

Synthesis of Havriliak-Negami functions for time-domain system identification

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Abstract: Fractional differentiation models have proven their usefulness in representing high dimensional systems with only few parameters. Generally, two elementary fractional functions are used in time-domain identification: Cole-Cole and Davidson-Cole functions. A third elementary function, called Havriliak-Negami, generalizes both previous ones and is particularly dedicated to dielectric systems. The use of this function is however not very popular in time-domain identification because it has no simple analytical impulse response. The only synthesis method of Havriliak-Negami elementary functions proposed in the literature is based on diffusive representation which sets restrictive conditions on fractional orders. A new synthesis method, with no such restrictions, is developed in this paper. For that purpose Havriliak-Negami function is first split into a Davidson-Cole function and a complementary one. Both functions are then synthesized in a limited frequency band using poles and zeros recursive distribution developed by Oustaloup (1995). As an example, this Havriliak-Negami function is used for a thermal system modeling.

Keywords: System identification; Fractional models; Fractional differentiation; Synthesis; Havriliak-Negami function.

1. INTRODUCTION

Although fractional (non integer) operators remained for a long time purely a mathematical concept, the rise of digital computers offered an easy way for simulating numerically non integer integro-differentiation of mathematical functions. The last two decades have witnessed considerable development in the use of fractional differentiation in various fields. Fractional differentiation is now an important tool for the international scientific and industrial communities. The use of fractional differentiation models in system identification was initiated in the late nineties and the beginning of this century (Lin (2001); Cois (2002); Aoun (2005)). They are now widely used in representing some diffusive phenomena (thermal diffusion, electrochemical diffusion) and in modeling viscoelastic materials.

Based on the synthesis of two elementary functions Cole-Cole (Cole and Cole (1941)) and Davidson-Cole (Davidson and Cole (1951)), both defined later, the objective of this paper is to propose a synthesis method for Havriliak-Negami function (Havriliak and Negami (1966, 1967)). Although this function is particularly dedicated to diffusive systems and generalizes both previous ones, it is, up to now, seldom used because its synthesis is problematic.

The paper is organized as follows. First, a mathematical background on fractional differentiation is presented. Then in section III, principles of the bandlimited frequency fractional operator synthesis is explained and the synthesis of the Davidson-Cole function is extended to complex zeros.

Next in section IV, Havriliak-Negami function is split up into two functions each of which is then synthesized. Finally, the Havriliak-Negami function is used for a thermal system modeling.

2. MATHEMATICAL BACKGROUND

The concept of differentiation to an arbitrary order (non-integer),

$$\mathbf{D}^\nu \triangleq \left(\frac{d}{dt} \right)^\nu \quad (1)$$

was defined in the 19th century by Riemann and Liouville. The ν fractional derivative of $f(t)$ is defined as being an integer derivative of order $[\nu] + 1$ ($[\cdot]$ stands for the floor operator) of a non-integer integral of order $\nu - [\nu]$ (Samko et al. (1993)):

$$\begin{aligned} \mathbf{D}^\nu f(t) &= \mathbf{D}^{[\nu]+1} \left(\mathbf{I}^{[\nu]+1-\nu} f(t) \right) \\ &\triangleq \frac{1}{\Gamma([\nu] + 1 - \nu)} \left(\frac{d}{dt} \right)^{[\nu]+1} \int_0^t \frac{f(\tau) d\tau}{(t-\tau)^{\nu-[\nu]}} \end{aligned} \quad (2)$$

where $t > 0, \forall \nu \in \mathbb{R}_+^*$, and the Euler's Γ function is defined as:

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt, \quad \forall x \in \mathbb{R}^* \setminus \{\mathbb{N}^-\}. \quad (3)$$

A more concise algebraic tool can be used to represent fractional systems: the Laplace transform. The Laplace transform of a ν order derivative ($\nu \in \mathbb{R}_+^*$) of a signal $x(t)$ relaxed at $t = 0$ is obtained by taking the Laplace transform of (2) Oldham and Spanier (1974):

$$\mathcal{L}\{\mathbf{D}^\nu x(t)\} = s^\nu X(s) \quad \text{if } x(t) = 0 \quad \forall t < 0. \quad (4)$$

Two elementary fractional-differentiation functions are generally used for representing fractional transfer functions: the Davidson-Cole function (Davidson and Cole (1951))

$$F_{dc}(s) = \frac{A}{(s + \omega_u)^\nu}, \quad (5)$$

and the Cole-Cole function (Cole and Cole (1941))

$$F_{cc}(s) = \frac{A}{s^\nu + \omega_u}, \quad (6)$$

where $\omega_u \in \mathbb{R}_+$ and $A \in \mathbb{R}$.

