Havriliak-Negami function for thermal system identification

Laurent Sommacal, Pierre Melchior and Alain Oustaloup

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 based on the splitting the Havriliak-Negami function into a Davidson-Cole function and a complementary one. Both functions are then synthesized in a limited frequency band using a recursive distribution of poles and zeros developed by [Ous95].

Havriliak-Negami function is then applied to model a thermal flux in the field of machining by turning, in the time domain.

I. INTRODUCTION

Although fractional (non integer) operators remained for a long time a purely 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 developments 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 ([Lin01], [Coi02], [Aou05]). 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, the Cole-Cole ([CC41]) and Davidson-Cole ([DC51]) functions, both defined later, the objective of this paper is to propose a synthesis method for Havriliak-Negami function ([HN66], [HN67]). 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 II, principles of the frequency-band-fractionalintegrator synthesis is explained. Part III is devoted to the synthesis of the Davidson-Cole function extended to complex

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zeros. Next in section IV, the Havriliak-Negami function is split into two functions each of which is then synthesized. In part V, the synthesis for internal order $\in \mathbb{R}_+$. Finally, a Havriliak-Negami function is applied to model a thermal system in the field of machining by turning.

II. MATHEMATICAL BACKGROUND

The concept of differentiation to an arbitrary order (noninteger),

$$\mathbf{D}^{\nu} \stackrel{\Delta}{=} \left(\frac{d}{dt}\right)^{\nu} \tag{1}$$

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 $|\nu| + 1$ (|.| stands for the floor operator) of a non-integer integral of order $\nu - |\nu|$ [SKM93]:

$$\mathbf{D}^{\nu}f(t) = \mathbf{D}^{\lfloor\nu\rfloor+1} \left(\mathbf{I}^{\lfloor\nu\rfloor+1-\nu}f(t) \right)$$
$$\stackrel{\Delta}{=} \frac{1}{\Gamma\left(\lfloor\nu\rfloor+1-\nu\right)} \left(\frac{d}{dt}\right)^{\lfloor\nu\rfloor+1} \int_{0}^{t} \frac{f(\tau) d\tau}{(t-\tau)^{\nu-\lfloor\nu\rfloor}} \quad (2)$$

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

$$\Gamma(x) = \int_{0}^{\infty} e^{-t} t^{x-1} dt, \quad \forall x \in \mathbb{R}^* \setminus \{\mathbb{N}^-\}.$$
 (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) [OS74]:

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

Two elementary fractional-differentiation functions are generally used for representing fractional transfer functions: the Davidson-Cole function ([DC51])

$$F_{dc}\left(s\right) = \frac{A}{\left(s + \omega_{u}\right)^{\nu}},\tag{5}$$

and the Cole-Cole function ([CC41])

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

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 [Ous83], [Ous95], $F_{cc}(s)$ might have s-poles at:

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

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

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

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

A third elementary function (Havriliak-Negami) was proposed by [HN66], [HN67]:

$$F_{hn}(s) = \frac{A}{(s^{\nu_1} + \omega_u)^{\nu_2}}.$$
(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 [Lau03] 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 behaviour.

The objective of this paper is to develop a rational realization of Havriliak-Negami elementary function on a bandlimited frequency for $\nu_1 \in \mathbb{R}_+$ and $\nu_2 \in \mathbb{R}$, and to prove its capability to model diffusive systems, such that thermal system, with very few parameters.

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 [Ous83], [Ous95].

III. 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. 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 [Ous83] 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

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

A dedicated study [Ous95] has shown that the edge effect is considerably reduced by choosing a frequency-band spreading factor (σ) up to 10 (the approximation is then closer to the fractional behavior on [ω_b, ω_h]). As a result, s^{ν} is approximated on the frequency band [ω_A, ω_B] by:

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

where

$$\omega_0' = \alpha^{\frac{1}{2}} \omega_b, \quad \omega_0 = \alpha^{\frac{1}{2}} \eta \,\,\omega_b, \tag{12}$$

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

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

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

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



Fig. 2. Fractional integrator $s^{-0.5}$ and its approximation $s^{-0.5}_{[0.1,10]}$ based on recursive poles and zeros realization [Ous95], for $\sigma = 10$ in (10)



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

IV. SYNTHESIS OF HAVRILIAK-NEGAMI FUNCTION

In this paper, Havriliak-Negami function:

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

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

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

$$F_{hn}(s) = \left[\prod_{m=1}^{M} \left(s - P_m\right)^{\nu_2} \left(s + \omega_u^{\frac{1}{(\nu_1 - M)}}\right)^{\nu_2(\nu_1 - M)}\right] \kappa(s)$$
(17)

where the asymptotic behaviors of $F_{hn}(s)$ and the function between the squared brackets are the same. Moreover, this asymptotic behavior and a Davidson-Cole lead to the same formulation of their approximation.

 $\kappa(s)$ is defined as the ratio of $F_{hn}(s)$ and the function between the squared brackets.

