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Numerical modeling of the benzene reaction with ozone in gas phase using differential neural networks

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ABSTRACT

In the present paper a mathematical model of a gas–gas reaction between ozone and benzene in a tubular reactor is considered. Usually, mathematical models of chemical process are governed by a set of ordinary differential equations assuming that the corresponding concentration dynamics depends only on time. On the other hand, the spatial distribution of the mass, energy and concentrations may be observed in the case of a more complex model structure that demands the use of models described by partial differential equations. The example of such complex model describing, the reaction between benzene and ozone in the gas phase, is considered here. The approach suggested in this study is based on the differential neural network (DNN) technique which permits to convert the task of mathematical modeling of a tubular reactor containing an uncertain (not well-defined) dynamics to a non-parametric identification problem. The asymptotic convergence of the obtained identification error to an ellipsoidal zone containing the origin is shown using the Lyapunov-like analysis. The coincidence between the benzene and ozone concentrations variation calculated by the suggested DNN-algorithm and those generated by a kinetic model is shown to be good enough.

1. Introduction

1.1. Volatile organic compounds treatment methods

The volatile organic compounds (VOCs) emission is one of the most important contributions to the atmospheric pollution, which leads to a decreasing of air quality content [1]. Moreover, VOCs are dangerous for the human health. Actually, it has been shown that they cause both nervous and bread system illnesses increasing the risk to provoke some kinds of cancers [2,3]. Among others effects, they give some important reasons to analyze and/or develop possible elimination methods to optimize the VOCs treatment in gaseous phase. The main source of VOCs emission is the liberation of these compounds from contaminated water and soil. This process is known as *stripping* that has been considered as a treatment method characterizing a liquid-to-gas mass transfer process. However, when the stripping occurs naturally, a big amount of air contaminants (such as gasoline, chlorinated compounds and solvents) are released to the atmosphere. Among others, benzene, toluene, xylene and ethylbenzene (BTEX's) are the most common contaminants moved from water and soil.

Most of treatment methods regarding to the VOCs elimination implies the transfer from one phase to another like the soil vapor extraction or the adsorption in activated carbon [4]. On the other hand, there are some methods applying microorganism's metabolism to reduce VOCs concentrations using special reactors usually referred to as biofilters [5,6]. More advanced methods require catalyst oxidation [7] or incineration. Among others, they represent some reasons to develop the VOC elimination methods by treatment in gas phase. One possible option is the gas phase reaction between ozone and VOCs, provoking a reduction of emitted contaminants. Several studies have analyzed ozonation in gas phase, but just considering the disinfection process or odour elimination.

A novel remediation method to eliminate VOC based on the high oxidation power of ozone has been proposed in the present study. The efficiency of this method to decompose contaminants in water and soil has been deeply studied [8–18]. However, the air treatment ozonation in gaseous phase has not been explored carefully. Indeed, a deep study of gas–gas reaction between ozone and VOC demands experimental setups with special reactors and analytical methods.

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1.2. Mathematical models of gas phase reaction

Experimental setups to determine the efficiency of ozonation treatment of VOCs generally require the usage of tubular reactors. This kind of reactor is selected due the very deep knowledge of their internal dynamics. Actually, they have been shown to be useful in controlled conditions of chemical reactions [19]. Most of the more profound studies regarding the tubular reactors are based on mathematical models describing the organics dynamics inside the reactor. Some of these mathematical models are normally governed by ordinary differential equations, assuming that organic movement inside the reactor depends only on time, but despising the diffusion, convection and advection processes. Nevertheless, exact and informative models require more complex mathematical descriptions. Therefore, to propose a mathematical description closer to a real chemical process behavior, it is necessary to use another framework. Actually, such systems should be described by a set of partial differential equations (PED's) trough a more complex modeling process. The tubular reactor models are usually given by linear second order parabolic PDE's. Indeed, this class of PDE's appear in time dependent compounds mass transfer, such as the gas flow in the reactor.

Even linear PDE's seem to be a good choice to describe the organics dynamics in the reactor, always there is a degree of uncertainty regarding to the parameters involved in the model, nonlinear relationships between mass transfer and chemical reaction. The uncertainties considered here can be treated using numerical approximation to solve PDE's. This assumption is valid when the relative size of the aforementioned uncertainties is small (compared with the numerical accuracy used for the algorithm to solve the PDE) or when the model uncertainties are not well defined.

