Mathematical Modelling and Analysis
Volume 11 Number 2, 2006, pages 149–160
© 2006 Technika ISSN 1392-6292 print, ISSN 1648-3510 online

IDENTIFICATION OF A NONLINEAR POLYNOMIAL COMPARTMENTAL SYSTEM OF $(\alpha+\beta)$ ORDER BY A LINEARIZATION METHOD

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Received March 9, 2005; revised April 19, 2006; published online May 25, 2006

Abstract. A linearization method is used for identifying a nonlinear polynomial compartmental system of $(\alpha+\beta)$ order. We bring back the nonlinear model to a linear one for which a method, developed for Michaelis-Menten systems in a previous paper, can be used.
Key words: Problem inverse, linear compartimental system, nonlinear compartmental system, identification, ordinary differential equation

1. Introduction

In general the compartimental systems are used in fields very varied such as medicine, biology, the chemistry. or the dynamics of the populations. Recently, Gian Italo Bischi [1] gave an application to the economic systems. The nonlinear systems occur particularly in dynamics of the populations. These systems are governed by the following law: "*the flow from compartment i to compartment j is proportional to the expression $x_i^\alpha x_j^\beta$*" ($\beta = 0$ if j designates the system's outside) (see [2, 3, 4]). The proportionality parameters k_{ij} denote the exchange parameters, α and β are positive constants characterizing the compartmental system, and $x_i(t)$ designates the quantity in compartment i at time t. These k_{ij} characterize the exchanges between compartments. This law is said of $(\alpha+\beta)$ order.

Our aim is to study an inverse problem consisting in identifying the exchange parameters k_{ij}. As for Michaelis-Menten systems (see [7]) a linearization method is used. The linear model obtained in the neighbourhood of the initial condition $(a, 0)$ gives a bad interpretation of the physical phenomenon. A " **temporization"** is necessary for obtaining an exact interpretation of the phenomenon. Furthermore the nonhomogeneity problem due to the initial condition encountered in Michaelis-Menten systems implies that the deduced linear system is not always real. The measures given by the practitioners will be used in association with a temporization technique allowing to adapt the results obtained for identification in linear compartmental systems.

2. Definitions and Notations

We consider the nonlinear bicompartmental system of polynomial type, namely (S_{NL}), shown in Figure 1.

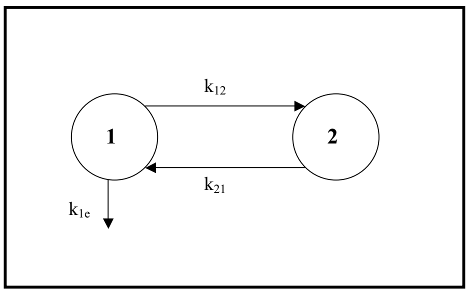

Figure 1. (S_{NL}): Nonlinear bicompartmental system.

The mass balance principle in each compartment leads to a nonlinear differential equations (see [2]). The identification is done by exciting the system with an instantaneous injection of substance quantity a in the compartment 1. Thus we can say that the compartmental system is governed by the following differential system with initial conditions :

$$\begin{cases} x_1^{'}(t) = k_{21} x_2^{\alpha}(t) x_1^{\beta}(t) - k_{12} x_1^{\alpha}(t) x_2^{\beta}(t) - k_{1e} x_1^{\alpha}(t), \\ x_2^{'}(t) = k_{12} x_1^{\alpha}(t) x_2^{\beta}(t) - k_{21} x_2^{\alpha}(t) x_1^{\beta}(t), \\ x_1(0) = a, \quad x_2(0) = 0. \end{cases} \tag{2.1}$$

