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A new Network Simulation Method for the characterization of delay differential equations

Manuel Caravaca Garratón [a], María del Carmen García-Onsurbe [b], Antonio Soto-Meca [a,*]

[a] Department of Science, University Centre of Defence at the Spanish Air Force Academy, c/ Coronel López Peña s/n, San Javier 30720, Spain
[b] Technical University of Cartagena, Campus Alfonso XIII, Paseo Alfonso XIII 48, Cartagena 30203, Spain

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ABSTRACT

In this work, we provide for the first time the characterization of delay terms in systems of delay differential equations within the frame of the Network Simulation Method, a procedure that sets a formal equivalence between the system of differential equations and an electrical network. The results were not achieved previously, which strengths the formalism of the model and provides new opportunities for the method. Free circuit software LTspice is employed to conduct the simulations, which requires few simulation rules and can be programmed either by electrical symbol code or text file. Very few devices are needed to design the network model, and the delay terms are easily implemented by voltage-controlled voltage sources. A practical example for delayed adsorption/desorption kinetics is employed to test the methodology, being the results compared with software Mathematica. Additionally, the modelling of pulse width in passively mode-locked quantum dot lasers by the application of a reverse bias voltage is addressed, which constitutes a promising application in communications and advanced sensing. The power, versatility and simplicity of the Network Simulation Method enables it as an exceptional alternative to solve complex systems described by delay differential equations, from both researching and educational points of view.

1. Introduction

Delay differential equations (DDEs) have gained importance in recent years, applied to the mathematical description of scientific-technical and socioeconomical systems [1], considering that is a common feature for natural processes to present memory effects. Examples include tumor-immune response via chemoimmunotherapy, synchronization of chaos for arrays of Josephson junctions applied to communications, adsorption kinetics, theory of chemical reactions, complex balanced kinetic systems with distributed time delays, or replicator dynamics with discrete multi-delays, among others [1–6]. Remarkably, the global pandemic situation due to COVID-19 has led to important advances in the dynamics of fractional-order delay models to study the disease, including delay terms associated to quarantine such as social distance, immigration and isolation [7]. Additionally, recent advances in mathematics focus on the study of random DDEs and new numerical procedures for DDEs with boundary conditions [8–10], which enables this discipline as a significant area of research.

Among the numerical approaches, the Network Simulation Method (NSM) is a highly efficient procedure to solve systems of coupled differential equations [11,12], based on the electrical analogy of transport processes [13]. Recent applications of the method include the thermal insulation of unmanned underwater vehicles, the evaluation of perturbed supply chains of a finite horizon, or the study of differential equations exhibiting singularities and chaotic behavior, qualifying the NSM as a powerful approach to characterize the nonlinear dynamics in diverse areas [14–16]. Besides, the authors developed NSM software FATSIM-A and SimKinet as free educational tools to simulate flow transport in porous media and chemical kinetic equations, respectively [13,17]. Despite all these advances, the implementation of delay terms

* Corresponding author.
E-mail addresses: manuel.caravaca@cud.upct.es (M. Caravaca Garratón), mariadelcarmen.garcia2@edu.upct.es (M.C. García-Onsurbe), antonio.soto@cud.upct.es (A. Soto-Meca).

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has not been previously addressed for the NSM, which results in a lack in its theoretical frame.

In this work we characterize for the first time the delay dependence for the NSM, which immediately opens new applications to the method. We will illustrate the implementation of the delay terms in the electrical analogy through the employment of a first order delay equation, the Hutchinson's model, and we will apply the approach to two practical examples of interest: (a) adsorption kinetics with time delay, extendable to the oscillatory molecular adsorption patterns in proteins [3], and (b) modeling of pulse width in quantum dot mode-locked lasers (QDMLLs), essential for communication, medical, micromachining and military applications, among others [18–22]. Additionally, we will compare the results with those obtained with software Mathematica [23], showing that they are orders of magnitude faster. The reason is that very few electrical devices and programming rules are required to design the network model.

In general, the NSM electrical analogy will lead to an equivalence between a system of DDEs and an electrical network, which is solved by means of appropriate circuit software. This last choice is not unique, but in this work we have selected the freeware LTspice [24], which adds value in terms of simplicity and usability, taking advantage of the powerful numerical codes embodied [25]. Additionally, LTspice presents a user-friendly environment, making the whole approach accessible for both researching and educational purposes in different areas.

