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PARAMETER ESTIMATION OF FRACTIONAL MODELS : APPLICATION TO THE MODELING OF DIFFUSIVE SYSTEMS

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Abstract : Black box modeling of diffusion processes can be performed by fractional models. The simulation of these particular models is based on a new fractional integrator, with limited spectral range. Parameter estimation of this class of systems is performed by an OE identification technique. This paper presents the application of this new methodology to the modeling of different diffusive systems dealing with electrochemistry, heat transfer and electromagnetism. *Copyright © 2002 IFAC*

Keywords : Partial differential equations - Parameter estimation - Output error identification - State space models - Special mathematical operator.

1. INTRODUCTION

Non integer order models, also known as fractional filters, have been introduced long ago in various fields such as electrochemistry (Ichise, *et al.*, 1971), acoustics (Matignon, *et al.*, 1994), heat transfer, … where they are fundamentally used for the modeling of diffusive processes. Their dynamics depend on a well-known Partial Derivative Equation and on the geometry of the considered problem. If the attention is focussed on the relation between variables at the boundary region, a theoretical modeling leads to an integrator with an order equal to ½. Generalization of this modeling to more complex situations needs to use a fractional model, characterized by its non integer order, whose value can vary from 0 and 1.

The objective of this paper is the black-box modeling of these diffusive processes, using a fractional integrator. This new operator has already been defined (Trigeassou, *et al.*, 1999 ; Lin and Poinot, 1999) : it is fundamentally characterized by its bounded spectral range and approximated by an equivalent state-space representation depending on a limited number of design parameters. Then, this fractional integrator is used to define a macro state space representation of the considered non integer system. Finally, identification is performed by OE classical parameter estimation, owing to the transformation of non integer order and its spectral range into design parameters.

The application of this black box modeling has already been performed experimentally on different type of diffusive systems (Lin, *et al.*, 2000a ; Lin, *et al.*, 2000b ; Lin, *et al.*, 2001a ; Lin, *et al.*, 2001b). Thus it is interesting in this paper to recall and to compare the main results in order to exhibit the capabilities of this new modeling methodology.

The paper is divided in four parts. Part 1 is devoted to diffusive processes and their modeling by fractional systems. In part 2, the modeling of non integer order systems is presented with the help of a fractional integrator and of a state-space representation. The identification procedure is presented in part 3. Finally in part 4, the application of this new methodology to different types of diffusive systems is analyzed.

2. DIFFUSIVE PROCESSES AND FRACTIONAL MODELS

2.1. Diffusive processes

The diffusion of particles in a one dimensional problem is related to two fundamental equations :

$$j(x,t) = -D\frac{\partial n(x,t)}{\partial x} \quad \text{(Fick's law)} \qquad (1)$$

$$\frac{\partial n(x,t)}{\partial t} = D\frac{\partial^2 n(x,t)}{\partial x^2} \qquad (2)$$

where n represents the concentration of particles, j is the particle current density and D is a coefficient characterizing diffusion.

The solution of the diffusion process ($n(x,t)$) is related to Partial Derivative Equation (2) and to the particular geometry of the problem. Equation (1) specifies the relation between $j(x,t)$ and $n(x,t)$, which will be considered respectively as the input and the output of the system when $x = 0$ (boundary region).

Many physical and chemical problems are based on diffusive processes. In the part 4 of this paper, one presents results obtained on three processes governed by equations (1) and (2) :

- Heat transfer in materials : in this case, j is related to the heat flux and n to the temperature.
- Electrochemical diffusion process : modeling of the transients of a lead-acid battery. In this example, j will be replaced by the current i and n by the voltage v of the battery cell.
- Electromagnetism : modeling of frequency effects in an induction motor. In this case, j will be replaced by the voltage of the rotor and n by the rotoric current.

2.2. Fractional integrator, fractional model

Consider a one dimensional idealized problem (see figure 1). $j(0,t)$ has the same value in each point of plane A ; plane B is insulated, i.e. $j(L,t) = 0$. $j(0,t)$ is considered as the actuator variable or input of the system ; $n(0,t)$ is the resulting variable or output of the system. The objective is to define the transfer function between $n(0,t)$ and $j(0,t)$.

