Application of ANN to Hydrodynamic Cavitation: Preliminary Results on Process Efficiency Evaluation

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The capability of hydrodynamic cavitation (HC) of degrading organic pollutants in water effluents is evaluated through the implementation of an Artificial Neural Network (ANN) analysis. Thanks to the construction and training of a multilayer ANN, the energy efficiency of the process has been correlated to measurable variables. These last have been accurately chosen in order to propose a novel modeling approach in the field of HC water treatment. One of the main peculiarity of the proposed model is to choose the ANN input neurons among both operating variables and physical-chemical characteristics of the pollutants. In this way, a powerful tool for prediction, optimization and control of the process, is realized. Preliminary results on the ANN training and on the simulation of factor influences are presented.

1. Introduction

The fulfilment of severe water quality standards and the safeguard of the water supplies with respect to emerging and persistent pollutants, leads to the development of innovative technologies to face the problem of tertiary treatment (Erto et al., 2010; Di Natale et al., 2010).

Hydrodynamic cavitation (HC) in a liquid occurs as a result of flow path constriction accompanied by a localized fall in the static pressure. This phenomenon represents a promising way for the generation of extreme local temperature and pressure conditions as well as the production of hydroxyl radical species. Thus, in the last decade, HC has been successfully studied as an Advanced Oxidation Process (AOP) (Rosa et al., 2012) to achieve the degradation of biological and chemically stable molecules. HC has shown a great potential in terms of power consumption, simplicity of construction and implementation in hybrid treatment solutions (Pradhan and Gogate, 2010). Despite promising results, there are few applications on full scale and there is still a lack of know-how for designing and optimizing the process (Capocelli et al., 2013a). Additionally, due to the stringent correlation among operating conditions, there are still many difficulties in linking experimental results obtained in different devices (Capocelli et al., 2013b).

A literature analysis has shown that, recently, there is a growing theoretical effort for numerically simulating the reactive cavitating bubble. The calculations, with different level of approximation, are aimed to the prediction of cavitation intensity in terms of pressure, temperature and radical species concentration (Capocelli et al., 2012).

Many difficulties arisen if taking into account bubble population phenomena and degradation reactions occurring in different phases. The influence of bubble dynamics and transport mechanisms (Prisciandaro et al., 2009) on the oxidation kinetic regime (Karatza et al., 2008, 2010) is still an unexplored field of research.

Similarly and even more than other AOP, hydrodynamic cavitation shows complex interdependences among system parameters: pollutant features and concentration, pH and volume of solution, geometrical

and hydraulic features of the system (Braeutigam et al., 2010). These have a direct consequence on bubble dynamics, radical generation, transport mechanisms of solutes and chemical reactions. Complex (deterministic) mathematical models have shown two main limits: the necessity of introducing theoretical hypotheses and the difficulties of measuring simulated or assumed variables. As consequence, most of the theoretical studies reported in literature do not propose a direct comparison with empirical observations. Moreover, there is still the need to address the phenomenology of HC oxidation and to develop predictive codes, correlations and theoretical models (Capocelli et al., 2013a-b) to facilitate the reactor design and the process control (Hidalgo et al., 2012).

On the basis of the aforementioned, artificial neural networks can be seen as a valid alternative to onnicomprehensive deterministic mathematical models. The ANN analysis is currently applied to many engineering problems and has been the subject of numerous research and review articles in this field (Kumar et al., 2010).

ANNs are directly inspired from the biology of the human brain, where billions of neurons are interconnected to process a variety of complex information. Accordingly, a computational neural network consists of simple processing units called neurons. Each network consists of artificial neurons grouped into layers and put in relation to each other by parallel connections. The strength of these interconnections is determined by the weight associated with them. The ANN flexibility and capability in modeling nonlinear phenomena make them useful in multivariate analysis of complex experimental data. Additionally they don't require mathematical interpretations with hypotheses and constrains but reproduce cause-effect relationships through training. With this black-box approach, they are extremely reliable in simulating and scaling up complex systems by observing and learning their behavior.

The present investigation discusses the use of a multilayer feed-forward neural network model to predict the energy efficiency in the HC degradation of different organic pollutants by taking into account both experimental parameters and pollutant characteristics. The proposed tool is virtually able to evaluate the process for different geometries, operating variables and organic pollutants to be removed.

2. Methods

2.1 Experimental data of hydrodynamic cavitation

Success in obtaining a reliable and robust network strongly depends on the choice of the involved process variables as well as the available set of data and the domain used for training purposes. In order to address the phenomenology of HC, a number of experimental results reported in literature has been considered. The system of variables implemented in this research are reported in Table 1. Molecular weight M_w, boiling temperature at atmospheric pressure T_{eb} and octanol-water partition coefficient k_{ow} are related to the pollutant. Initial concentration C_0, temperature T, inlet pressure P_{in}, pipe diameter D, orifice-to-pipe ratio d/D, cavitation number C_v and pH are representative of the experimental conditions. The chosen parameters are the most commonly reported in the literature and, for the purpose of our research, have been extrapolated from the cited research articles: Bagal and Gogate, 2013; Joshi and Gogate, 2012; Mishra and Gogate, 2010; Gogate and Boshale, 2013; Pradhan and Gogate, 2010; Saharan et al., 2011, 2012, 2013. The last variable in Table 1 is the energy consumption EC, calculated as in the following Eq (1):

$$EC = \frac{Energy}{mass} = \frac{W \cdot t}{V(C_0 - C_t)} \tag{1}$$

where W is the mechanical power put into the system, t is the treatment time, V the volume of the solution and C_0 and C_t are the pollutant concentration at the initial and treatment time, respectively.