2. Network simulation method and delay differential equations

2.1. NSM and DDEs electrical analogy

The NSM is a numerical procedure for the study of physical systems modeled by sets of differential equations, which is based on the electrical analogy of transport processes [26,27]. The approach consists of two well differentiated stages. Firstly, an electrical circuit equivalent to the mathematical model, including the initial and boundary conditions, is obtained. Secondly, subsequent numerical resolution of the network model is conducted by means of a suitable electrical circuit software. An independent electrical circuit corresponds to each differential equation of the mathematical model, being all connected by a common ground node, thus constituting an electrical network. For physical transport processes, the NSM establishes a correspondence between flow and potential variables with electric currents and electric potentials, respectively [11].

In order to show how the electrical analogy establishes equivalence between a set of coupled differential equations and an electric circuit network, it is particularly useful to visualize the process through the example of the kinetics of a chemical reaction, which is well known to be described by a set of coupled ordinary differential equations.

Consider the balance equation of a multiple chemical reaction that represents the relative amounts of reactants, R_i, and products, P_j:

$$\left\{\sum_i \nu_{R_i} R_i \underset{k_b}{\overset{k_f}{\rightleftarrows}} \sum_j \nu_{P_j} P_j\right\}_s ; s = 1, 2, \cdots \tag{1}$$

where ν_{R_i} and ν_{P_j} stand for the stoichiometric coefficients of R_i and P_j, and k_f, k_b are the forward and backward kinetic constants, respectively. The index s labels each equation.

With the aim to assign sign to the stoichiometric coefficients, which will be useful for the derivation, $\nu^*_{R_i}$ and $\nu^*_{P_j}$ are introduced in Eq. (1):

$$\left\{0 \underset{k_b}{\overset{k_f}{\rightleftarrows}} \sum_i \nu^*_{R_i} R_i + \sum_j \nu^*_{P_j} P_j\right\}_s ; s = 1, 2, \cdots \tag{2}$$

where $\nu^*_{R_i} = -\nu_{R_i}$ and $\nu^*_{P_j} = \nu_{P_j}$.

The molar flows J_{R_i} and J_{P_j} for each reaction s are defined as follows [28]:

$$J_{R_i} = \frac{dn_{R_i}}{dt} \quad J_{P_j} = \frac{dn_{P_j}}{dt} \tag{3}$$

being n_{R_i} and n_{P_j} the number of moles of species R_i and P_j, respectively. Since the molar concentration and the number of moles are related through the volume of the reactive medium V by $c_{R_i} = \frac{n_{R_i}}{V}$ (equivalent for products), Eq. (3) can be rewritten as:

$$J_{R_i} = V\frac{dc_{R_i}}{dt} \quad J_{P_j} = V\frac{dc_{P_j}}{dt} \tag{4}$$

The molar flows can be expressed in terms of the so-called reaction rate $J^{\mathscr{R}}_s$, a measure of the change in the concentrations of the reactants and products per unit time, according to [13]:

$$-\frac{J_{R_i}}{\nu_{R_i}} = \frac{J_{P_j}}{\nu_{P_j}} = J^{\mathscr{R}}_s \tag{5}$$

$$\frac{V}{\nu^*_{R_i}}\frac{dc_{R_i}}{dt} = \frac{V}{\nu^*_{P_j}}\frac{dc_{P_j}}{dt} = J^{\mathscr{R}}_s \tag{6}$$

Eq. (6) establishes the mass local balance corresponding to both R_i and P_j, where there is a creation-annihilation term given by reaction rate $J^{\mathscr{R}}_s$, determined by the mass action law [28]:

$$J^{\mathscr{R}}_s = k_f \prod_i {c_{R_i}}^{\nu_{R_i}} - k_b \prod_j {c_{P_j}}^{\nu_{P_j}} \tag{7}$$

Eq. (6) can be rewritten for reactants and products, respectively, as follows:

$$J^{\mathscr{R}}_s - J_{\gamma_i} = 0 \text{ and } J^{\mathscr{R}}_s - J_{\gamma_j} = 0 \tag{8}$$

where $J_{\gamma_i} = \frac{V}{\nu^*_{R_i}}\frac{dc_{R_i}}{dt}$ and $J_{\gamma_j} = \frac{V}{\nu^*_{P_j}}\frac{dc_{P_j}}{dt}$ are known as the cumulative flows.