$F_{cc}(s)$ has one s^ν -pole at $-\omega_u$ and, as shown by Oustaloup (1983, 1995), $F_{cc}(s)$ might have s -poles at:

$$P_k = (\omega_u)^{\frac{1}{\nu}} e^{j\pi \frac{2k+1}{\nu}}, \quad (7)$$

provided there exists $k \in \mathbb{Z}$ such that:

$$-\frac{(1+\nu)}{2} < k < \frac{(1+\nu)}{2}. \quad (8)$$

Hence, the number of s -poles equals:

- 0 when $\nu < 1$,
- 1 when $\nu = 1$,
- 2 when $1 < \nu < 3$,
- 3 when $\nu = 3$,
- 4 when $3 < \nu < 5$.

The s -pole locus is plotted in Fig. 1 versus differentiation order ν varying from 1 to 3. For $0 \leq \nu < 1$, F_{cc} is stable since it has no s -pole. When $1 < \nu < 2$, F_{cc} has two stable complex conjugate poles. Beyond $\nu = 2$, it has at least two unstable poles.

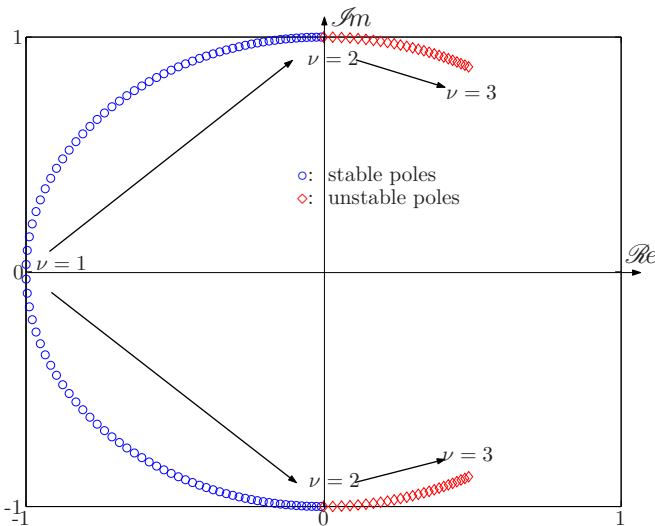


Fig. 1. Pole locus of F_{cc} versus differentiator order for $1 < \nu \leq 3$. F_{cc} has two complex conjugate poles, unstable beyond $\nu = 2$

A third elementary function (Havriliak-Negami) was proposed by Havriliak and Negami (1966, 1967):

$$F_{hn}(s) = \frac{A}{(s^{\nu_1} + \omega_u)^{\nu_2}}. \quad (9)$$

Although, it generalizes the two previous ones, it is rarely used in time domain-simulations because of the difficulty of its synthesis.

A rational realization of the Havriliak-Negami elementary function is proposed in Laudebat (2003) for $(\nu_1, \nu_2) \in (]0, 1[)^2$ and is based on diffusive representation. Nevertheless, this representation does not allow to have a band limited fractional behavior, which is generally present in physical systems, i.e. physical systems do not have an infinite band fractional behavior.

The objective of this paper is to define a rational realization of Havriliak-Negami elementary function on a bandlimited frequency for $\nu_1 \in \mathbb{R}_+$ and $\nu_2 \in \mathbb{R}$.

This new realization is based on the splitting of Havriliak-Negami elementary function into a Davidson-Cole and a complementary function. Then, the rational realization of both functions is obtained by using the principle of recursive poles and zeros synthesis of a bandlimited fractional integrator as described by Oustaloup (1983, 1995).

3. SYNTHESIS OF FRACTIONAL OPERATORS IN A BANDLIMITED FREQUENCY

Considering the bandlimited fractional behavior of real physical systems and the practical limitations of input and output signals (Shannon's cut-off frequency and the spectrum of the input signal), fractional operators are usually approximated by high order rational models within a limited frequency band. This physical limitation is all the more interesting as until now, there is no mathematical tool leading to an approximation for every frequencies. As a result, a fractional model and its rational approximation have the same dynamics within a limited frequency band. The most commonly used approximation of the fractional integro-differentiator s^ν in the bandlimited frequency $[\omega_A, \omega_B]$ is the recursive distribution of zeros and poles proposed by Oustaloup (1983) and explained below.