2. Differential neural network for PDE solution

2.1. Application of Neural Networks to model PDE's

The main PDE's based modeling disadvantage is the difficulty of finding their exact solutions. Indeed, when a best description of a phenomenon under study is achieved, one must expect that application of conventional solution methods is unviable. Actually the classical methods such as the variable separation or series schemes are not longer applicable when the mathematical description of PDE's has any uncertainty degree [20,21]. Instead of analytical solutions, some numerical methods have been introduced to obtain an approximate solution for the PDE's trajectories. Within the numerical methods framework, some numerical techniques (such as the finite-difference method (FDM) and the finite element method (FEM)) have been introduced [20,21]. Shortly speaking, they are well-defined if the PDE structure is perfectly known and when the PDE's is unaffected by external perturbations. Therefore, the existence of modeling errors and "unmodeled dynamics" arise naturally. Nevertheless, there are not so many methods to solve or approximate the PDE solution when its structure (even in linear case) is uncertain.

Neural networks (NNs) seem to be a good tool to obtain numerical reproductions of nonlinear PDE's in general. Using this method, one can avoid the necessity to obtain the mathematical description model. Actually, if the mathematical model of a real process is incomplete or partially known, the NN method provides an effective way to solve a wide spectrum of problems such as nonparametric identification, state estimation and trajectories tracking [22].

Several approaches dealing with state estimation problem are widely used in practical applications. Among them there are the Lie-algebraic method [23], Lyapunov-like observers [24], high gain observation [25], the reduced-order nonlinear observers [26] and others. However, all of them require the complete knowledge on the mathematical description of the system to be estimated, and they demands some constrains on the dynamics structure which are difficult to be fulfilled in real situations. Special attention is paid during this study to neural state observer providing the state estimates for uncertain dynamic systems because the assumption that all states of a dynamic process to be identified are completely accessible seems to be unrealistic.

Artificial Neural Network (ANNs) has shown good identification properties in the presence of some uncertainties or external disturbances. However, the more extended class of these ANN are the referred to as static neural networks dealing with global optimization problems by means of weights adjustment of such ANN to minimize a desired performance index [14]. Static class of ANN uses back-propagation technique as common analysis method, with good results to reproduce uncertain dynamics but just given a functional map between the input action and the corresponding states dynamics. This particular fact makes useless the static approach when the state estimation or parameter identification is tried to be solved for uncertain systems.

The second approach, exploiting DNN feedback properties, permits to avoid many problems related to global extreme search converting the learning process to an adequate feedback design to regulate and adjust the parameters (weights) using dynamic structures [27,28].

The main objective of this study is the application of a numerical solution based on differential neural networks (DNNs) to realize the identification of benzene–ozone reaction carried out in tubular reactor.

There are some methodologies on designing of identifiers, which have been widely used in practical situations [27]. Indeed, they require an almost complete knowledge of the mathematical model. Nevertheless, there are not so many methods to solve or approximate the PDE solution when its structure (even in linear case) is uncertain. It is well known that Radial Basis Function Neural Networks (RBFNNs) and Multi-Layer Perceptrons (MLPs) can perform good approximation for any continuous function defined on a compact set. NN have demonstrated effective performance to identify nonlinear uncertain systems. In general, there are two types of NN: the *static* (related with a search of a global extreme [20]) and the *recurrent* NNs [22], which work in a discrete time. One novel option is the *continuous time* DNN [27,28] that uses some feedback systems properties. Since the solutions of benzene–ozone reaction in gas phase carried out in a tubular reactor are continuous and the viable sets are compact, DNN seem to be a good proposal for the identification problem. This DNN-identifier uses a set of adjustable parameters, which usually are called "weights". The weights dynamics are supported by some *learning laws* which are also described here using an appropriated theory based on the Lyapunov functions method [28].

In this study, a strategy based on DNN for the trajectories identification in a mathematical model described by PDE's is proposed. *The main idea* here is to reproduce the concentration profiles of ozone and benzene along the reactor and during the ozonation time. The identification problem is reduced to finding an exact expression for the weights dynamics based on the DNN properties. To investigate the qualitative behavior of the suggested methodology, here the non-parametric modeling problem for a distributed parameter plant is considered [29–31]. The model tackles a gas phase reaction between ozone and benzene in a tubular reactor, where the interaction between both gases is represented by two second order PDE's. The numerical example is realized considering two practical scenarios: ozone and benzene are injected to the reactor in gaseous form and the second one involves the benzene's stripping from contaminated water.