For the general case, each species takes part in more than one reaction. For instance, if species A takes part in each reaction, a partial balance equation is obtained for each reaction, following the form:

$$\left[\frac{V}{\nu^*_A}\frac{dC_A}{dt} = J^{\mathscr{R}}\right]_s \tag{9}$$

or

$$\left[\frac{dc_A}{dt}\right]_s = \pm\left[\frac{\nu_A}{V}J^{\mathscr{R}}\right]_s \tag{10}$$

The total change in concentration c_A sums up the contributions of each reaction s, whose expression is given by [28]:

$$\frac{dc_A}{dt} = \sum_s \left[\frac{dc_A}{dt}\right]_s = \pm\frac{1}{V}\sum_s \nu_{As} J^{\mathscr{R}}_s \tag{11}$$

The total flow $J_{\gamma A}$ is defined by:

$$\sum_s J^{\mathscr{R}}_s - J_{\gamma A} = 0 \tag{12}$$

Eq. (12) can be considered as Kirchhoffs current law (KCL) at the node c_A from the point of view of the network model, and it is equivalent to the corresponding differential equations of each chemical species. The flow term $J_{\gamma A}$ resembles the expression of

the current through a capacitor when the voltage c_A is applied at its ends, since the constitutive equation between the current I and voltage $\mathscr{V}$ at a capacitor is given by $I = \mathscr{C}\frac{d\mathscr{V}}{dt}$, $\mathscr{C}$ being the capacity of the capacitor.

Because of this similarity, the first-order derivative of the concentration is easily implemented in the model via a capacitor, whose voltage $\mathscr{V}$ is then equivalent to c_A. The term $\sum_s J_s^{\mathscr{R}}$ in Eq. (12) represents the relations between the flows of the reactants and the products. These terms are easy to determine since each equation must satisfy KCL, because they represent mass local balanced equations. They can be implemented in the network model through devices named voltage-controlled current sources. These generators are able to model any kind on non-linearity [11].

Concentration c_A is always a positive quantity, so if a ground node at one end of the capacitor to design the equivalent circuit is chosen, the current branch is always outgoing from a particular node c_A (see Fig. 1). Its related voltage is just the voltage of the capacitor. Since the first derivative has units of current, the rest of the addends also have, representing $J_s^{\mathscr{R}}$ all the remaining addends. Each of these addends must be considered in the electric circuit as a parallel branch to verify KCL. Since all the species concentrations are positive, also all the node voltages are, and the mathematical sign of each addend determines if the branch current is incoming or outgoing.

After visualizing the general formalism of the NSM, now we describe the implementation of delay terms for the model. To illustrate the procedure, we will choose a system of delay differential equations, where the i-th equation has the form:

$$\frac{dx_i(t)}{dt} = f_i\left(t, \{x_j(t-\tau_j)\}_{j=1,\cdots,n}\right) \tag{13}$$

where f_i is a function of time t and variables x_j, which depend on time delays τ_j that can be zero or not. As mentioned, the NSM adopts the following correspondence between mathematical and electrical variables:

$$x_i \equiv V_{x_i} \quad \frac{dx_i}{dt} \equiv I_{\gamma_i} \tag{14}$$

where $\mathscr{V}_{x_i}$ is the electric potential (V) and I_{γ_i} is the electric current (A). Each addend in Equation (13) is considered as an electric current flowing through a branch which balances with the rest of the terms according to KCL [11]:

$$J_{\gamma_i} = I_{\gamma_i} = \frac{dx_i}{dt} \tag{15}$$

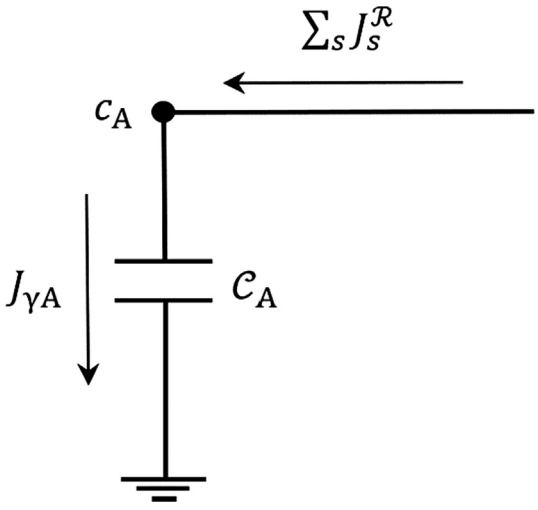

Fig. 1. Current flows $\sum_s J_s^{\mathscr{R}}$ and $J_{\gamma A}$ at the concentration node c_A, satisfying KCL.