Rational realization of fractional operators in the bandlimited frequency $[\omega_A, \omega_B]$ induces deterioration around the edge frequencies ω_A and ω_B as shown in Fig. 2 and 3. This deterioration is known as edge effect and is generally reduced by extending the frequency band on which the realization is carried out from $[\omega_A, \omega_B]$ to $[\omega_b, \omega_h]$, where

$$\begin{aligned} \omega_b &= \frac{\omega_A}{\sigma} \\ \omega_h &= \omega_B \cdot \sigma \end{aligned} \quad (10)$$

A dedicated study (Oustaloup (1995)) has shown that the edge effect is considerably reduced by choosing a spreading factor of $\sigma = 10$ or 100 . As a result, s^ν is approximated on the frequency band $[\omega_A, \omega_B]$ by:

$$s^\nu \rightarrow s_{[\omega_A, \omega_B]}^\nu = C_0 \left(\frac{1 + \frac{s}{\omega_h}}{1 + \frac{s}{\omega_b}} \right)^\nu \approx C_0 \prod_{k=1}^N \frac{1 + \frac{s}{\omega_k}}{1 + \frac{s}{\omega_k}} \quad (11)$$

where

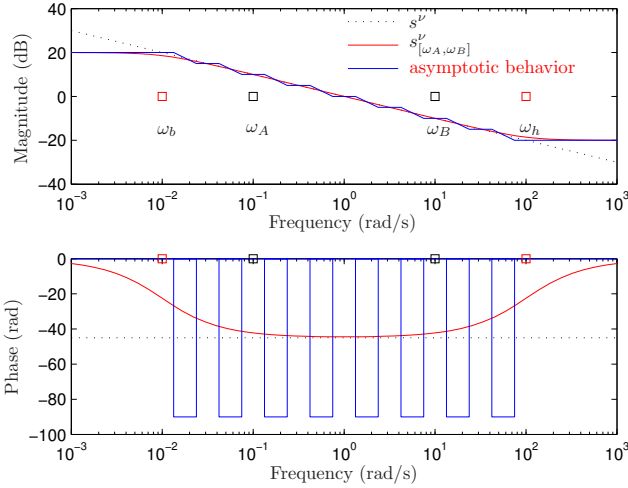


Fig. 2. Fractional integrator $s^{-0.5}$ and its approximation $s_{[0.1,10]}^{-0.5}$ based on recursive poles and zeros realization Oustaloup (1995), for $\sigma = 10$ in (10)

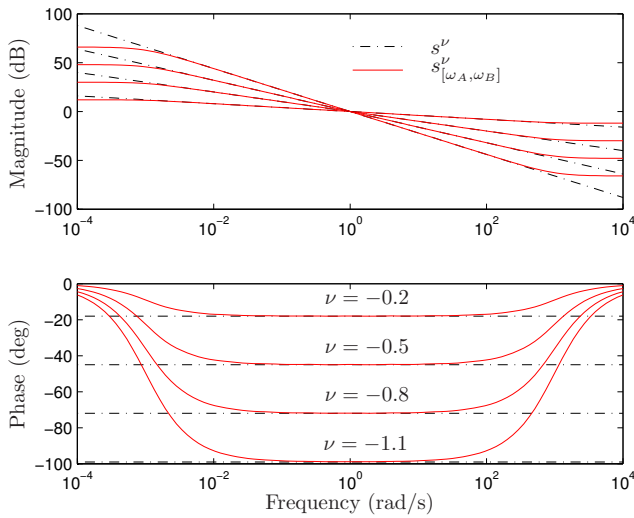


Fig. 3. Fractional integrators s^ν and their approximation $s_{[10^{-2}, 10^2]}^\nu$ for $\nu = -0.2, -0.5, -0.8$ and -1.1 , for $\sigma = 10$

$$\omega'_0 = \alpha^{\frac{1}{2}} \omega_b, \quad \omega_0 = \alpha^{\frac{1}{2}} \eta \omega_b, \quad (12)$$

$$\frac{\omega_{k+1}}{\omega'_k} = \alpha, \quad \frac{\omega'_{k+1}}{\omega_k} = \eta, \quad (13)$$

$$C_0 = \left(\frac{\omega_h}{\omega_b} \right)^\nu \left(\frac{1 + \omega_b^2}{1 + \omega_h^2} \right)^{\frac{\nu}{2}}. \quad (14)$$

The real parameters α and η define by their own the differentiation order ν :

$$\nu = \frac{\log(\alpha)}{\log(\alpha \cdot \eta)}. \quad (15)$$

N is the number of poles and zeros used to approximate $s_{[\omega_A, \omega_B]}^\nu$, which tends theoretically to ∞ . But, an approximation with 2 poles and zeros per decade leads already to an acceptable error.