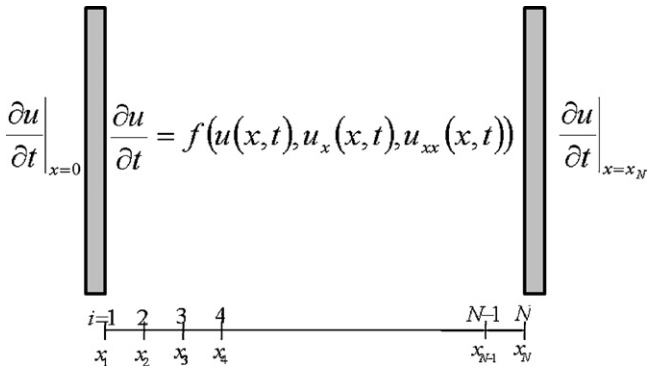

Fig. 1. Mesh based division for the domain $x \in [0,1]$ in N equidistant sections.

The contributions given in this paper regard to the development of a non-parametric identifier for uncertain systems described by partial differential equations. The method produces an artificial mathematical model that is able to describe the partial differential equations dynamics. The required numerical algorithm to solve the non-parametric identifier was also developed as an additional part of the theoretical development.

2.2. Finite-difference approximation for uncertain PDE's

The problem requires the proposal of a non-parametric identifier based on DNN. The problem here may be treated within the PDE's framework. Therefore, this section introduces the DNN approximation characteristics to reconstruct the trajectories profiles for a family of parabolic PDE's. Let assume that ozone–benzene reaction carried out in the tubular reactor is given by a set of second order parabolic PDE's with uncertain structure and disturbed by unknown, but bounded perturbations. In general, this reaction may be described as follows:

$$u_t(x,t) = f(u(x,t), u_x(x,t), u_{xx}(x,t)) \tag{1}$$

Here $u(t)$ has n components ($u(t) \in \Re^n$) defined in a domain given by $x \in [0,1]$, $t \geq 0$. Considering the reaction conditions, the set of PDE's (1) is armed with the boundary (Neumann and Dirichlet) and initial conditions given by

$$\begin{aligned} &u_x(0,t) = 0 \in \Re^n,\ u(0,t) = u_0 \in \Re^n \\ &u(x,0) = c \in \Re^n \end{aligned} \tag{2}$$

In (1), $u_t(x,t)$ stands for $\partial u(x,t)/\partial t$ and

$$u_x(x,t) = \frac{\partial u(x,t)}{\partial x}, \quad u_{xx}(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} \tag{3}$$

The main idea behind the application of DNN [27] to approximate the PDE's solution is to use a class of modified finite-difference methods for uncertain nonlinear functions. So, it is necessary to construct an interior set (commonly called grid or *mesh*) that divides the domain $x \in [0,1]$ in N equidistant sections (Fig. 1) defined as x_i in such a way that $x_0 = 0$ and $x_N = 1$.

Using this mesh based description one can introduce the following definitions:

$$\begin{aligned} &u_i(t) := u(x_i,t),\ u_{i,t}(t) := \left.\frac{\partial u(x,t)}{\partial t}\right|_{x=x_i} \\ &u_{i,x}(t) := u_x(x,t)\big|_{x=x_i},\ u_{i,xx}(t) := u_{xx}(x,t)\big|_{x=x_i} \end{aligned} \tag{4}$$

Now, applying the finite-difference representation:

$$u_{i,x}(t) = \frac{u_i(t) - u_{i-1}(t)}{\Delta x}, \quad u_{i,xx}(t) = \frac{u_{i,x}(t) - u_{i-1,x}(t)}{\Delta x} \tag{5}$$

We obtain the so-called Δx-*approximation* of the nonlinear PDE (1) that can be expressed as

$$\begin{aligned} \dot{u}_i(t) = u_{i,t}(t) &= f\left(u_i(t), \frac{u_i(t) - u_{i-1}(t)}{\Delta x}, \frac{u_i(t) - 2u_{i-1}(t) + u_{i-2}(t)}{(\Delta x)^2}\right) \\ &= \Phi(u_i, u_{i-1}, u_{i-2}), \quad (i = 0, \ldots, N) \end{aligned} \tag{6}$$

Based on the neural network methodology, by simple adding and subtracting, the corresponding terms, one can represent the previous equation as

$$\begin{aligned} &u_t(x,t) = Au(x,t) + V_1\sigma(x) + V_2\varphi(x) + V_3\gamma(x) + \tilde{f}(x,t) \\ &A \in \Re^{n\times n},\ V_1 \in \Re^{n\times s_1},\ V_2 \in \Re^{n\times s_2},\ V_3 \in \Re^{n\times s_3} \\ &\tilde{f}(x,t) := f(u(x,t), u_x(x,t), u_{xx}(x,t)) - Au(x,t) - V_1\sigma(x) - V_2\varphi(x) \\ &-V_3\gamma(x) \end{aligned} \tag{7}$$

