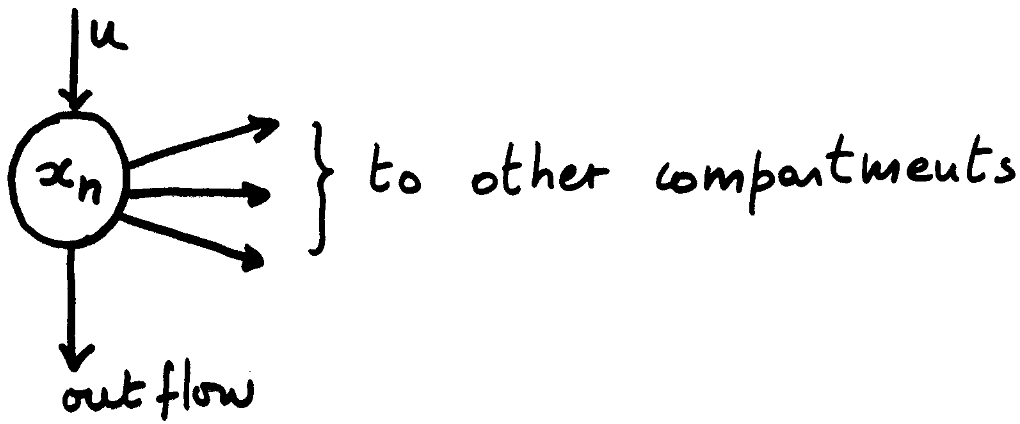
The proposed controller achieves the control objective.

CASE II . BIBS Systems

- **Problem** : avoid undesirable attracting equilibria

- **Solution** : Regulate some output at a set point y^* which uniquely assigns the equilibrium

- **Special case** : output $y = x_n$ = "initial" compartment



$$\left.\begin{aligned}
\dot{x}_1 &= r_1(x) - a_1 x_1 \\
\dot{x}_2 &= r_2(x) - a_2 x_2 \\
&\;\vdots \\
\dot{x}_{n-1} &= r_{n-1}(x) - a_{n-1} x_{n-1}
\end{aligned}\right\} \quad \dot{z} = \psi(z,y) \quad = \begin{cases} \text{Compartmental system with input } y \\ \text{zero dynamics} \end{cases}$$

$$\dot{x}_n = r_n(x) - a_n x_n + u \longrightarrow \dot{y} = -(\underbrace{\phi(z,y) + a_n}_{>0})\, y + u$$

A control law

$$u = (\underbrace{\phi(z,y) + a_n}_{>0})\left[(1-\lambda)\, y + \lambda y^*\right] \quad \text{positive!}$$

set point

$$0 < \lambda < 1$$

Closed loop

$$\dot{z} = \psi(z,y)$$

$$\dot{y} = -(\phi(z,y) + a_n)\, \lambda\, (y^* - y) \qquad y \rightarrow y^*$$

Mass balance systems in stirred tanks.

Special case : single control u = volumetric flow rate

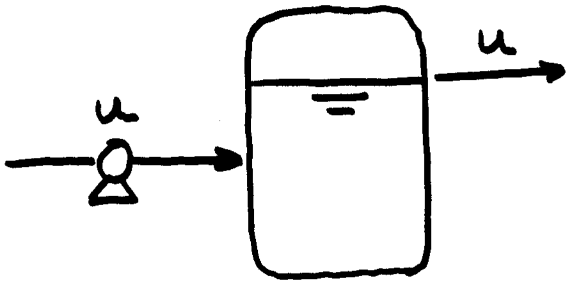
$$\dot{x} = r(x,u) - q(x,u) + p(x,u)$$

$$\swarrow \qquad\qquad \downarrow \qquad\qquad \searrow$$

independent of u	bilinear	linear
$r_i(x)$	$q_i = u x_i$	$p_i = u b_i$

$$\boxed{\begin{array}{ll} \text{General form :} & \dot{x} = r(x) + u(b-x) \\ \text{Stoichiometric form :} & \dot{x} = C\rho(x) + u(b-x) \end{array}}$$

Example : Depollution process



Exchange : $d \longrightarrow u$

$u \longrightarrow b$

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \mu_1 x_1 x_2 \\ \mu_2 x_1 x_3 \end{pmatrix} + u \begin{pmatrix} -x_1 \\ -x_2 \\ b - x_3 \end{pmatrix}$$

Obviously : exactly the same open loop equilibria !

State boundedness.

$$\dot{x} = r(x) + u(b - x) \qquad u(t) \geq 0$$

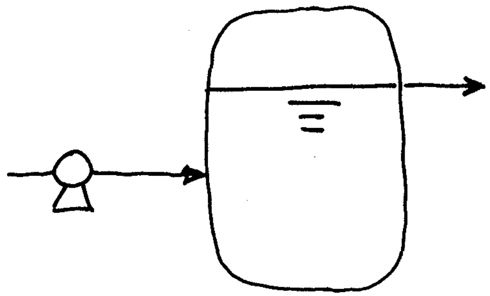
- Dynamics of the total mass : $\frac{d}{dt} M(x) = u\left(\sum_i b_i - M(x)\right)$

- $M(x)$ bounded $\Rightarrow$ x bounded independently of u !

- The simplex $\Delta = \{ x \in R^n_+ : \sum_i x_i \leq \sum_i b_i \}$ is forward invariant (also int Δ)

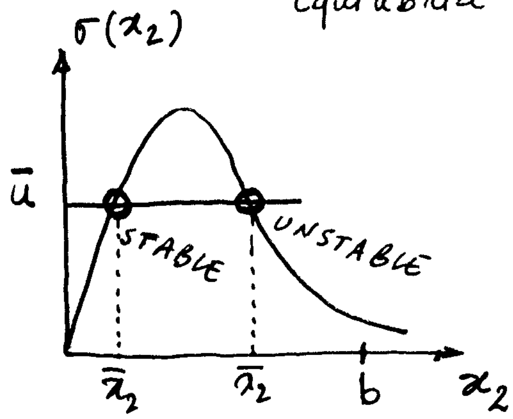
- If $u(t) \geq \varepsilon > 0 \ \forall t$, then $M(x) \longrightarrow \sum_i b_i$

A simple example of Lyapunov control design



$$\begin{cases} \dot{x}_1 = x_1 \sigma(x_2) - u x_1 \\ \dot{x}_2 = -x_1 \sigma(x_2) + u(b - x_2) \end{cases}$$

Equilibria



$$\bar{x}_1 = b - \bar{x}_2$$

Stabilization set point x_1^*

Control law $\quad u = \sigma(x_2)\left(1 - \lambda x_1^* + \lambda x_1\right)$

$$0 < \lambda x_1^* < 1 \Rightarrow u \text{ positive!}$$

Lyapunov function $\quad V = \frac{1}{2}(x_1^* - x_1)^2 + \frac{1}{2}\left(b - (x_1 + x_2)\right)^2$

$$\Rightarrow \dot{V} = -\lambda \sigma(x_2)(x_1^* - x_1)^2 - \sigma(x_2)(1 - \lambda x_1^* + \lambda x_1)\left(b - (x_1 + x_2)\right)^2$$

< 0 along the trajectories

Conclusions.

- Positivity and mass conservation conditions are explicitely used
  - → in control design
  - → in stability analysis

- Dissipativity of the unforced system may also be critical in inflow controlled systems – Otherwise no hope to stabilise the total mass at an <u>arbitrary</u> set point