Let us set:

$$X : [0, +\infty[\longrightarrow \mathbb{R}^2,$$
$$t \longrightarrow X^T(t) = \big(x_1(t), x_2(t)\big)$$

the state function associated to compartmental system (S_{NL}), and

$$F : \mathbb{R}^2 \longrightarrow \mathbb{R}^2,$$
$$(x_1, x_2) \longrightarrow F(x_1, x_2) = (f_1(x_1, x_2), \ f_2(x_1, x_2))$$

the vectorial function defined by :

$$\begin{cases} f_1(x_1,x_2) = k_{21}x_2^{\alpha}x_1^{\beta} - k_{12}x_1^{\alpha}x_2^{\beta} - k_{1e}x_1^{\alpha}, \\ f_2(x_1,x_2) = k_{12}x_1^{\alpha}x_2^{\beta} - k_{21}x_2^{\alpha}x_1^{\beta}. \end{cases}$$

With these notations we can write the differential system (2.1) under the vectorial form :

$$\begin{cases} X'(t) = F(X(t)), \\ X(0) = \begin{pmatrix} a \\ 0 \end{pmatrix}. \end{cases} \tag{2.2}$$

3. Linearization of the Differential System

The partial derivatives of the function F are defined as follows:

$$\frac{\partial f_1}{\partial x_1}(x_1,x_2) = \beta k_{21}x_2^{\alpha}x_1^{\beta-1} - \alpha k_{12}x_1^{\alpha-1}x_2^{\beta} - \alpha k_{1e}x_1^{\alpha-1}k_{1e}x_1^{\alpha},$$

$$\frac{\partial f_1}{\partial x_2}(x_1,x_2) = \alpha k_{21}x_2^{\alpha-1}x_1^{\beta} - \beta k_{12}x_1^{\alpha}x_2^{\beta-1},$$

$$\frac{\partial f_2}{\partial x_1}(x_1,x_2) = \alpha k_{12}x_1^{\alpha-1}x_2^{\beta} - \beta k_{21}x_2^{\alpha}x_1^{\beta-1},$$

$$\frac{\partial f_2}{\partial x_2}(x_1,x_2) = \beta k_{12}x_1^{\alpha}x_2^{\beta-1} - \alpha k_{21}x_2^{\alpha-1}x_1^{\beta}.$$

The function F is differentiable in all point (x_1,x_2) such that $x_1 \neq 0$ and $x_2 \neq 0$ for all $\alpha > 0$ and all $beta > 0$, and the Jacobian matrix is given by:

$$(DF)_{(x_1,x_2)} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{pmatrix}.$$

For linearizing the system (2.2) we apply the Taylor formula in the neighbourhood of the initial condition $(a,0)$. Furthermore:

$i)$ F is not differentiable in $(a,0)$ if $\alpha < 1$ or $\beta < 1$.

$ii)$ If $\alpha \geq 1$ and $\beta \geq 1$ F is differentiable in $(a,0)$. The Taylor formula applied in neighbourhood of $(a,0)$ leads to:

$$X'(t) = F^T(a,0) + (DF)_{(a,0)}(x_1 - a, 0)^T$$
$$+ \frac{1}{2}\left(D^2F\right)(a + \theta(x_1 - a), \theta x_2)\left((x_1 - a, 0)^T\right)^2, \quad 0 < \theta < 1.$$

The *linear* bicompartmental system approximating the nonlinear system (S_{NL}) is given as follows:

$$X^{'}(t) = F^{T}(a,0) + (DF)_{(a,0)}(x_1 - a, 0)^{T}.$$

Then the explicit formulation is

$$\begin{cases} x_1^{'}(t) = p_{21}x_2(t) - p_{12}x_1(t) - p_{1e}x_1(t), \\ x_2^{'}(t) = p_{12}x_1(t) - p_{21}x_2(t), \\ x_1(0) = a, \quad x_2(0) = 0. \end{cases}$$

This means that this linear bicompartmental system has the following figure:

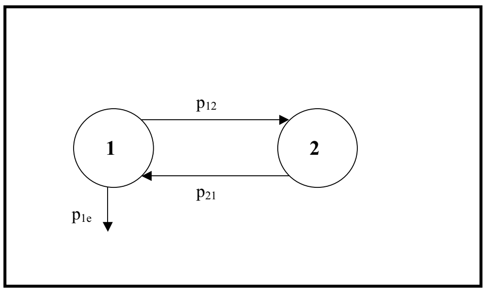

Figure 2. (S_L): A linear bicompartmental system.

with

$$\begin{cases} p_{12} = \dfrac{\partial f_2}{\partial x_1}(a,0) = 0, \\ p_{21} = \dfrac{\partial f_1}{\partial x_2}(a,0) = \begin{cases} 0, & \text{if } \alpha \geq 1 \text{ and } \beta > 1, \\ -a^{\alpha}k_{12}, & \text{at } \beta = 1, \\ a^{\beta}k_{21}, & \text{if } \alpha = 1 \text{ and } \beta > 1 \end{cases} \\ p_{1e} = \alpha k_{1e}a^{\alpha-1} \end{cases}$$

$p_{12} = 0$ involves that there is no exchange between compartment 1 and 2. Moreover if $\alpha = 1$ and $\beta > 1$, then the proposed model is not real because $p_{21} < 0$. So the initial condition $x_2(0) = 0$ is not well adapted for applying the method of temporization.

We suggest to introduce a "*temporization* ". It means that we "*wait a moment* t^*" after injecting the quantity a for permitting exchange in the system (S_{NL}), and we measure the compartment 1 at this time t^*. Then for $t > t^*$ the system (S_{NL}) is governed by the following Cauchy problem:

$$\begin{cases} x_1^{'}(t) = k_{21}x_2^{\alpha}(t)\,x_1^{\beta}(t) - k_{12}x_1^{\alpha}(t)\,x_2^{\beta}(t) - k_{1e}x_1^{\alpha}(t), \quad t > t^*, \\ x_2^{'}(t) = k_{12}x_1^{\alpha}(t)\,x_2^{\beta}(t) - k_{21}x_2^{\alpha}(t)\,x_1^{\beta}(t), \\ x_1(t^*) = a^*, \quad x_2(t^*) = b. \end{cases}$$

Generally, compartment 2 is not accessible to the measurement and thus b is unknown. This differential system can be written under the vectorial form:

$$\begin{cases} X^{'}(t) = F^{T}\left(X^{T}(t)\right), \\ X^{T}(t^{*}) = (a^{*}, b). \end{cases} \tag{3.1}$$

F being a regular function, we can apply the Taylor formula to F in the neighbourhood of (a^{*}, b). There exists a time t_0 sufficiently small such that the system (3.1) can be approached by the linear differential system with initial condition on the interval $[t^{*}, t_0]$:

$$\begin{cases} X^{'}(t) = F^{T}(a^{*}, b) + (DF)_{(a_*, b)}\left(x_1 - a_*, (x_2 - b)\right)^{T}, \ t > t^{*}, \\ X^{T}(t^{*}) = (a^{*}, b), \end{cases} \tag{3.2}$$

where :

$$F^{T}(a_*, b) = \left(k_{21} b^{\alpha} a_*^{\beta} - k_{12} a_*^{\alpha} b^{\beta} - k_{1e} a_*^{\alpha} \ , \ _{12} a_*^{\alpha} b^{\beta} - k_{21} b^{\alpha} a_*^{\beta}\right).$$

The error due to the linearization will be studied in another paper.

4. Reduction of the System (3.2) to the Canonical Form

For applying results of [5, 6, 7] relating to the linear systems, it is necessary to reduce the differential system (4.2) to the general form:

$$Y^{'}(t) = AY(t).$$

This form is said to be *canonical form* (A being a matrix of order 2). We are going to operate in two steps:

First step:

Lemma 1. *Suppose that the system* (S_{NL}) *is open. If* t^{*}*is chosen such that*

$$\alpha k_{21} b^{\alpha - 1} - \beta k_{12} a_*^{\alpha} b^{\beta - 1} \neq 0,$$

then there exists a unique set (γ, δ) *in* $\mathbb{R}^2$ *such that:*

$$(DF)_{(a_*, b)} \begin{pmatrix} \gamma \\ \delta \end{pmatrix} = F(a_*, b).$$

More precisely:

$$\gamma = \frac{a_*}{\alpha}, \quad \delta = \frac{(\alpha - \beta) a_*^{\beta}}{\alpha} \frac{k_{21} b^{\alpha}}{\alpha k_{21} b^{\alpha - 1} a_*^{\beta} - \beta k_{12} a_*^{\alpha} b^{\beta - 1}}.$$

Proof. Equation

$$(DF)_{(a_*,b)}\begin{pmatrix}\gamma\\ \delta\end{pmatrix}=F\left(a_*,b\right)$$

is a linear algebraic system according to (γ,δ), whose determinant, namely D_1, is:

$$D_1=\alpha k_{1e}a_*^{\beta-1}\left(\alpha k_{21}b^{\alpha-1}a_*^{\beta}-\beta k_{12}a_*^{\alpha}b^{\beta-1}\right).$$

If the system is open ($k_{1e}\neq 0$), then $D_1\neq 0$ and consequently the previous algebraic system has a unique solution:

$$\gamma=\frac{a_*}{\alpha}=\gamma^*.$$

We denote $\gamma=\gamma^*$ because it is calculable, and

$$\delta=\frac{(\alpha-\beta)\,a_*^{\beta}}{\alpha}\,\frac{k_{21}b^{\alpha}}{\alpha k_{21}b^{\alpha-1}a_*^{\beta}-\beta k_{12}a_*^{\alpha}b^{\beta-1}}.$$

■

Second step:

Previous Lemma permits to write the differential system (4.2) under the form:

$$X'(t)=(DF)_{(a^*,b)}\begin{pmatrix}x_1(t)-a^*+\gamma\\ x_2(t)-b+\delta\end{pmatrix}. \tag{4.1}$$

The change of the state variables

$$Y(t)=\begin{pmatrix}y_1(t)\\ y_2(t)\end{pmatrix}=\begin{pmatrix}x_1(t)-a^*+\gamma_*\\ x_2(t)-b+\delta\end{pmatrix} \tag{4.2}$$

reduces system (4.2) to its canonical form:

$$\begin{cases}Y'(t)=(DF)_{(a^*,b)}\,Y(t),\\ Y^T(t^*)=(\gamma_*,\delta).\end{cases}$$

Remark 1. The system (S_{NL}) is approximated by the compartmental linear model, namely (S_{CL}) shown in Figure 3, where

$$p_{12}=\alpha k_{12}a_*^{\alpha-1}b^{\beta}-\beta k_{21}b^{\alpha}a_*^{\beta-1},\quad p_{21}=\alpha k_{21}b^{\alpha-1}a_*^{\beta}-\beta k_{12}a_*^{\alpha}b^{\beta-1}.$$

5. Choice of the Initial Condition and Induced Problem

The parameters k_{12}, k_{21} and the constants α,β characterize the system. But the initial condition a^* and b depend on the choice of the time t^*. This involves that the signs of p_{12} and p_{21} are related to $t^*$and are not known. To be sure

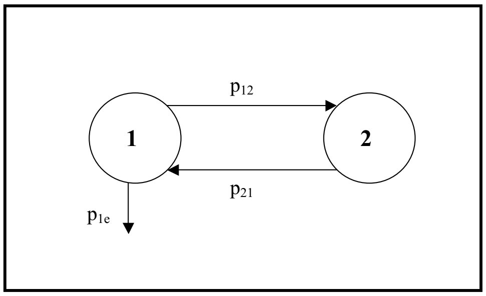

Figure 3. (S_{CL}): Approximation linear model.