$$J_{f_i} = I_{f_i} = f_i\left(t, \{x_j(t-\tau_j)\}_{j=1,\cdots,n}\right) \tag{16}$$

$$J_{\gamma_i} - J_{f_i} = 0 \tag{17}$$

The last equation represents KCL at node $x_i(t)$ (equivalently, $\mathscr{V}_{x_i}$) of the circuit.

The next step is to find appropriate electrical devices to implement J_{γ_i} and J_{f_i}. Expression $J_{\gamma_i} = dx_i/dt$ resembles the characteristic equation relating the current I flowing in a capacitor with the electric potential $\mathscr{V}$, $I = \mathscr{C}\frac{d\mathscr{V}}{dt}$. Addend J_{γ_i} is implemented by means of a capacitor of unit value ($\mathscr{C} = 1$F). In general, function f_i is implemented by a voltage-dependent current source containing all the dependence [11]. Notwithstanding, the characterization of addends exhibiting delay has not been previously addressed for the NSM method. The key ingredient is to implement them in the circuit network through open voltage-controlled voltage sources, as showed in Fig. 2 (right branch). In this fashion, whenever a term with delay in the current source is needed, the corresponding auxiliary node (node $x_i(t-\tau)$ in Fig. 2) is called as a function, which retains the value of x_i at previous times, depending on τ. For our simulations, we use freeware LTspice to run the circuit model, making use of the sophisticated numerical techniques of analysis that this code embodies (see details in section 2.2). It is worth pointing out that only three simple electrical devices are needed to model the whole mathematical system.

To show how a network model with time delay is designed, let us analyze Hutchinson's delayed logistic equation [29]. This equation plays a fundamental role in the mathematical modeling of ecology problems:

$$\frac{dx(t)}{dt} = \alpha x(t) - \frac{\alpha}{K}x(t)x(t-\tau) \tag{18}$$

where $\alpha > 0$ and $K > 0$ are the intrinsic growth rate and the carrying capacity of resources, respectively. Variable x usually represents a population.

As mentioned, the derivative term $\frac{dx(t)}{dt}$ is implemented by means of a capacitor of 1F. Function $f = \alpha x(t) - \frac{\alpha}{K}x(t)x(t-\tau)$ is implemented via a voltage-dependent current source. To characterize the term showing time delay, $x(t-\tau)$, a voltage-controlled voltage source is employed (see Fig. 2). The whole electric network consists of one circuit, corresponding to Eq. (18).

Remarkably, both the design and the solution of analogical electric networks constitute an important alternative to other classical numerical procedures. Examples include predator–prey models modeled via analog multipliers, capacitors and resistors and delay Lotka-Volterra via operating amplifiers and multipliers powered by a continuous voltage [30,31]. However, one of the main advantages of the NSM against other electrical analogies is that very few simple electrical devices are required to implement the network model [11]. As mentioned, the solution presented in this work for the implementation of the time-delayed addends in NSM was not achieved previously, thus completing the theoretical frame for the procedure.

2.2. Numerical algorithms in LTspice

LTspice offers three different integration methods in its control panel. Since certain circuits (containing time constants of very different values) can give rise to stiff equations, it is convenient the integration algorithm to be stiff-stable. To achieve this objective, trapezoidal (trap) and Gear integration methods of variable order, from two to six, are internally considered. After achieving convergence, the solution is stored, and the process is restarted for the next instant. The time step is variable: the program adjusts it according to the precision required for the computation time to