A classical approach is to apply Laplace Transform to equations (1) and (2). Thus, equation (2) is equivalent to :

$$N(x,s) = L[n(x,t)] = L_1(s)e^{\sqrt{s/D}\,x} + L_2(s)e^{-\sqrt{s/D}\,x} \qquad (3)$$

Using (3), the Laplace transform of (1), and the two boundary conditions $j(0,t)$ and $j(L,t)$, one get :

$$J(0,s) = -\sqrt{s\,D}\,[L_1(s) - L_2(s)] \qquad (4)$$

and

$$L_2(s) = L_1(s)e^{2\sqrt{s/D}\,L} \qquad (5)$$

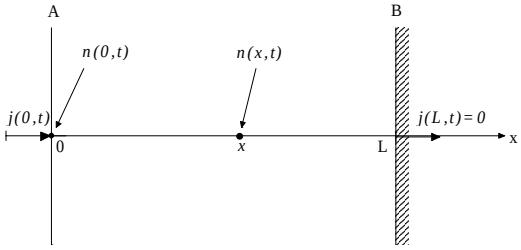

Figure 1 : One dimensional problem

Then, combining (3), (4) and (5), it is straightforward to get :

$$\frac{N(0,s)}{J(0,s)} = -\frac{1}{\sqrt{s\,D}}\,\frac{1+e^{2\sqrt{s/D}\,L}}{1-e^{2\sqrt{s/D}\,L}} \qquad (6)$$

Finally, if the semi-infinite problem where $L \to \infty$ is considered, then

$$\frac{N(0,s)}{J(0,s)} = -\frac{1}{\sqrt{D}\sqrt{s}} \equiv -\frac{K}{s^n} \quad with\ n = \frac{1}{2} \qquad (7)$$

Equation (7) exhibits a fractional integrator whose order n is equal to ½. Practically, n depends on the geometry of the problem ; moreover, when plane B is not completely insulated, then $j(L,t) \neq 0$ *and* $n(o,t) \xrightarrow[t\to\infty]{}$ finite value when a step input $j(0,t)$ is applied to the system. Thus K/s^n has to be replaced by :

$$\frac{G}{1+\tau\,s^n} = \frac{b_0}{a_0 + s^n}, \quad 0 < n < 1 \qquad (8)$$

Equation (8) represents the fractional model of the diffusive process at the point $x = 0$ (boundary region).

3. MODELING OF NON INTEGER ORDER SYSTEMS

(Trigeassou, *et al.*, 1999 ; Lin and Poinot, 1999)

3.1. Fractional integrator

Consider the Bode diagram of a modified integrator on figure 2.

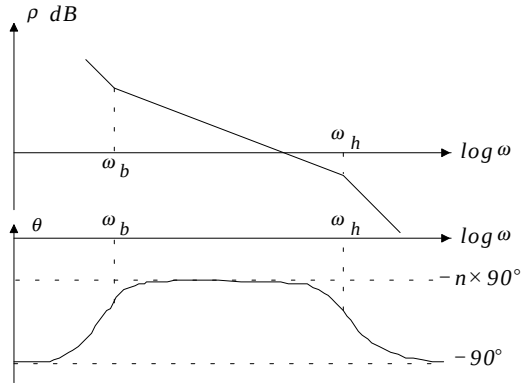

Figure 2 : Bode diagram of the non-integer integrator

It is composed of three parts :

- The intermediate part corresponds to non integer action, characterized by *n* (experiments show that it is necessary to restrict the non integer action to a limited fractional band).
- In the two other parts, the integrator has conventional action, characterized by *n = 1*.