Here $\tilde{f}(x,t) \in \Re^n$ represents the *modeling error* term, A and V_k ($k = 1, 2, 3$) are any constant matrices and the set of functions (usually called activation functions) $\sigma(x) \in \Re^{s_1}$, $\varphi(x) \in \Re^{s_2}$, $\gamma(x) \in \Re^{s_3}$. Following the DNN ideas introduced in [27] and applying the same representation to (7), we get for each $i \in (1,\ldots,N)$:

$$\begin{aligned} u_{i,t}(t) &= A^i u_i(t) + W_1^i\sigma(x_i) + W_2^i\varphi(x_i)u_{i-1}(t) \\ &\quad + W_3^i\gamma(x_i)u_{i-2}(t) + \tilde{f}^i(t) \end{aligned} \tag{8}$$

where

$$\begin{aligned} &\tilde{f}^i(t) := \Phi(u_i, u_{i-1}, u_{i-2}) - A^i u_i - W_1^i\sigma(x_i) - W_2^i\varphi(x_i)u_{i-1}(t) \\ &-W_3^i\gamma(x_i)u_{i-2}(t) \\ &W_1^i \in \Re^{n\times s_1},\ W_2^i \in \Re^{n\times s_2},\ W_3^i \in \Re^{n\times s_3} \end{aligned} \tag{9}$$

2.3. DNN approximation for uncertain PDE's

The differential form of the neural-identifier, based on DNN is the following:

$$\begin{aligned} \frac{d}{dt}\hat{u}_i(x,t) &= A^i\hat{u}_i(x,t) + W_{1,t}^i\sigma(\hat{u}_i) + W_{2,t}^i\varphi(\hat{u}_i)\hat{u}_{i-1}(x,t) \\ &\quad + W_{3,t}^i\gamma(\hat{u}_i)\hat{u}_{i-2}(x,t) \end{aligned} \tag{10}$$

where $A^i \in \Re^-$, $W_{1,t}^i \in \Re^{s1}$, $W_{2,t}^i \in \Re^{s2}$, $W_{3,t}^i \in \Re^{s3}$, are the parameters or weights that should be adjusted to ensure a good neural network approximation; $\sigma(\hat{u}_i) \in \Re^{s1}$, $\varphi(\hat{u}_i) \in \Re^{s2}$, $\gamma(\hat{u}_i) \in \Re^{s3}$ are three vector fields composed with standard sigmoid functions as it was describe above; $\hat{x}_t$ is the state vector of the neural-identifier of the reaction parameters. An adequate learning procedure for the neural-identifier (10) provides a sufficiently small upper level (in a sense averaged value) for the estimation error $\Delta_t = \hat{u}_t - u_t$. The procedure of learning is given for the variable in time weight matrices:

$$\begin{aligned} \dot{W}_s &= -k_s^{-1}\sum_{i=1}^{N}(2[\Delta_i^T P^i\psi_s(u_i) + \Delta_x^{Ti}S^i\nabla_x\psi_s(u_i) + \hat{u}_i T^i\psi_s(u_i)] \\ &\quad + \alpha_m^i k_s\tilde{W}_s^i) \end{aligned} \tag{11}$$

Matrices P^i, S^i and T^i are solutions for a set of three uncoupled Riccati equations [31]. If these solutions exist and they are positive definite, then the parameters adjustment schemes (11) are valid. Here it should be noticed that the identifier (1) does not use any information on the PDE structure. This means that, no dynamic model is necessary to develop the pre-identification DNN-algorithm. In this sense, the suggested technique is treated as an identifier for model uncertainties. Considering the identifier defined in (10) with the nonlinear adjustments laws (11) to tune the weights described in (11), it is possible to ensure an upper limit for the identification process depending on the noises power.