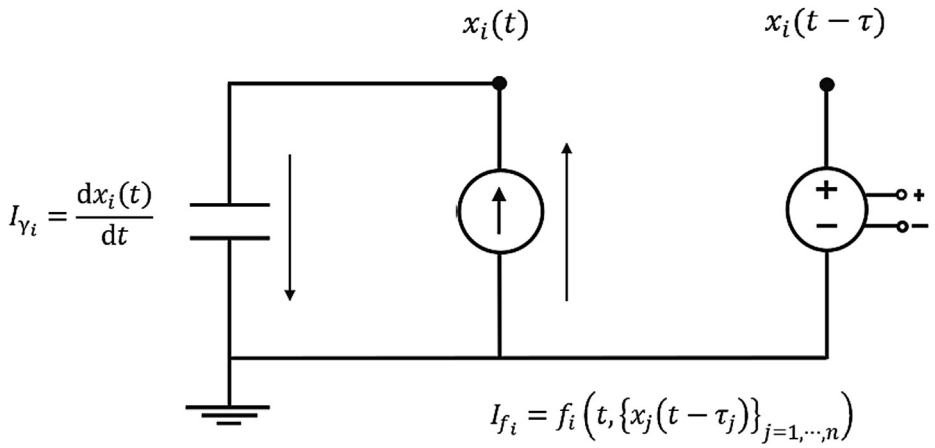

Fig. 2. General NSM circuit equivalent to Hutchinson's delay differential equation, Eq. (18). The right branch represents the auxiliary voltage-controlled voltage source which controls the delay.

be minimum. The trapezoidal method is usually the best integration option, generally stable and accurate, where the time penalty is to calculate the underlying function at each time. Gear integration is also effective, but requires greater step time work to reach the same accuracy, being generally slower than trapezoidal methods [32]. However, the trapezoidal is just marginally stable on stiff circuits, and may cause a numerical artifact called trap ringing, in which the integrated solution oscillates step by step over the true continuous time behavior. This phenomenon represents a recurring topic in the literature, also present when circuits switch [33]. For this reason, LTspice incorporates an additional method called *modified trap*, which is identical to the standard trap, except for one additional post-processing that eliminates the oscillation by using interpolation. Subsequently, LTspice calculates upper and lower interpolation lines, saving the average value in place of the original result [24]. In section 3, an application of the NSM procedure on adsorption kinetics exhibiting delay will be performed, comparing the LTspice numerical algorithms with those from software Mathematica.

3. Applications

3.1. Adsorption kinetics

Adsorption processes that naturally present delay must be described by means of DDEs. As an example to test the method, let us apply the NSM formalism to solve a practical model of adsorption kinetics involving the surface tension of gelatin solution at an interface air/solution, originally developed by Ohshima et al. in 2004 [34]. The introduction of time delay in adsorption kinetics at the interface between air and a polymer solution leads, under certain conditions, to overshoot and oscillation in the time course of the surface tension of aqueous gelatin solution [34]. The equations describing the model are:

$$\frac{dN(t)}{dt} = k_a c_0 [N_m - N(t)] - k_d N(t-\tau) \tag{19}$$

$$\sigma(t) = \sigma(0) - [\sigma(0) - \sigma(\infty)]\left(\frac{1+K}{K}\right)\frac{N(t)}{N_m} \tag{20}$$

In this problem, $N(t)$ and $c(t)$ are the polymer concentration in the solution and on the interface, respectively, and $\sigma(t)$ represents the surface tension. Constants k_a, k_d are the rate constants for adsorption and desorption, respectively, $c_0 = c(0)$, $N_m = \frac{1+K}{K}N(\infty)$, K is a characteristic constant for the adsorption and desorption processes and τ is the time delay [34]. Parameters and initial conditions for simulations are: $\alpha = 0.56\text{h}^{-1}$, $K = 4.0$, $\tau = 7.4\text{h}$, $\sigma(0) = 59.42\text{mN m}^{-1}$, $\sigma(\infty) = 54.34\text{mN m}^{-1}$ and $N_m = 100$, where $\alpha = k_a c_0$ and $k_d = \frac{\alpha}{K}$.

Fig. 3 shows the dependence of the surface tension $\sigma(t)$ (mN/m) on time t(h) obtained via NSM (black line) and software Mathematica [23] (empty red dots), exhibiting agreement. The NSM formalism can be extended to describe other related complex phenomena exhibiting delay, such as the oscillatory molecular adsorption patterns of proteins, which study is connected to the time scale needed for self-organization [3].