In this way, a new operator $I_n(s)$ is defined which is a conventional integrator, except on a limited band $[\omega_b, \omega_h]$ where it is acting like a "*n*" non integer integrator. The operator $I_n(s)$ is defined using a fractional phase lead filter (A. Oustaloup,1995) :

$$I_n(s) = \frac{1}{s} \prod_{i=1}^{N} \frac{1 + \frac{s}{\omega'_i}}{1 + \frac{s}{\omega_i}} \tag{9}$$

This operator is characterized by five parameters :

- ω'_1 and ω_N define the frequency range (equivalently to ω_b and ω_h),
- *N* is the number of cells (it is directly related to the quality of the approximation),
- α and η are recursive parameters related to non integer order *n*.

This operator is completely defined by the following relations :

$$\omega_i = \alpha\, \omega'_i, \omega'_{i+1} = \eta\, \omega_i, n = 1 - \frac{\log \alpha}{\log \alpha\eta} \tag{10}$$

3.2. State-space representation of the operator

The pseudo-integrator is defined by (9). Practically, a state-space representation is associated to $I_n(s)$.

Because $I_n(s)$ is composed of a product of cells, the state variables are defined as the output of each cell, according to figure 3.

Each state variable x_n is only related to the preceding x_{n-1} by :

$$-\frac{\omega_{n-1}}{\omega'_{n-1}} \dot{x}_{n-1} + \dot{x}_n = \omega_{n-1}(x_{n-1} - x_n) \tag{11}$$

where $\omega_{n-1}/\omega'_{n-1} = \alpha$.

Then, considering x_{n+1}

$$-\alpha\, \dot{x}_n + \dot{x}_{n+1} = \omega_n(x_n - x_{n+1}) \tag{12}$$

The connection between these two lines is realized by $\omega_n = \alpha\, \eta\, \omega_{n-1}$. Thus, this particular state-space representation uses only α and η, plus ω'_1 or ω_N .

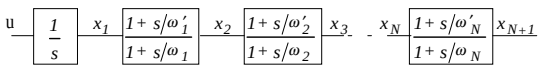

Figure 3 : $I_n(s)$ block diagram

So, one can write :

$$\begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ -\alpha & 1 & & & \vdots \\ 0 & -\alpha & 1 & & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -\alpha & 1 \end{bmatrix} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \vdots \\ \vdots \\ \dot{x}_{N+1} \end{bmatrix} = \begin{bmatrix} 0 & 0 & \cdots & \cdots & 0 \\ \omega_1 & -\omega_1 & & & \vdots \\ 0 & \omega_2 & -\omega_2 & & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \omega_N & -\omega_N \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_{N+1} \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix} u \tag{13}$$

Then, defining M_I , A_I , $\underline{B}_I$ and $\underline{x}_I$, one can write (where M_I , A_I and $\underline{B}_I$ are parsimonious matrixes) :

$$M_I\, \dot{\underline{x}}_I = A_I\, \underline{x}_I + \underline{B}_I\, u \tag{14}$$

or equivalently :

$$\dot{\underline{x}}_I = A_I^*\, \underline{x}_I + \underline{B}_I^*\, u \tag{15}$$

where

$$\begin{cases} A_I^* = M_I^{-1}\, A_I \\ \underline{B}_I^* = M_I^{-1}\, \underline{B}_I \end{cases}$$

are full matrixes necessary for the numerical simulation of the operator.

3.3. State-space representation of a non-integer system

Principle. Using the fractional integrator operator, the state-space model of a non-integer system can be constructed. Consider the non integer differential equation (with *0 < n < 1*) :

$$\frac{d^n y(t)}{dt^n} + a_0\, y(t) = b_0\, u(t) \tag{16}$$

Define $x(t)$ such as

$$X(s) = \frac{1}{s^n + a_0} U(s) \tag{17}$$

Thus, a "macro" state-space representation of this system is associated to model (17) (with "macro" parameters a_0 and b_0).

$$\begin{cases} \frac{d^n x(t)}{dt^n} = -a_0\, x(t) + u(t) \\ y(t) = b_0\, x(t) \end{cases} \tag{18}$$

or equivalently using the operator defined previously :

$$\begin{cases} \dot{x}_1 = -a_0\, x_{N+1} + u \\ y = b_0\, x_{N+1} \end{cases} \tag{19}$$

This "macro" model is only convenient for compact writing. Practically, there are two imbricated state-space representations, one for the "macro" model, the

other for the operator. Notice that $\underline{x} = \underline{x}_I$ in this simple example.