4. SYNTHESIS OF HAVRILIAC-NEGAMI FUNCTION

In this paper, Havriliak-Negami function:

$$F_{hn}(s) = (s^{\nu_1} + \omega_u)^{\nu_2} \quad (16)$$

is synthesized for $\nu_2 \in \mathbb{R}$, and $(\nu_1, \omega_u) \in \mathbb{R}_+^2$.

Consider M as the number of s -roots P_1, P_2, \dots, P_M of $F_{hn}(s)$. M depends on ν_1 as explained in part I. Hence, $F_{hn}(s)$ can be written as:

$$F_{hn}(s) = \left[\prod_{m=1}^M (s - P_m) F(s) \right]^{\nu_2} \kappa(s) \quad (17)$$

with

$$F(s) = \left(s + \omega_u \frac{1}{(\nu_1 - M)} \right)^{(\nu_1 - M)}. \quad (18)$$

The part between squared brackets has the same asymptotic behavior than $F_{hn}(s)$. $\kappa(s)$ is then defined as the ratio of $F_{hn}(s)$ and its asymptotic behavior (the function between the squared brackets). $F_{hn}(s)$ is then

$$F_{hn}(s) = \left[\prod_{m=1}^M (s - P_m)^{\nu_2} \left(s + \omega_u \frac{1}{(\nu_1 - M)} \right)^{\nu_2(\nu_1 - M)} \right] \kappa(s). \quad (19)$$

Since the s -roots (obtained when $\nu_1 > 1$), introduce nothing else but additional Davidson-Cole functions which synthesis are known (Oustaloup (1995)), **only the case $\nu_1 \in]0, 1[$ is considered in this paper.**

Thus, $F_{hn}(s)$ can be split into the product of two functions:

$$F_{hn}(s) = F_1(s) \cdot \kappa(s) \quad (20)$$

where F_1 corresponds to a Davidson-Cole elementary function:

$$F_1(s) = \left(s + \omega_u \frac{1}{\nu_1} \right)^{\nu_1 \cdot \nu_2}. \quad (21)$$

The asymptotic behaviors of $F_{hn}(j\omega)$ and $F_1(j\omega)$ when $\omega \rightarrow 0$ and $\omega \rightarrow +\infty$ are the same, since

$$\lim_{\omega \rightarrow 0} F_{hn}(j\omega) = \lim_{\omega \rightarrow 0} F_1(j\omega) = \omega_u^{\nu_2}. \quad (22)$$

$$\lim_{\omega \rightarrow \infty} F_{hn}(j\omega) = \lim_{\omega \rightarrow \infty} F_1(j\omega) = j\infty. \quad (23)$$

Moreover, in the vicinity of $\omega \rightarrow \infty$, both functions converge to the same rate:

$$F_{hn}(j\omega) \sim (j\omega)^{\nu_1 \nu_2}, \quad \text{as } \omega \rightarrow \infty \quad (24)$$

$$F_1(j\omega) \sim (j\omega)^{\nu_1 \nu_2}, \quad \text{as } \omega \rightarrow \infty. \quad (25)$$

As seen previously, $F_1(s)$ is approximated by a recursive distribution of poles and zeros. The additional function

$$\kappa(s) = \frac{F_{hn}(s)}{F_1(s)}, \quad (26)$$

plotted in Fig. 4, plays a significant role in median frequencies (around $\omega_u^{\frac{1}{\nu_1}}$). Its synthesis is developed in section 4.1.

Remarks

- (1) When ν_1 tends to 1, the Havriliak-Negami function (16) tends to the Davidson-Cole function (21), $\kappa(s)$ tends to 1, and hence, $F_{hn}(s)$ tends to $F_1(s)$.
- (2) When ν_1 tends to 0, the Havriliak-Negami function (16) is far from the Davidson-Cole function, $\kappa(s)$ tends to $F_{hn}(s)$ (20), and hence, $F_1(s)$ tends to 1.