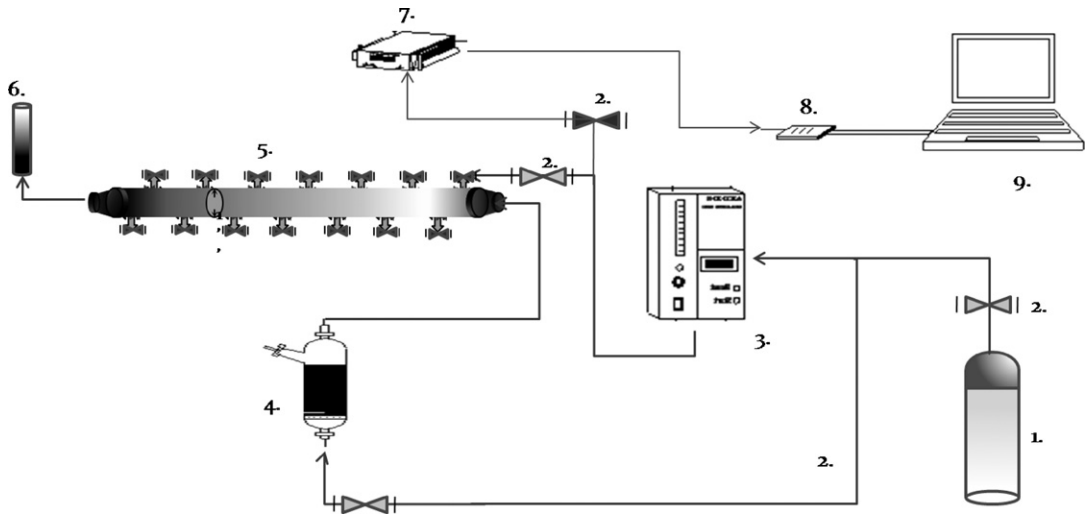

Fig. 2. Schematic diagram of the experimentation at laboratory scale: (1) oxygen tank, (2) valve step, (3) ozone generator, (4) liquid reactor, (5) tubular gas phase reactor with sample valves distributed uniformly (6) activated carbon, (7) ozone analyzer, (8) data acquisition board and (9) PC.

2.3.1. PDE's identification

State *identification* (estimation) problem for nonlinear uncertain PDE's (1), could be now formulated as follows:

Problem. For the nonlinear system, described by a vector PDE (1), the problem considered in this paper can be stated as follows: to analyze the quality of the DNN-identifier (10) supplied with the adjustment (learning) laws (11), identification error δ given by

$$\delta := \overline{\lim_{t\to\infty}} \sum_{i=0}^{N} \left\| \hat{u}_i(t) - u_i(t) \right\|_{Pi}^2 \tag{12}$$

One additional problem, if possible, is to reduce the estimation error to its lowest possible value. This minimization is carried out by the selection of free parameters participating into the DNN-identifier. Using the well-known Lyapunov method applied within the adaptive control framework, the main result of this paper can be presented as follows:

Consider the nonlinear model (1), given by the system of PDE's with uncertainties (perturbations) in the states and the outputs, under the border conditions (2). The DNN-identifier is given by (10) which parameters are adjusted by the learning laws (11) with positive parameters α_m^i ($i = 0,\ldots,N$), provides for all $i = 0,\ldots,N$ the following ρ upper bound for the adaptive identification problem:

$$\overline{\lim_{t\to\infty}} \sum_{i=0}^{N} [\left\| \hat{u}_i(t) - u_i(t) \right\|_{Pi}^2 + \left\| \hat{u}_{i,x}(t) - u_{i,x}(t) \right\|_{Si}] \le \mu \tag{13}$$

is ensured with $\mu_0 := \sqrt{N}[\min_i(\alpha_m^i)]^{-1/2}$ and

$$\mu := \mu_0 \left[\sqrt{\max_i(\lambda_{\max}([\Lambda_P^i]^{-1})F_4^i)} + \sqrt{\max_i(\lambda_{\max}([\Lambda_S^i]^{-1})F_9^i)} + \sqrt{\max_i(\lambda_{\max}([\Lambda_T^i]^{-1})f_3^i)} \right] \tag{14}$$

Moreover, the weights $W_{1,t}$, $W_{2,t}$ and $W_{3,t}$ remain bounded and being proportional to μ, that is

$$\left\| W_{1,t} \right\| \le K_1\mu, \left\| W_{2,t} \right\| \le K_2\mu, \left\| W_{3,t} \right\| \le K_3\mu \tag{15}$$

This means that reconstructed trajectories involved in the chemical benzene-ozone reaction inside the reactor tube are so close to their real values as small as disturbances are affecting the state. To guarantee that identification error be the less small as possible, the DNN parameters (1) must be elected carefully. There are two main ways to solve the training [29]:

1. Using the simplified reaction model of benzene with ozone. This model is applied to generate an idealized set of best fitted weight values. This set of best fitted weights is employed in the correction of the DNN parameters, as well as, it is used in the selection of the identifier initial conditions.
2. Using a set of experimental data to produce the best fitted weights values required in the DNN-identifier. Here it is important to say that the training is only made once, and then, the neural-identifier could be used without the information of the reaction conditions.