Thus, since it is not a s-root for $\nu_1 \in [0, 1]$, $F_{hn}(s)$ can be split into the product of two functions:

$$F_{hn}(s) = F_1(s) \cdot \kappa(s) \tag{18}$$

where F_1 corresponds to a Davidson-Cole elementary function:

$$F_1(s) = \left(s + \omega_u^{\frac{1}{\nu_1}}\right)^{\nu_1 \cdot \nu_2}.$$
 (19)

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

$$\lim_{\omega \to 0} F_{hn} \left(j\omega \right) = \lim_{\omega \to 0} F_1 \left(j\omega \right) = \omega_u^{\nu_2}.$$
 (20)

$$\lim_{\omega \to \infty} F_{hn} \left(j\omega \right) = \lim_{\omega \to \infty} F_1 \left(j\omega \right) = j\infty.$$
 (21)

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

$$F_{hn}(j\omega) \sim (j\omega)^{\nu_1\nu_2}, \quad \text{as } \omega \to \infty$$
 (22)

$$F_1(j\omega) \sim (j\omega)^{\nu_1\nu_2}, \quad \text{as } \omega \to \infty.$$
 (23)

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

$$\kappa\left(s\right) = \frac{F_{hn}\left(s\right)}{F_{1}\left(s\right)},\tag{24}$$

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

Remarks

- 1) When ν_1 tends to 1, the Havriliak-Negami function (16) tends to the Davidson-Cole function (19), $\kappa(s)$ 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 $F_{hn}(s)$ (18), and hence, $F_1(s)$ tends to 1.
- A. 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 III is now used to synthesize $\kappa(s)$ in the frequency band $\left[\frac{\omega_u}{\Delta}, \omega_u \Delta\right]$ where

$$\Delta = \max\left(\Delta_1, \Delta_2\right),\tag{25}$$

$$\Delta_1 = \max\left(\frac{\omega_u}{\sigma \cdot \omega_h}, \frac{\sigma \cdot \omega_h}{\omega_u}\right),\tag{26}$$

$$\Delta_2 = \max\left(\frac{\sigma \cdot \omega_u}{\omega_b}, \frac{\omega_b}{\sigma \cdot \omega_u}\right). \tag{27}$$

and $\sigma = 100$.

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

$$\omega_{e_1} = \frac{\omega_u}{\Delta},\tag{28}$$



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

and

$$\frac{\omega_{e_{k+1}}}{\omega_{e_k}} = \Delta^{\frac{1}{N}}.$$
(29)

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:

$$\omega_{k,0}' = \alpha_k^{\frac{1}{2}} \,\omega_{e_k}, \quad \omega_{k,0} = \alpha_k^{\frac{1}{2}} \,\eta_k \,\,\omega_{e_k}, \tag{30}$$

$$\frac{\omega_{k,m+1}}{\omega'_{k,m}} = \alpha_k, \quad \frac{\omega'_{k,m+1}}{\omega_{k,m}} = \eta_k.$$
(31)

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

$$\nu_k = \frac{\log\left(\alpha_k\right)}{\log\left(\alpha_k \cdot \eta_k\right)}.$$
(32)

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

$$\kappa(s) \approx \kappa_1(s) = \prod_{k=1}^{2N} \prod_{m=1}^{M_k} \frac{s + \omega'_{k,m}}{s + \omega_{k,m}}$$
(33)

2 poles and zeros per decade are 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



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

the following product:

$$\kappa_1(s) = \prod_{i=1}^{2N \cdot M_k} \frac{s + \omega'_i}{s + \omega_i}.$$
(34)

B. Improved synthesis of $\kappa(s)$

While synthesizing $\kappa_1(s)$, the modulus of the error $(\kappa(j\omega) - \kappa_1(j\omega)), \omega \in \left[\frac{\omega_u}{\Delta}, \omega_u \Delta\right]$, is maximum at $\omega_u^{\frac{1}{\nu_1}}$. For $\nu_1 \to 0$, the gain of the Davidson-Cole function is much less than the gain of $\kappa_1(s)$ at $\omega_u^{\frac{1}{\nu_1}}$.

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

An improved synthesis of κ (s) is obtained by using κ_2 (s), which is a weighted κ_1 (s) approximation:

$$\kappa_2\left(s\right) = \nu_1 \cdot \kappa_1\left(s\right). \tag{35}$$

The use of $\kappa_2(s)$ allows to reduce considerably the synthesis error around $\omega_u^{\frac{1}{\nu_1}}$. Fig. 5 shows the improvements introduced by the approximation $\kappa_2(s)$ of $\kappa(s)$ as compared to the approximation $\kappa_1(s)$.

C. 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. 6. The frequency band used for synthesis is symbolized by squares and corresponds to [0.1, 10] rad/s.