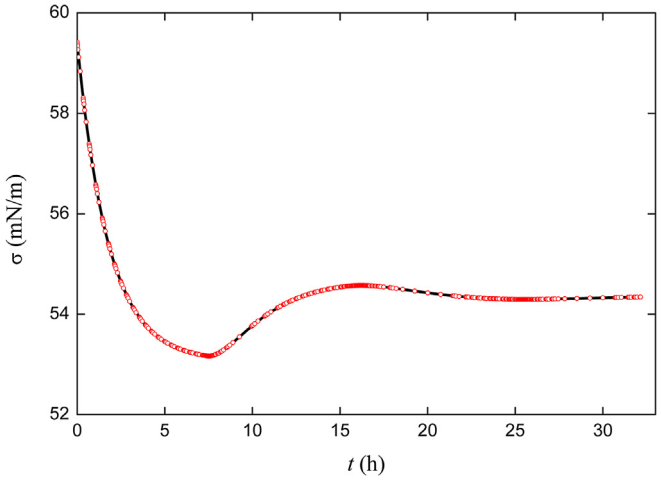

Fig. 3. Dependence of surface tension $\sigma(t)$ on time t for the NSM (black line) and Mathematica (empty red dots).

Table 1
Comparison between LTspice and Mathematica algorithms for simulation of the adsorption problem introduced by Eqs. (19)-(20).

	Numerical integration method	Computing time (s)
LTspice	Gear	0.023
	Trapezoidal	0.024
	Modified trapezoidal	0.022
Mathematica	Explicit Runge-Kutta	3.345
	Adams	3.407
	Stiffness	3.454

Table 2
Experimental QDMDLL parameters employed in the NSM simulations.

Parameter	$0V$	$-3V$
T	3.23	5.00
$G(0)$	3.33	4.18
$Q(0)$	2.33	3.20
α_g	0.1	0.2
α_q	0.1	0.2
s	2.68	4.65
Γ	0.13	0.08
γ	29.14	39.15
k	0.55	0.55

Table 1 shows the computing time for numerical algorithms computed in LTspice and Mathematica applied to Eqs. (19)-(20). For LTspice, the best computing time is 0.022 s by using the modified trapezoidal method, while Mathematica gives 3.407 s by employing the explicit Runge-Kutta method. Moreover, any choice in LTspice is orders of magnitude faster, which could lead to advantages for slow running numerical problems. The power and robustness of the powerful numerical algorithms implemented in the electrical circuit simulation programs confirm the feasibility and precision of the NSM, enabling the approach as an outstanding alternative for the resolution of DDE problems.

3.2. Control of pulse width in passively mode-locked quantum dot lasers

Quantum-dot semiconductor lasers operating in mode-locking are outstanding optical sources for generating ultrashort pulses, exhibiting low-jitter, high repetition rates and less sensitiveness