Because $\dot{x}_1 = -a_0\ x_{N+1} + u$, the global state-space model is :

$$\dot{\underline{x}} = A\,\underline{x} + \underline{B}\,u \tag{20}$$

with

$$A = A_I^* + \begin{bmatrix} 0 & \cdots & 0 & -a_0 \\ \vdots & \ddots & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 \end{bmatrix}, \quad \underline{B} = \underline{B}_I^*$$

and for the observation equation :

$$y = \underline{C}^T\,\underline{x} \tag{21}$$

with $\underline{C}^T = [0 \quad \cdots \quad 0 \quad b_0]$.

4. OUTPUT ERROR IDENTIFICATION OF THE FRACTIONAL SYSTEM

The model of the system is in continuous time representation, thus it is preferable to use an output error technique (OE) to estimate its parameters *(*Richalet, et al.*, 1971)*.

The state-space model of the non integer system is :

$$\dot{\underline{x}} = A(\underline{\theta})\,\underline{x} + \underline{B}(\underline{\theta})\,u \tag{22}$$

$$y = \underline{C}^T(\underline{\theta})\,\underline{x} \tag{23}$$

with $\underline{\theta}^T = [a_0 \quad b_0 \quad \omega_1' \quad \omega_N \quad \alpha \quad \eta]$.

The data set is composed of *K* data pairs $\{u_k, y_k^*\}$ with $t = k\,T_e$ (T_e : sampling period) ; b_k is an output disturbance.

$$y_k^* = y_k + b_k \tag{24}$$

The state-space model is simulated using a numerical integration algorithm, thus one get $\hat{y}_k = f_k(u, \hat{\underline{\theta}})$ where $\hat{\underline{\theta}}$ is an estimation of $\underline{\theta}$. Then, defining output prediction error

$$\varepsilon_k = y_k^* - \hat{y}_k(u, \hat{\underline{\theta}}) \tag{25}$$

The optimal value of $\hat{\underline{\theta}}$ ($\underline{\theta}_{opt}$) is obtained by minimization of the quadratic criterion :

$$J = \sum_{k=1}^{K} \varepsilon_k^2 \tag{26}$$

Because $\hat{y}(t)$ is not linear in $\hat{\underline{\theta}}$, a Non Linear Programming technique is used to estimate iteratively $\hat{\underline{\theta}}$:

$$\underline{\theta}_{i+1} = \underline{\theta}_i - \left\{ [J''_{\theta\theta} + \lambda\, I]^{-1}\ \underline{J}'_\theta \right\}_{\underline{\theta} = \underline{\theta}_i} \tag{27}$$

with (Ljung, 1987) :

$$\begin{cases} \underline{J}'_\theta = -2 \sum_{k=1}^{K} \varepsilon_k\ \underline{\sigma}_{k,\underline{\theta}_i} & : \textit{gradient} \\ J''_{\theta\theta} \approx 2 \sum_{k=1}^{K} \underline{\sigma}_{k,\underline{\theta}_i}\ \underline{\sigma}^T_{k,\underline{\theta}_i} & : \textit{hessian} \\ \lambda : \textit{monitoring parameter} \\ \underline{\sigma}_{k,\underline{\theta}_i} = \dfrac{\partial \hat{y}_k}{\partial \underline{\theta}_i} & : \textit{output sensitivity function} \end{cases}$$

This algorithm, known as Marquardt's one (Marquardt, 1963), insures robust convergence, even with a bad initialization of $\hat{\underline{\theta}}$. Fundamentally, this technique is based on the calculation of gradient and hessian, themselves dependant on the numerical integration of the sensitivity functions $\underline{\sigma}_{k,\underline{\theta}_i}$ *(*Richalet, *et al.*, 1971*)*, which are equivalent to the regressors in the linear case.