that the linear model (S_{CL}) corresponds to a measurable physical reality, p_{12} and p_{21} must be positive :

$$\begin{cases} p_{12} > 0 \\ p_{21} > 0 \end{cases} \Leftrightarrow \begin{cases} \alpha k_{12} a_*^\alpha - \beta k_{21} b^{\alpha-\beta} a_*^\beta > 0, \\ \alpha k_{21} b^{\alpha-\beta} a_*^\beta - \beta k_{12} a_*^\alpha > 0. \end{cases}$$

Two questions arise:

i) Do there exist values of a_* and b such that $\begin{cases} p_{12} > 0, \\ p_{21} > 0 \end{cases}$?

ii) Moreover, a_* and b being tied, does it exist a couple (a^*, b) satisfying the condition, or in other words, does it exist a value t^* verifying this condition?

A first answer is given by the following

Proposition 1. *For all value of* a_* *fixed,* $0 < a_* < a$ *, there exists* $b > 0$ *such that:*

$$p_{12} > 0, \quad p_{21} > 0 \text{ if and only if } \alpha > \beta.$$

Proof. Set $x = k_{12} a_*^\alpha$ and $y = k_{21} b^{\alpha-\beta} a_*^\beta$ $(x > 0$ and $y > 0)$

$$\begin{cases} p_{12} > 0 \\ p_{21} > 0 \end{cases} \Leftrightarrow \begin{cases} \alpha x - \beta y > 0, \\ \alpha y - \beta x > 0. \end{cases}$$

If $\alpha < \beta$ the solutions set $\begin{cases} \alpha x - \beta y > 0 \\ \alpha y - \beta x > 0 \end{cases}$ is empty.

If $\alpha > \beta$ the solutions set $\begin{cases} \alpha x - \beta y > 0 \\ \alpha y - \beta x > 0 \end{cases}$ is not empty.

■

Next we should check if the values found above are suitable. We are going to show that the choice of t^* is compatible with one real system as soon as the eigenvalues λ_1^* and λ_2^* obtained by the minimization of an error functional (defined below) are negative.

The compartment 1 of the system (S_{NL}) is measured at instants t_j, $1 \leqslant j \leqslant m$. Let us consider the functional:

$$J_{(i_1,i_p)}\left(\beta_1^1, \beta_2^1, \lambda_1, \lambda_2\right) = \sum_{j=i_1}^{i_p} \left(x_1\left(t_j\right) - \left(\beta_1^1 e^{\lambda_1 t_j} + \beta_2^1 e^{\lambda_2 t_j}\right)\right)^2,$$

where $1 \leqslant i_1 \leqslant m-1$ and $2 \leqslant i_p \leqslant m$. Parameters i_1 and i_p are chosen such that:

$$\min J_{(i_1,i_p)}\left(\beta_1^1, \beta_2^1, \lambda_1, \lambda_2\right)$$

is realized for $\lambda_1 < 0$ and $\lambda_2 < 0$. As matter of fact let us prove the following proposition:

Proposition 2. *Let λ_1^*, λ_2^* , β_1^{1*}, and β_2^{1*} be the values such that:*

$$\min J_{(i_1,i_p)}\left(\beta_1^1, \beta_2^1, \lambda_1, \lambda_2\right) = J_{(i_1,i_p)}\left(\beta_1^{1*}, \beta_2^{1*}, \lambda_1^*, \lambda_2^*\right).$$

If $\lambda_1^* < 0$, $\lambda_2^* < 0$, $\beta_1^{1*} \neq 0$ and $\beta_2^{1*} \neq 0$, then $p_{12} > 0$, $p_{21} > 0$.

Proof. Note the compartmental matrix of the linear model (S_{CL})

$$A = \begin{pmatrix} -p_{1e} - p_{12} & p_{21} \\ p_{12} & -p_{21} \end{pmatrix} \quad \Rightarrow \quad \det A = \lambda_1^* \lambda_2^* = p_{1e} p_{21}.$$

But $p_{1e} = \alpha k_{1e}$, thus $p_{1e} > 0$ and consequently $p_{21} > 0$.