2.3.2. Mathematical model of benzene–ozone reaction in a tubular reactor

Previously, it has been settled the benzene feeding by its liberation from contaminated water (by the stripping). The solution for mathematical model of PDE's describing the reaction between ozone and benzene is not well-defined and it is necessary to make a big effort to estimate the stoichiometric coefficient (here it is considered one to one for the benzene–ozone reaction). In this section, it has been considered a mathematical model using PDE's to describe the dynamics involving the benzene–ozone reaction in a tubular reactor. This reaction is preceded of the benzene's striping from the contaminated water contained in a supplementary reactor (see Fig. 2).

The more common hypothesis in the chemical reactors modeling is to suppose that the gas flow through the reactor is uniform or laminar [32], the molecules are diffused at a specific rate, depending of the position inside the tubular reactor and a chemical reaction between two gases is being done. Therefore, there are a lot of possible sources of uncertainties when the reaction is modeled. DNN adjustment demands a large set of experimental data to obtain enough information for the second training method described above. This is the main reason to present a simplified PDE's model, describing the reaction between benzene and ozone. Besides, an isothermal reaction is assumed to avoid the presence of an extra parabolic PDE. Mathematical description of aforementioned cou-

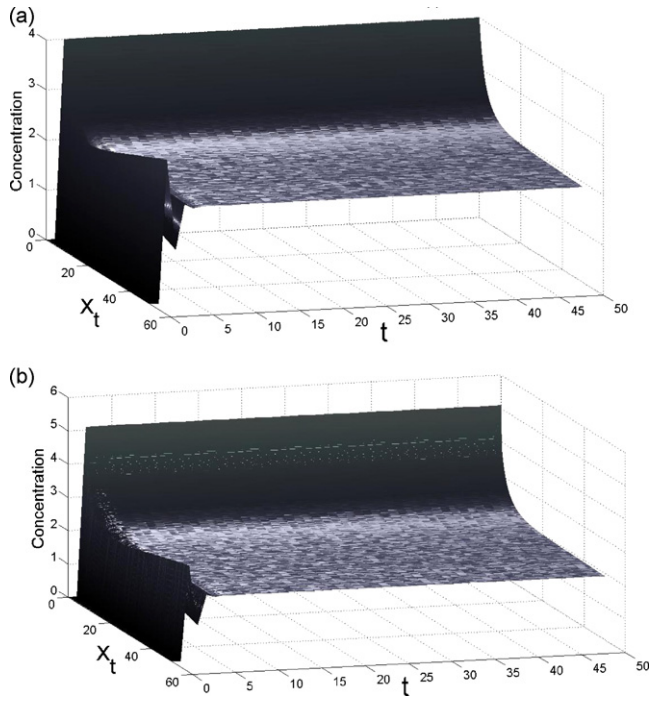

Fig. 3. Comparison between the benzene concentration simulated using the model (16) (a) and reconstructed by the DNN-identifier (b).

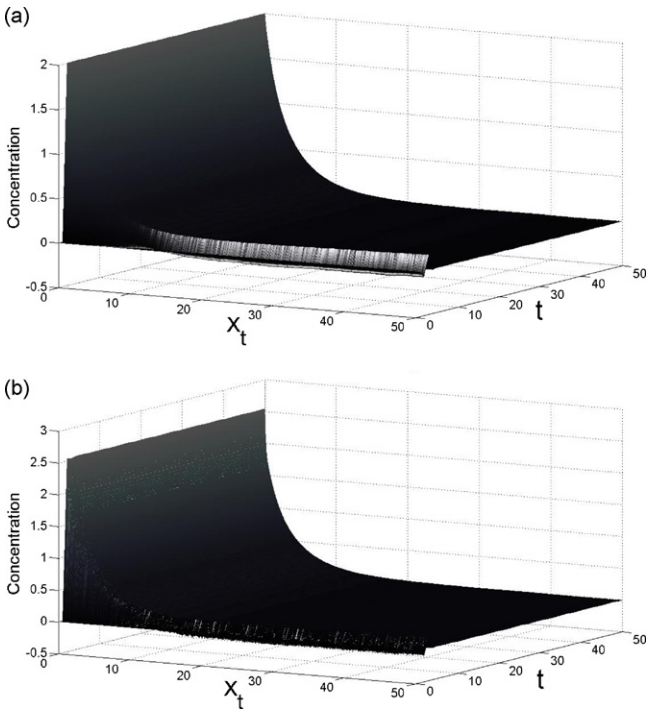

Fig. 4. Comparison between the ozone concentration simulated using the model (16) (a) and reconstructed by the DNN-identifier (b).