5. EXPERIMENTAL RESULTS

5.1. Introduction

One presents here results obtained on three diffusive processes : electrochemical diffusion process (Lin, *et al.*, 2000b), heat transfer in materials (Lin, *et al.*, 2001a ; Lin, *et al.*, 2001b) and electromagnetism (Lin, *et al.*, 2000a ; Lin, *et al.*, 2001a).

Electrochemical diffusion process : modeling of the transients of a lead-acid battery. Usually, the transfer function between voltage and current of the battery is represented by a fractional impedance, obtained by frequential experiments. The objective is to replace this impedance by a fractional model, derived from classical input/output data, thus by the new black box model :

$$H(s) = \frac{b_0}{a_0 + s^n} \tag{28}$$

where $0 < n < 1$.

Heat transfer in materials. Classically, heat transfer systems can be modeled by *RC* cells connected together as shown in figure 4. *P* is the source of heat flux equivalent to a current source. θ_{in} is the temperature at the boundary source and θ_{ext} is the fixed temperature in the enclosure.

The use of a large number of *RC* cells permits to take into account the specific geometry of the system, that is to say any fractional order. However, identification of this model can be very difficult beyond 2 or 3 cells. So, a fractional model can be equivalently used. The major interest is that the complexity of *RC* cells is summarized by a few design parameters. The model is also given by (28).

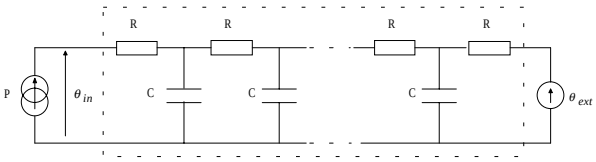

Figure 4 : Modeling of the heat transfer system

Electromagnetism : modeling of frequency effects in an induction motor. Induced currents in a conductive volume caused by a variable magnetic field are governed by diffusive mechanism. In concrete terms, this mechanism is characteristic of an induction machine, where stator windings, traversed by three-phase currents, are the cause of induced currents in rotor bars.

A model of fixed order equal to ½ can be used (Retière and Ivanes, 1998) but this model is unable to take into account the real geometry of the conductors. Another solution is to use a model like for heat transfer with a high number of parameters (Kabbaj, 1997) but identification of this model is difficult beyond 3 cells. So, the modeling of the rotor behavior is performed using a non integer impedance given by ($0 < n < 1$) :

$$Z_n(s) = \frac{a_0 + s^n}{b_0} \qquad (29)$$

5.2. Identification results

Tables 1, 2 and 3 present identification results obtained on these three processes. The parameters of the previous models (28) (or (29)) have been estimated using the identification technique presented in part 3. For each process, two experiments have been used.

One can notice that, in each case, the two experiments lead approximately to the same parameters, thus to the same model. On the other hand, the value of the non integer order *n* is very different from the expected theoretical value, that is to say 0.5. Thus, *n* varies from 0.22 (electrochemical system) to 0.7/0.8 ; these values are derived from experimentation and are necessary to a good fit of the model to real data. At the present time, no theoretical approach has been able to explain the difference with 0.5 value : our hypothesis is that geometry of each system is perhaps the cause of this important difference.

Consider now values of ω_1' and ω_N . One can notice that for the same process, values are similar ; between processes, obtained values are different and the spectral range of the non integer action can be very large. Identification results show that these parameters are not sensitive and final values of the optimization algorithm depend highly on initial ones. Practically, this spectral range is limited by the sampling period of the data acquisition system and by the time length of excitation steps. In a next research step, it will be interesting to use this remark in order to simplify the identification algorithm, because ω_1' and ω_N are not sensitive parameters.