4.1 Basic synthesis of $\kappa(s)$

The gain diagram of $\kappa(s)$, is log-symmetric with respect to $\omega_u^{\frac{1}{\nu_1}}$ (Fig. 4). The principle of poles and zeros recursive distribution underlined in section 3 is now used to synthesize $\kappa(s)$ in the frequency band $[\frac{\omega_u}{\Delta}, \omega_u \Delta]$. Δ leads to the necessary log-symmetry of this frequency band,

$$\Delta = \max(\Delta_1, \Delta_2), \quad (27)$$

with Δ_1 and Δ_2 such that:

$$\Delta_1 = \max\left(\frac{\omega_u}{\sigma \cdot \omega_h}, \frac{\sigma \cdot \omega_h}{\omega_u}\right), \quad (28)$$

$$\Delta_2 = \max\left(\frac{\sigma \cdot \omega_u}{\omega_b}, \frac{\omega_b}{\sigma \cdot \omega_u}\right). \quad (29)$$

as presented by figure 4, and $\sigma = 100$.

This frequency band $[\frac{\omega_u}{\Delta}, \omega_u \Delta]$ is subdivided into $2N$ bands, namely $[\omega_{e_k}, \omega_{e_{k+1}}]$ for $k = 1, 2, \dots, 2N$, such as

$$\omega_{e_1} = \frac{\omega_u}{\Delta}, \quad (30)$$

and

$$\frac{\omega_{e_{k+1}}}{\omega_{e_k}} = \Delta^{\frac{1}{2N}}. \quad (31)$$

Then, a recursive distribution of M_k poles and zeros is applied on every $[\omega_{e_k}, \omega_{e_{k+1}}]$ frequency band. Hence, for each m^{th} frequency band:

$$\omega'_{k,0} = \alpha_k^{\frac{1}{2}} \omega_{e_k}, \quad \omega_{k,0} = \alpha_k^{\frac{1}{2}} \eta_k \omega_{e_k}, \quad (32)$$

$$\frac{\omega'_{k,m+1}}{\omega'_{k,m}} = \alpha_k, \quad \frac{\omega'_{k,m+1}}{\omega_{k,m}} = \eta_k. \quad (33)$$

The real parameters α_k and η_k define a local differentiation order ν_k :

$$\nu_k = \frac{\log(\alpha_k)}{\log(\alpha_k \cdot \eta_k)}. \quad (34)$$

Thus, the approximation $\kappa_1(s)$ of $\kappa(s)$ in the frequency band $[\frac{\omega_u}{\Delta}, \omega_u \Delta]$ is given by:

$$\kappa(s) \approx \kappa_1(s) = \prod_{k=1}^{2N} \prod_{m=1}^{M_k} \frac{s + \omega'_{k,m}}{s + \omega_{k,m}}. \quad (35)$$

If M_k is defined by ν_1 , N is fixed such that 2 poles and zeros per decade for the frequency band, which is typically enough to synthesis κ and F_1 functions.

Finally, by ordering all the poles and all the zeros as a global non recursive distribution, $\kappa_1(s)$ can be written as the following product:

$$\kappa_1(s) = \prod_{i=1}^{2N \cdot M_k} \frac{s + \omega'_i}{s + \omega_i}. \quad (36)$$

4.2 Improved synthesis of $\kappa(s)$

While synthesizing $\kappa_1(s)$, the modulus of the error $(\kappa(j\omega) - \kappa_1(j\omega))$, $\omega \in [\frac{\omega_u}{\Delta}, \omega_u \Delta]$, is maximum at $\omega_u^{\frac{1}{\nu_1}}$.

For $\nu_1 \rightarrow 0$, the gain of the Davidson-Cole function is much less than the gain of $\kappa_1(s)$ at $\omega_u^{\frac{1}{\nu_1}}$.