V. EXTENSION OF THE METHOD FOR $\nu_1 \in \mathbb{R}_+$

As explained in section II, a function

$$F_{cc}\left(s\right) = s_{1}^{\nu} + \lambda \tag{36}$$



Fig. 6. Bode diagram of function $F_{hn}(s) = (s^{\nu_1} + 1)^{-0.5}$ on the frequency band [0.1, 10] pour ν_1 =0.1, 0.25, 0.5, 0.75 and 0.9

has M s-roots, depending on the fractional order ν_1 . The synthesis when $\nu \geq 1$, which implies $M \geq 1$, is then developed.

Due to these M s-roots, the Havriliak-Negami function, $F_{hn}(s)$ becomes (17). Thus, every Davidson-Cole function, such that $(s + \omega_a)^{\nu}$ (with $\omega_a = \lambda_k$ or λ), are approximated with recursive poles and zeros distributions (section III). Indeed, as ω_b is replaced by λ and considering $\omega_h >> \lambda$, equation (11) leads to

$$(s+\lambda)^{\nu} \approx \left(\frac{s+\lambda}{s+\omega_h}\right)^{\nu} \approx \prod_{k=1}^{N} \frac{s+\omega'_k}{s+\omega_k}.$$
 (37)

where ω' and ω are calculated by the relations (12)-(15). It leads to the following relation for $\nu > 0$:

$$\tilde{F}_{hn}(s) = \prod_{m=1}^{M} \prod_{k_{1}=1}^{K_{1}} \frac{s + \omega'_{mk_{1}}}{s + \omega_{mk_{1}}} \bigg|_{\nu_{1} > 1} \\
\prod_{k_{2}=1}^{K_{2}} C_{2} \frac{s + \omega'_{k_{2}}}{s + \omega_{k_{2}}} \bigg|_{K_{3}=1} C_{3} \frac{s + \omega'_{k_{3}}}{s + \omega_{k_{3}}} \bigg|_{\kappa_{2}(s)}$$
(38)

and finally, by ordering all poles and all zeros, to the relation:

$$\tilde{F}_{hn}\left(s\right) = \prod_{i=1}^{M \cdot K_1 K_2 \cdot K_3} \frac{s + \omega'_i}{s + \omega_i}.$$
(39)

The result of this synthesis is shown on the Bode diagram for $F_{hn}(s) = (s^{\nu_1} + 1)^{-0.5}$ with $\nu_1 = .1, 0.25, ..., 0.9$ (Fig. 6) and for $F_{hn}(s) = (s^{\nu_1} + 1)^{-1.5}$ with $\nu_1 = 1.1, 1.3, ..., 1.9$ (Fig. 7).

VI. EXAMPLE

Thermal systems have a fractional nature. Cole-Cole function had been previously used to model the thermal flux in a thermal bench with few parameters ([SMO05], [MASO06]). A model based on Havriliak-Negami functions



Fig. 7. Bode diagram of function $F_{hn}(s) = (s^{\nu_1} + 1)^{-1.5}$ on the frequency band [0.1, 10] pour ν_1 =1.1, 1.3, 1.5, 1.7 and 1.9



Fig. 8. Description of operation

allow even more to reduce the number of model parameters ([SMMO08]).

In this paper, the example concerns a thermal application in the field of machining by turning (See [BCPO01] for a more complete description of the experimental protocole). The goal is to estimate the heat flux $\phi(t)$ during machining, by using an inverse model obtained off-line and using system identification (as direct measurement of heat flux is not possible).

To obtain the machining tool model, a thermocouple (type T) is embedded close to the tip of the insert tool (Fig. 8). Heat flux is then generated using a heat resistor formed by a platinum film (10 μ m) placed on a thin ceramic substrate (250 μ m). This leads to neglect the thermal inertia of such a resistor compared to the sampling interval (h=0.4s). Two sequences have been generated, one for parameter estimation and the second one for model validation. A first pseudorandom binary sequence is used as input signal. The system is identified by applying output error model. Due to its flexibility in the frequency domain with only 4 parameters, our model is then based on the Havriliak-Negami function. In fact, a fractional integrator proved to be necessary, and



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



Fig. 10. Validation data and modeling error using Havriliak-Negami function

the model is therefore set to:

$$F(s) = \frac{k}{s^{\nu} \left(s^{\nu_1} + \omega_u\right)^{\nu_2}}.$$
 (40)

 s^{ν} is then approximated as in section III and $(s^{\nu_1} + \omega_u)^{\nu_2}$ as in IV. 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 ([Sub89], [Woo85]). The obtained model has then only five parameters:

$$\mathscr{M}(s) = \frac{T(s)}{\phi(s)} = \frac{2.54\,10^3}{s^{0.27}\left(s^{0.93} + 0.29\right)^{1.49}} \tag{41}$$

for a variance $\sigma^2 = 1.41 \, 10^{-5}$. Fig. 9 shows model/system outputs and error. Model validation with the second pseudo-random binary sequence is shown on Fig. 10.

VII. 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 function and a complementary one, both of which are then synthesized in a limited frequency band using a recursive distribution of poles and zeros developed by [Ous95].

Finally, to prove the capability of this function for diffusive systems identification, a real thermal system in the field of machining by turning is modeled.

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