Table 1 : Application to electrochemistry

a_0	b_0	n	ω_1' (rd/s)	ω_N (rd/s)
2.522	0.1300	0.2299	0.1549	115.64
2.531	0.1308	0.2165	0.1483	131.74

Table 2 : Application to heat transfer

a_0	b_0	n	ω_1' (rd/s)	ω_N (rd/s)
0.2318	0.0016	0.7112	0.0008	6.2831
0.2310	0.0015	0.7452	0.0003	6.2860

Table 3 : Application to electromagnetism

a_0	b_0	n	ω_1' (rd/s)	ω_N (rd/s)
12.27	4.32	0.763	0.157	10^6
16.91	6.03	0.865	10^{-8}	10^6

5.3. Illustration example : Fractional modeling of a lead-acid battery (Lin, *et al.*, 2000b)

In order to illustrate our results, one presents the fractional modeling of the lead-acid battery. Identification results are given in table 1. As exhibited by figure 5, there is a good fit between measured and estimated voltage.

The harmonic responses H(jω) of the two models are plotted on figure 6 : it is evident that the two models are very close (same variation of magnitude, same phase), even if there are small differences between parameters.

In order to exhibit the role of the fractional integrator, its Bode plots have been represented figure 7. In the two cases, the curves are very close and correspond to the theoretical ones, plotted on figure 2. The same results can be verified on the other diffusion processes. As a conclusion, the proposed black box fractional model $b_0 / a_0 + s^n$ can be considered as a satisfying approximation of diffusive systems either in time domain or in frequential one.

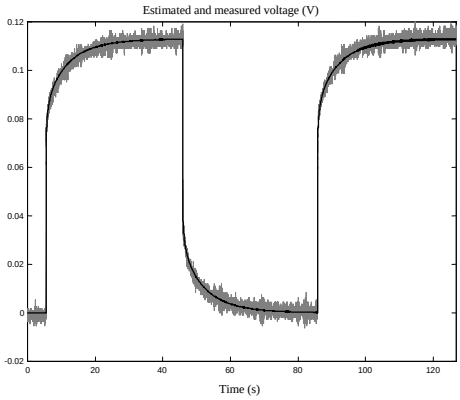

Figure 5 : Measured and estimated voltage

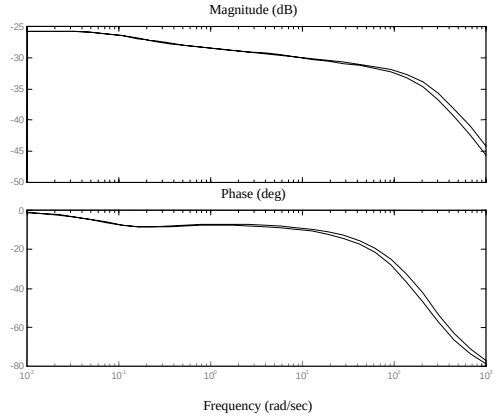

Figure 6 : Bode plot of estimated models

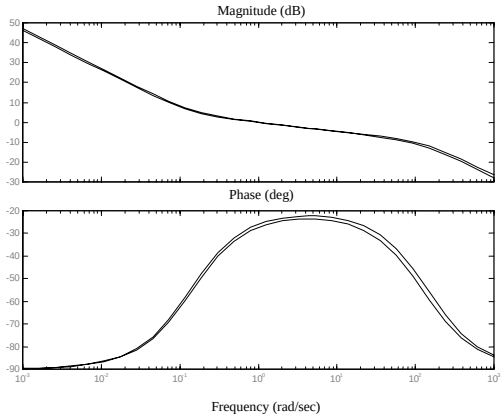

Figure 7 : Bode plot of estimated integrators

6. CONCLUSION

In this paper, the application of fractional modeling and identification to three diffusive processes has been presented and analyzed. The simulation of these systems is performed using a fractional integrator operator, associated to a *N* dimension state-space representation. Global identification of the system is performed by an Output Error technique.

The proposed black box fractional model is characterized by a good fit between experiments and predicted outputs. The harmonic responses of these models are very close, despite some differences between estimated parameters. Experiments show that fractional modeling is well suited to represent the dynamics of diffusive processes ; particularly, the success of this approach is due to the special fractional integrator operator with limited spectral range.

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