It is proved in [3] that

$$p_{12} = -\frac{\left(\lambda_1^* + p_{1e}\right)\left(\lambda_2^* + p_{1e}\right)}{p_{1e}}$$

then, supposing that $\lambda_2^* < \lambda_1^*$, we get

$$p_{12} > 0 \quad \Leftrightarrow \quad \left(-\lambda_1^*\right) < p_{1e} < \left(-\lambda_2^*\right).$$

According to [3] we have:

$$\left(\beta_1^{1*} \neq 0, \text{ and } \beta_2^{1*} \neq 0\right) \quad \Rightarrow \quad \left(-\lambda_1^*\right) < p_{1e} < \left(-\lambda_2^*\right).$$

This proves the result. ■

Corollary 1. We can set $t^* = t_{i1}$.

6. Identification of the Systems (S_{CL}) and (S_{NL})

6.1. Identification of the system (S_{CL})

The following hypothesis for identification of the linear nonhomogeneous compartmental systems shown in Figure 4 are satisfied (see [7]): the system is

- *linear, open,*
- *nonhomogeneous,*
- *undeterminated,*
- *satisfying initial conditions*

$$\begin{cases} y_1(0) = \dfrac{a_*}{\alpha}, \\ y_2(0) = \delta. \end{cases}$$

We use a new variable $s = t - t^*$ and δ is unknown.

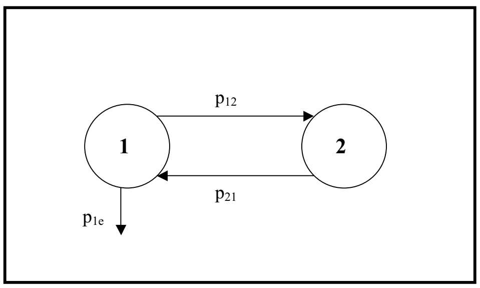

Figure 4. Linear nonhomogeneous bicompartmental system.

The excretion coefficient p_{1e} is identified (see [3]) by

$$p_{1e} = k_{1e} = \frac{-(\lambda_1^* + \lambda_2^*) - \sqrt{(\lambda_1^* + \lambda_2^*)^2 - 8\lambda_1^*\lambda_2^*}}{2},$$

then the matrix of partial measures is completed as follows:

$$\begin{cases} \beta_1^2 = -\left(1 + \dfrac{p_{1e}}{\lambda_1^*}\right) \beta_1^{1*}, \\ \beta_2^2 = -\left(1 + \dfrac{p_{1e}}{\lambda_2^*}\right) \beta_2^{1*} \end{cases}$$

and consequently the exchange parameters p_{12} and p_{21} are identified by solving a linear algebraic system giving identification (see Hebri, B. & Cherruault, Y. 2002a [6, 7]). Let:

$$\begin{cases} \nu_2^* = p_{12} = \alpha k_{12} a_*^{\alpha-1} b^\beta - \beta k_{21} b^\alpha a_*^{\beta-1}, \\ \nu_3^* = p_{21} = \alpha k_{21} b^{\alpha-1} a_*^\beta - \beta k_{12} a_*^\alpha b^{\beta-1} \end{cases}$$

be this solution, and set $\nu_1^* = p_{1e}$. This notation will be used in the next section.

6.2. Identification of the nonlinear system (S_{NL})

For obtaining an approximation of the non linear system (S_{NL}), it suffices to determine b.