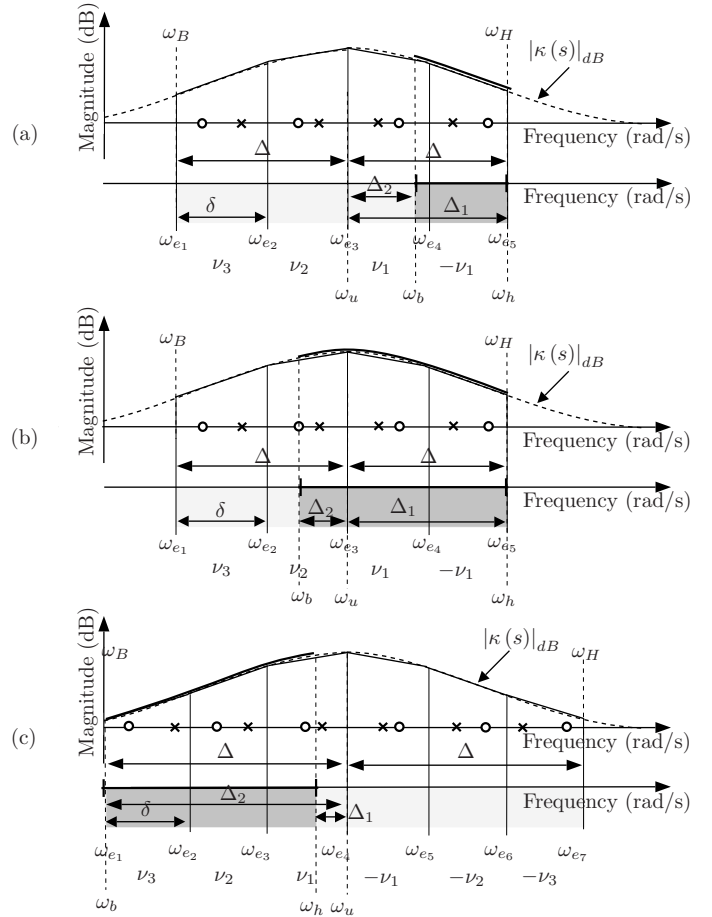


Fig. 4. Principles of the non recursive distribution of poles (\times) and zeros (\circ) for the synthesis of $\kappa(s)$ on the frequency band $[\omega_b, \omega_h]$, for (a) $\omega_u \leq \omega_b \leq \omega_h$, (b) $\omega_b \leq \omega_u \leq \omega_h$ and (c) $\omega_b \leq \omega_h \leq \omega_u$

In the opposite case, for $\nu_1 \rightarrow 1$, the gain of $\kappa_1(s)$ is much less than the gain of the Davidson-Cole function at $\omega_u^{\frac{1}{\nu_1}}$.

Based on remarks about influences of ν_1 on κ (see part Remarks), an improved synthesis of $\kappa(s)$ is obtained by using $\kappa_2(s)$, which is a weighted $\kappa_1(s)$ approximation:

$$\kappa_2(s) = (1 - \nu_1) \cdot \kappa_1(s). \quad (37)$$

The use of $\kappa_2(s)$ allows to reduce considerably the synthesis error around $\omega_u^{\frac{1}{\nu_1}}$ by attenuating edge effects as ν_1 tends to 1 (κ tends to 0 in this case). Fig. 5 and 6 show the improvements introduced by the approximation $\kappa_2(s)$ of $\kappa(s)$ as compared the approximation $\kappa_1(s)$.

4.3 Synthesis of Havriliak-Negami elementary function using κ_2 approximation

Syntheses for $F_{hn}(s) = (s^{\nu_1} + 1)^{\nu_2}$ with $\nu_2 = -0.5$ and ν_1 respectively equal to 0.1, 0.25, 0.5, 0.75 and 0.9 are presented on Fig. 7. The frequency band used for synthesis is symbolized by squares and corresponds to $[0.1, 10]$ rad/s.

5. IDENTIFICATION OF A THERMAL SYSTEM

To illustrate the use of fractional models in system identification, a semi-infinite dimensional thermal system is

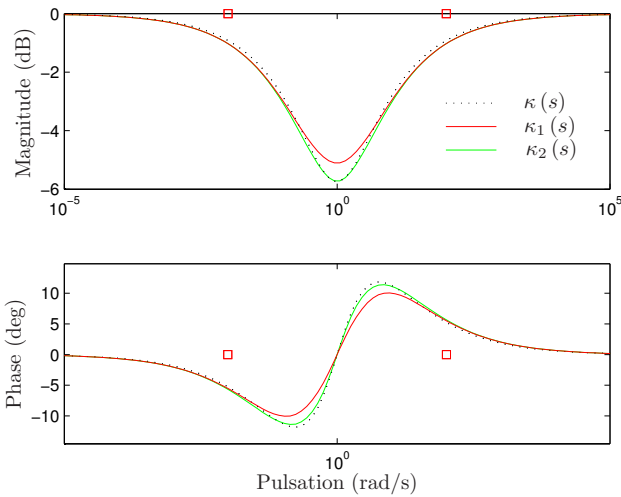


Fig. 5. Comparison between synthesis of $\kappa_1(s)$ and $\kappa_2(s)$ linked to the Havriliak-Negami function $F(s) = (s^{0.5} + 1)^{-1.5}$ on the frequency band $[0.01, 100]$ (\square symbols) with two poles and two zeros per decade and the frequency band spreading factor $\sigma = 100$