pled system is as follows:

$$\begin{aligned}
\frac{\partial c_v}{\partial t} &= D_{c_v}\frac{\partial^2 c_v}{\partial x^2} + u_v\frac{\partial c_v}{\partial x} + g_{t,v}(Hc_l - c_v) - k_c^{gas}c_v^{m_1}(c_{O_3}^{gas})^{n_1}\\
\frac{\partial c_{O_3}^{gas}}{\partial t} &= D_{O_3}\frac{\partial^2 c_{O_3}^{gas}}{\partial x^2} + u_{O_3}\frac{\partial c_{O_3}^{gas}}{\partial x} + g_{t,O_3}(Hc_{O_3}^{l} - c_{O_3}^{gas})\\
&\quad - k_c^{gas}c_v^{m_1}(c_{O_3}^{gas})^{n_1}\\
\frac{dc_l}{dt} &= -g_t(Hc_l - c_v)
\end{aligned} \tag{16}$$

First equation describes the decomposition dynamics of gas reacting (c_v, mol/L) with ozone in gas phase. This equation considers diffusion ($D_{c_v}(\partial^2 c_v/\partial x^2)$), dragging ($u_v(\partial c_v/\partial x)$) processes, the decomposition produced by reaction with ozone ($k_c^{gas}c_v^{m_1}(c_{O_3}^{gas})^{n_1}$) and the contribution produced by striped contaminant from water ($g_{t,v}(Hc_l - c_v)$). Second equation is similar, but in this case, ozone dynamics ($c_{O_3}^{gas}$, mol/L) is described here. Last pair of equations considers contaminants decomposition (c_l, mol/L) in water and dissolved ozone dynamics ($c_{O_3}^{l}$, mol), respectively. Parameters involved in this process were: D_{c_v} is the contaminant's diffusion coefficient: D_{O_3} is the ozone's diffusion coefficient; u_v is the velocity of injected contaminant; u_{O_3} is the velocity of injected ozone; k_c^{gas} is reaction rate constant of ozone and contaminant in gas phase. Term $g_t(Hc_l - c_v)$ refers to striping of dissolved benzene. This description uses the Henry law constant H. In this paper, the ozonation is only considered in gas phase. Using the previous model [28], it is possible to get numerical results for the benzene's ozonation [32–34].

3. Results and discussion

Under the idea of guarantee the best identification, the neural network parameters (2) must be chosen very carefully. The parameter A is adjusted out off line by a trail-and-error procedure. With the purpose of showing the NN training process, it is considered the model in (4). It is assumed that there is possible to measure the benzene concentration along the reactor in specific sites (Fig. 2).

This section discusses a pair of reaction conditions. In the first case, the main supposition is that benzene is feeding as gas with constant initial concentration. The second case considers that benzene is stripped from contaminated water (200 mg/L). In the last case, a moving boundary problem is achieved, which is not simple to solve by classical methods.

3.1. Tubular reactor feeding without the benzene stripping

Numerical reconstruction of variation for the benzene and ozone concentrations, created by the DNN, provides a closely correspondence to the trajectory obtained by the mathematical model (see Figs. 3 and 4). The proposed algorithm to adjust the identifier allows an almost complete trajectory's reconstruction in short time (all identification cases were finished before 2 s of numerical simulation), whereas the profiles of gases concentrations agreed with the data obtained from the ozonation mathematical model. The correspondence between these variations obtained by the model (16) and those based on DNN is acceptable considering the

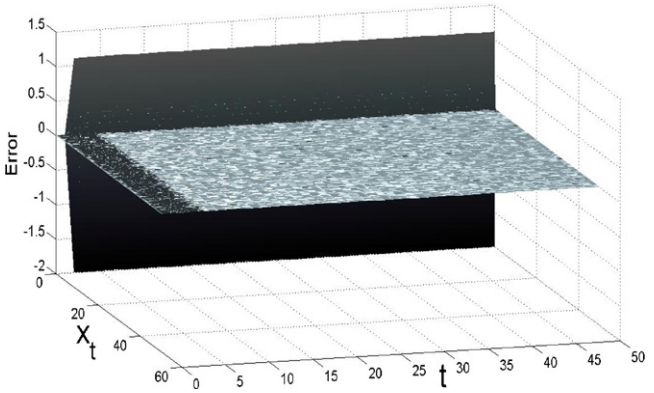

Fig. 5. Identification error of benzene concentration in the tubular reactor.