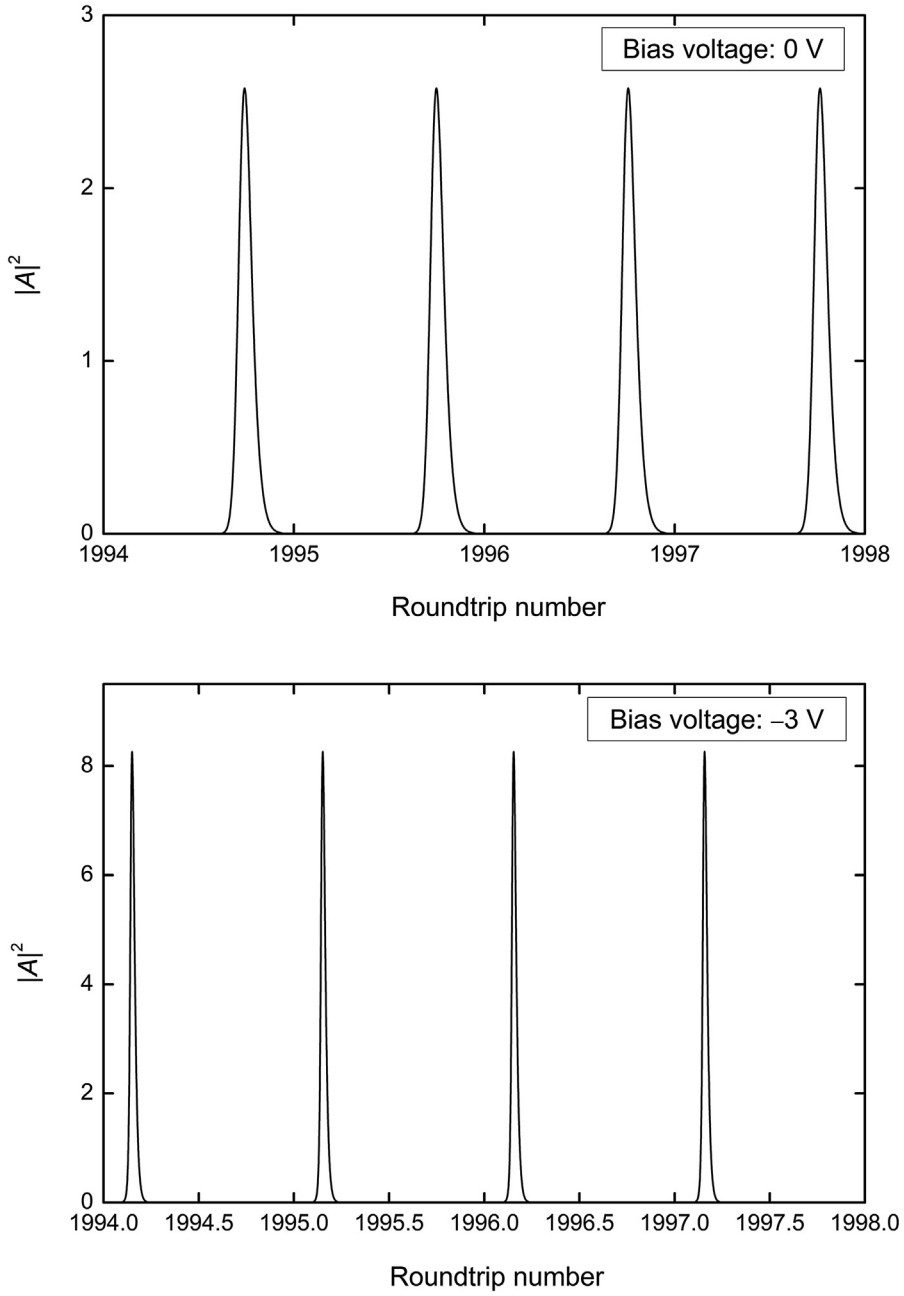

Fig. 4. Optical power for passively mode-locked quantum dot lasers with monolithic saturable absorber at reverse bias voltage equal to 0 (top image) and −3 V (bottom image). Pulse widths are 16.20 and 5.27 ps, respectively.

to temperature changes. QDMLLs are of particular interest in a plethora of applications, highlighting communication and detection systems [35]. Experimentally, it is well known that the increase of a reverse bias on the saturable absorber section shortens the laser pulse width [36], but the numerical simulations remain scarce. The authors are currently developing a line of research involving the modelling of ultrashort pulses in passively mode-locked quantum dot lasers by means of the NSM delay approach, applied to LiDAR technologies in military and aerospace environments, which constitutes a prominent area of research [37]. The absorber section is monolithically integrated in the device, making the unit a compact and portable source, and Lorentzian spectral filtering is considered.

The DDE model that describes the QDMLL is given by [36,38]:

$$\gamma^{-1}\frac{dA}{dt} = -A + \sqrt{k}\left[e^{\left(\frac{(1-iz_g)}{2}G(t-T)-\frac{(1-iz_q)}{2}Q(t-T)\right)}\right]A(t-T) \tag{21}$$

$$\frac{dQ}{dt} = q_0 - Q - s\left[1-e^{-Q}\right]|A|^2 \tag{22}$$

$$\frac{dG}{dt} = g_0 - \Gamma G - e^{-Q}\left[e^{G}-1\right]|A|^2 \tag{23}$$

Here, A is the envelope of the electric field in the complex domain, Q is the saturated loss in the absorber section and G represents the saturated gain of the device. Time t is the renormalized time, T is the cold cavity roundtrip delay time, q_0 and g_0 are the unsaturated gain and adsorption parameters, Γ is the ratio between the absorber and gain relaxation times, s is the saturation parameter, while α_g and α_q are the line enhancement factors for gain and absorber sections, respectively. Additionally, γ describes the spectral filtering bandwidth and k accounts for losses in the cavity. The values of these parameters employed in the NSM simulations are obtained from real experiments for reverse bias voltages equal to 0 and −3 V, summarized in Table 2. The unsaturated gain and adsorption parameters are determined as follows:

$$g_0 = \Gamma G(0), q_0 = \frac{Q(0)}{s} \tag{24}$$

Fig. 4 shows the time dependence of stable optical power $|A|^2$ for voltages 0 (top image) and −3 V (bottom image). The results clearly indicate that voltage −3 V shortens the laser pulse width. Besides, a noticeable increase in the optical power is achieved. In order to measure the pulse width, full width at half maximum (FWHM) is the standard employed, along with pulse repetition rate, set equal to 4.96 GHz [36]. The results are summarized in Table 3, compared with the experimental values.

The agreement between the experiment and the NSM simulations, along with the simplicity of the network model, enables the method as an excellent approach to model QDMLL pulses. Further simulations are focused on the effect of temperature on the devices, study of threshold values for α_g and α_q, application of Bragg spectral filtering, effect of noise sources, and the inclusion of dispersive time delays. The characterization of these phenomena and the control of the pulse dynamics has led to collaborations with researching groups of microelectronic design, for the study of advanced sensing applications.

Table 3
Experimental and NSM simulation values for the pulse width corresponding to the QDMLL described in [36].

Bias voltage	Experimental	NSM
0 V	16.25ps	16.20ps
−3 V	5.12ps	5.27ps

4. Conclusions

In this paper, we introduce the first model for delay terms in DDEs within the frame of the NSM, goal not achieved previously. The procedure is easy to implement, requiring very few devices to complete the network model. The key ingredient is to employ open voltage-controlled voltage sources that retain the values of the variables for selected time delays. Remarkably, the model can be run in free circuit software such as LTspice, which accurate numerical algorithms present advantages over powerful software such as Mathematica in terms of computing time, also exhibiting equivalent results. The work presented strengths and completes the formalism of the NSM, enabling it as a formal and outstanding alternative to the resolution of DDE problems in a fast and simple way, accessible to both researchers and scholars. In order to illustrate the power of the method applied to real problems, the modelling of ultrashort pulses in passively mode-locked quantum dot lasers was conducted, a fascinating topic that presents vast applications in medicine, remote sensing or communications. Concretely, it was found that the implementation of a reverse bias voltage in the absorber section produces a remarkable shortening of the pulse width, in agreement with the experiments. The future lines of research of the NSM include the implementation of delay terms for partial differential equations, with special application to density-driven flow in porous media.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Dr. Manuel Caravaca Garratón, Graduate and Doctor in Physics is a professor at the University Centre of Defence, Spanish Air Force Academy. He has extensive experience in physical aspects of adsorption processes (with emphasis in thermodynamics and kinetics), as well as surface characterization by microscopy techniques (TEM, FESEM). Likewise, he has experience in computational physics applied to materials of high technological interest such as Coulomb glasses. He is a collaborator at Umea University, Sweden, studying the effect of pollution in the genetic makeup of different plants, and how to mitigate the effect. He is author of recent publications of high impact on removal of pollutants, and developer of proprietary sofware SimKinet and EcoPhys along with Dr. Antonio Soto Meca.

María del Carmen García Onsurbe received a dregree in Engineering in Agri-Food Industries and Biological Systems. She currently belongs to the Advanced Techniques in Food Research and Development doctorate program. She developed her master degree project in computation, applying the Network Simulation Method to biological pest control. Her publications are focused on nanostructured materials employed as adsorbents for aquatic pollutants, with the aim of maximizing the removal of hazardous materials by employing low-cost and environmentally friendly methods.

Dr. Antonio Soto Meca, Graduate and Doctor in Physics is a professor at the University Centre of Defence, Spanish Air Force Academy. His area of expertise is related to the theoretical and computational aspects of the Network Simulation Method, which establishes an analogy between an electrical circuit and a system of differential equations. He is author of high impact publications in this area, as well as proprietary software (FATSIM-A, FAHET, SimKinet, EcoPhys). Other areas of study include discriminated dimensional analysis, adsorption of water pollutants by using nanoparticles (with recent high impact articles), and spectroscopy techniques for surface characterization.