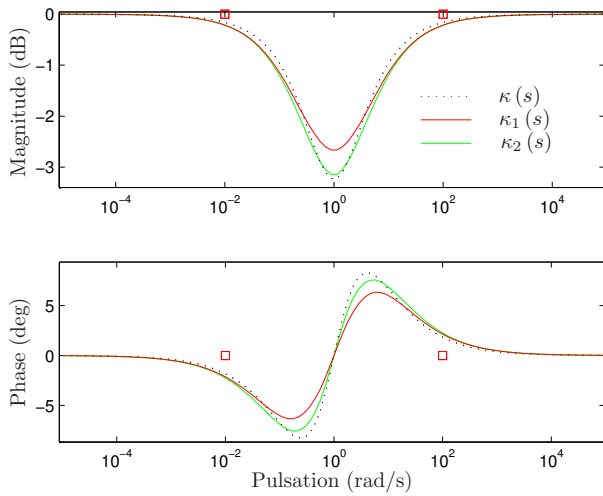


Fig. 6. Comparison between synthesis of $\kappa_1(s)$ and $\kappa_2(s)$ linked to the Havriliak-Negami function $F(s) = (s^{0.75} + 1)^{-1.5}$ on the frequency band $[0.01, 100]$ (\square symbols) with two poles and two zeros per decade and the frequency band spreading factor $\sigma = 100$

considered (Sabatier et al. (2005)). It is constituted of a long aluminium rod heated by a resistor. To ensure unidirectional heat transfer, the entire surface of the rod is insulated. The temperature of the rod is measured at a distance $x = 5\text{mm}$ from the heated end (Fig. 8).

The thermal system is considered as a semi-infinite plane homogenous medium initially at ambient temperature. Losses on the surface where the thermal flux is applied are neglected.

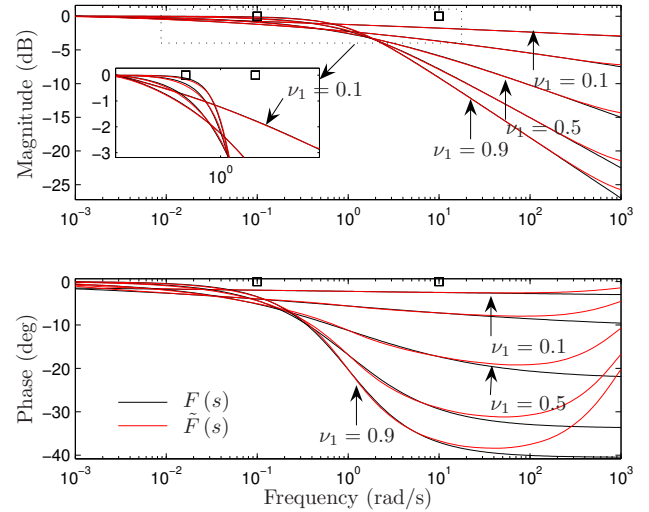


Fig. 7. Bode diagram of function $F_{hn}(s) = (s^{\nu_1} + 1)^{-0.5}$ on the frequency band $[0.1, 10]$ and $\nu_1 = 0.1, 0.25, 0.5, 0.75$ and 0.9

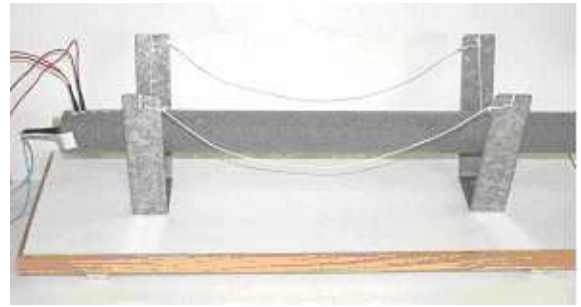


Fig. 8. Insulated long aluminium rod heated by a resistor. A pseudorandom binary sequence is used as input signal. The sampling period is fixed to $T_e = 0.5\text{s}$. $[\omega_b, \omega_h]$ are then as $[\frac{1}{100 N_{points} T_e}, 100 * \frac{2\pi}{T_e}]$ with $N_{points} = 4400$. For Δ equal to 4 decades, the number of poles and zeros (N) for the approximation of the Havriliak-Negami is then 16. The fractional integrator approximation leads to the same number of poles and zeros on this frequency band.