Proposition 3. *Let*

$$B^{*2} = \begin{pmatrix} \beta_1^{1*} & \beta_1^{2*} \\ \beta_2^{1*} & \beta_2^{2*} \end{pmatrix}$$

be the completude of the partial measures matrix of the algebraic masses associated to the model (S_{CL}). *We suppose that this system is identified. Then the initial condition* b *is obtained by the relationship:*

$$b = \frac{1}{\nu_3^*} \left[(\alpha + \beta) \left(-\lambda_1^* \beta_1^{2*} - \lambda_2^* \beta_2^{2*} \right) + a_* \nu_2^* \right]. \tag{6.1}$$

Proof. (S_{CL}) being identified, the coefficients k_{12} and k_{21} verify

$$\begin{cases} \nu_2^* = p_{12} = \alpha k_{12} a_*^{\alpha-1} b^\beta - \beta k_{21} b^\alpha a_*^{\beta-1}, \\ \nu_3^* = p_{21} = \alpha k_{21} b^{\alpha-1} a_*^\beta - \beta k_{12} a_*^\alpha b^{\beta-1}. \end{cases}$$

We deduce that

$$\begin{aligned} b\nu_3^* - a_* \nu_2^* &= (\alpha + \beta) \left(k_{21} b^\alpha a_*^\beta - k_{12} a_*^\alpha b^\beta \right) \\ &= (\alpha + \beta) x_2' (0) \\ &= (\alpha + \beta) \left(-\lambda_1^* \beta_1^{2*} - \lambda_2^* \beta_2^{2*} \right). \end{aligned}$$

In conclusion, we have

$$b = \frac{1}{\nu_3^*} \left[(\alpha + \beta) \left(-\lambda_1^* \beta_1^{2*} - \lambda_2^* \beta_2^{2*} \right) + a_* \nu_2^* \right].$$

■

Theorem 1. *Let* (S_{NL}) *be a nonlinear polynomial system, and* (S_{CL}) *the linear associated model. If* $\alpha > \beta$ *an approximation of the parameters of* (S_{NL}) *are given by*

$$\begin{cases} k_{12} = \dfrac{\alpha \nu_2^* a_* + \beta \nu_3^* b}{(\alpha^2 - \beta^2) a_*^\beta b^\alpha}, \\ k_{21} = \dfrac{\alpha \nu_3^* b + \beta \nu_2^* a_*}{(\alpha^2 - \beta^2) a_*^\beta b^\alpha}, \end{cases}$$

where ν_2^* *and* ν_3^* *are the coefficients of* (S_{CL}).

Proof. If $\alpha > \beta$ we can approach the nonlinear system (S_{NL}) by the real linear model (S_{CL}) shown in Figure 3. This system is identified by

$$\begin{cases} p_{12} = \nu_2^*, \\ p_{21} = \nu_3^*, \end{cases} \qquad (\mathrm{S_{alg}})$$

b being determinated by the relationship (6.1). S_{alg} is a linear algebraic system according to (k_{12}, k_{21}) whose determinant namely $D_{S\mathrm{alg}}$ is

$$D_{S\mathrm{alg}} = \left(\alpha^2 - \beta^2\right)(a_* b)^{\alpha+\beta-1} \neq 0.$$

Then S_{alg} admits a unique solution (k_{12}, k_{21}) given by

$$\begin{cases} k_{12} = \dfrac{\alpha\nu_2^* a_* + \beta\nu_3^* b}{(\alpha^2 - \beta^2)\, a_*^{\beta} b^{\alpha}}, \\ k_{21} = \dfrac{\alpha\nu_3^* b + \beta\nu_2^* a_*}{(\alpha^2 - \beta^2)\, a_*^{\beta} b^{\alpha}}. \end{cases}$$

■

7. Conclusion

The linear model associated to the nonlinear polynomial compartmental system of $(\alpha + \beta)$ order involves three important difficulties :

i) The initial condition at time $t = 0$ does not permit to give a complete information about the model (S_{NL}). A "*temporization* t^*" is introduced to suppress this difficulty.

ii) If this temporization is not modulated, the linear model is not necessarily real. We have shown that the measures done on the compartment 1 permit to choose one measure at instant $t_{i_1} = t^*$ such that we can develop a linearization method as for the Michaelis-Menten system (see [3]).

iii) The nonhomogeneous condition $x_2(t^*) = b$ being unknown is identified from measures done on compartment 1.

The error on the system's coefficients due to the linearization will be developed in another paper.

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