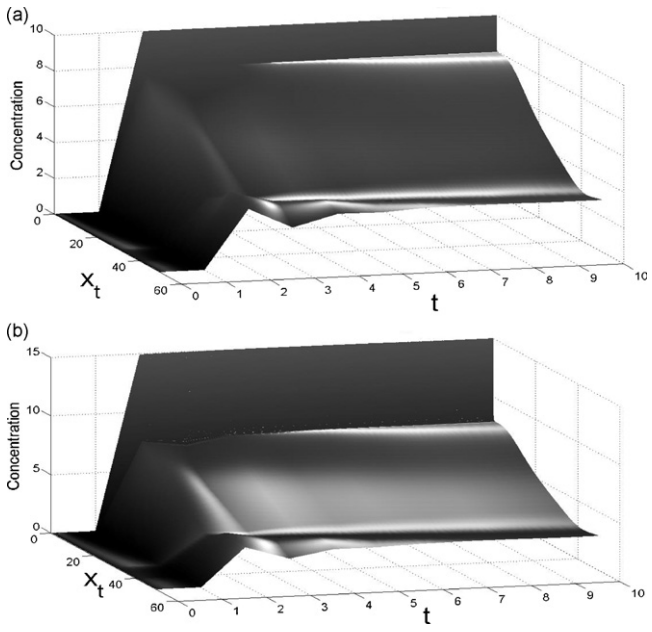

Fig. 6. Comparison between the benzene concentration simulated using the model (16) (a) and reconstructed by the DNN-identifier (b) in the case of benzene's stripping from contaminated water.

identification error obtained along the whole domain in x and t (Fig. 5).

In Fig. 3, one can observe the benzene concentration's similarity obtained by model and DNN-identifier numerical simulations. This solution demonstrates the DNN capability to approximate uncertain PDE's. Even more, the correspondence between both figures is presented not only for the PDE's solution, but also for their derivatives with respect to t and x. Even when the both simulations are almost equivalent, there is a zone when x and t is close to zero where a big difference between real and estimated trajectories is observed. This dissimilarity is dependent on the learning period (approximately 2 s) that is required to adjust the DNN-identifier. This result shows the efficiency of the identification provided by the DNN-algorithm.

3.2. Tubular reactor feeding by the benzene stripped from contaminated water

The more complex problem discussed in this paper arises when benzene was stripped from the contaminated water. The benzene concentration reconstruction was solved successfully as can be seen in Fig. 6. In this case, the closeness between both trajectories is again evident. Main characteristics described in the previous case remain valid for this more complex case. Figs. 6 and 7 demonstrate the quality achieved by the proposed methodology based on DNN-identifier. As one can understand, it is quiet difficult to observer some details in the errors graphics presented in 2D. However, Fig. 7 includes the norm of error throughout the time. This graphic is one-dimensional and can show the convergence of the proposed method based on DNN.

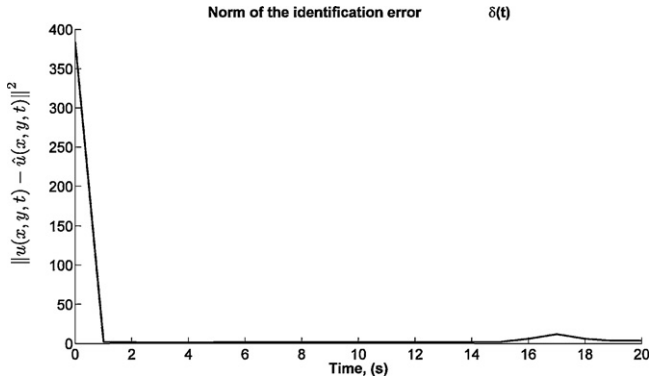

Fig. 7. This figure shows the norm's time evolution of the identification error.

4. Conclusions

The method proposed in this study based on DNN to obtain the uncertain PDE's approximation has been applied for the ozone–benzene reaction in a tubular reactor. The non-parametric neural-identification method to reconstruct the benzene and ozone concentrations in the tubular reactor has been shown to be efficient in two studied cases: without and with benzene stripping. The results obtained by the DNN-identifier, are good approximations of modeled concentrations obtained by numerical simulations. Identification error converges to zero in short time (less than 2 s), which also shows the DNN's high velocity to reconstruct the benzene and ozone concentrations. This was shown for both cases considered in this study.

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