Prior knowledge shows the presence of a fractional integrator in the model which is therefore set to:

$$F(s) = \frac{k}{s^\nu (s^{\nu_1} + \omega_u)^{\nu_2}} \quad (38)$$

One can notice that a Havriliak-Negami elementary function is chosen in the model (38). Its synthesis is carried out as described in this paper with the following parameters. The spreading factor is set to $\sigma = 100$ to reduced edge effect and the number of poles and zeros, used to synthesize $\kappa_2(s)$ and F_1 functions, is set to 2 per decade.

The system is identified by applying output error model. Parameter vector $[k, \nu, \nu_1, \nu_2, \omega_u]$ is optimized by using the non-linear Simplex optimisation algorithm (Subrahmanyam (1989); Woods (1985)). The obtained model is:

$$F(s) = \frac{5 \times 10^{-3}}{s^{0.32} (s^{0.50} + 0.51)^{3.49}} \quad (39)$$

and has only five parameters.

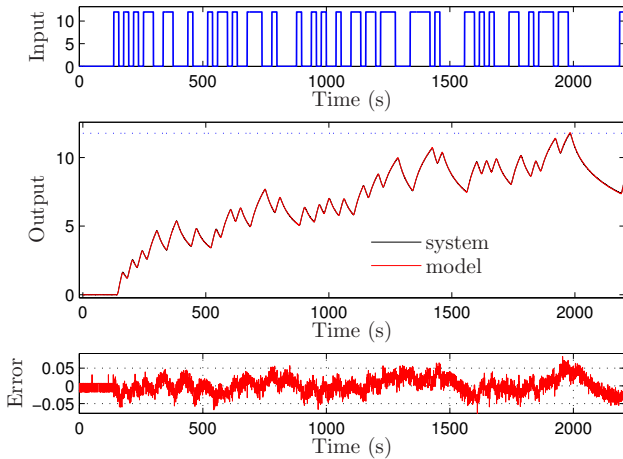


Fig. 9. System identification using a Havriliak-Negami function and modeling error

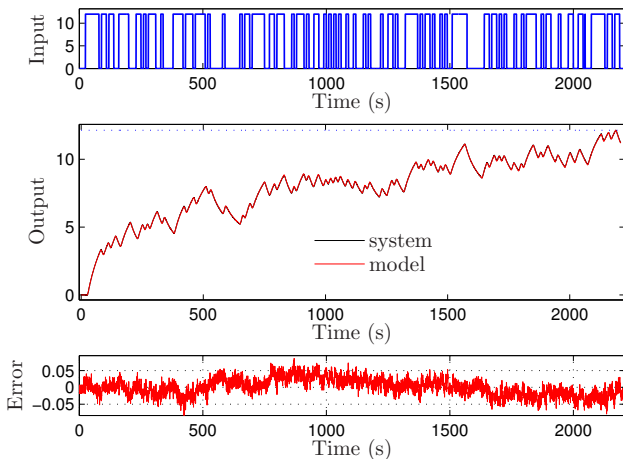


Fig. 10. System identification using a Havriliak-Negami function and modeling error on validation data

As shown on validation data of Fig. 10, the identified model (Fig. 9) gives satisfactory results. The error variance is $\sigma^2 = 5.1 \cdot 10^{-4}$ with this model, while by using Cole-Cole functions, a variance $\sigma^2 = 9.4 \cdot 10^{-4}$ for 6 parameters (Malti et al. (2006)).

6. CONCLUSION

Fractional (non integer) operators has proven their usefulness in representing high dimensional systems with only few parameters.

Among different fractional elementary functions, the Havriliak-Negami function is not very popular because of the difficulty of its synthesis. Hence, a new synthesis method is developed in this paper. Havriliak-Negami function is first split into a Davidson-Cole and a complementary functions, both of which are then synthesized in

a limited frequency band using poles and zeros recursive distribution developed by Oustaloup (1995).

Finally, to illustrate the usefulness of Havriliak-Negami function a real thermal diffusive system is identified on the basis of this function.

The next step of our study would provide a method to control the synthesis approximation error.

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