Table 1: Experimental parameters of HC degradation

Parameter	M_w	T_{eb}	$logP_{ow}$	C_0	T	P_{in}	pH	V	D	d/D	C_v	EC
unit	g/mol	°C	-	mg/L	°C	bar	-	L	Mm	-	-	kJ/mg
min	$1.2 \cdot 10^2$	$1.4 \cdot 10^2$	$4.6 \cdot 10^{-1}$	$9 \cdot 10^0$	$1.8 \cdot 10^1$	$9.0 \cdot 10^1$	$1.8 \cdot 10^0$	$6.5 \cdot 10^2$	$3.6 \cdot 10^0$	$1 \cdot 10^1$	$7.2 \cdot 10^{-2}$	$1.1 \cdot 10^1$
max	$1.6 \cdot 10^3$	$1.9 \cdot 10^3$	$7.1 \cdot 10^0$	$1.1 \cdot 10^2$	$4.4 \cdot 10^1$	$1.1 \cdot 10^1$	$1.2 \cdot 10^1$	$5.6 \cdot 10^{-1}$	$1.6 \cdot 10^1$	$2.7 \cdot 10^1$	$1.8 \cdot 10^{-1}$	$3.3 \cdot 10^3$

2.2 ANN training and validation

The ANN topology has been optimized in order to find the best configuration. The ANN was trained using the back-propagation algorithm, the mean square error (MSE) was used as the error function. All samples were normalized in the 0-1 range. The simulations indicated that the introduction of 7 hidden neurons minimizes MSE ($8 \cdot 10^{-4}$). Thus, in this work, a multilayer feed-forward ANN with seven hidden layers and sigmoid activation function was used; its structure is shown in Figure 1. Al the calculation are developed in Matlab. In total, 185 experimental sets were used to feed the ANN structure. The data sets were divided into training, validation and test subsets (respectively containing 70 %, 15 % and 15 % of the data).
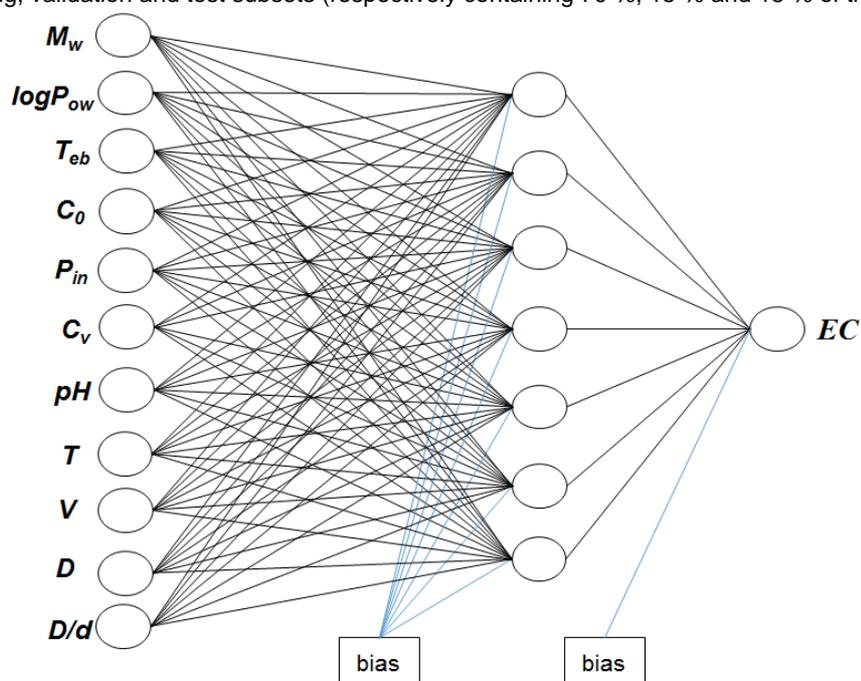
Figure 1: Structure of ANN multilayer feed-forward

3. Results and discussion

Figure 2 illustrates, in a parity diagram, the simulation of the ANN in comparison with the whole set of experimental data; a good agreement is found after the ANN validation.

As the ANN is tested and valuated, it represents a tool for simulating the behavior of HC devices in different configurations. In this paper, two different results are presented in order to address the effect of important parameters on the degradation efficiency. Figure 3 reports the simulation of Orange Acid II degradation for different inlet pressure and pH value. The geometrical configuration chosen for the simulation is the one reported in the work of Gogate and Bhosale (2013). Thus the ANN has been tested with a matrix of 144x11 virtual experiments for generating 144 simulated EC values. Results have been reported as contour plot in Figure 3. It is possible to observe that lowering pH values has a positive effect on the process: at a fixed P_{in} is more convenient to operate in acidic conditions. This is a direct consequence of higher generation capacity of oxidation of hydroxyl radicals at low *pH* (Pradhan and Gogate, 2010) (In further analysis this parameter could be also correlated to pKa of organic molecules). P_{in}, on the contrary, shows a negative effect: the higher the inlet pressure, the greater the energy consumption. Controversial discussion can be found in literature on the effect of inlet pressure: higher P_{in} (consequently higher flow rate) can increase the degradation rates until a maximum is reached (Capocelli et al., 2013a-b); obviously the higher the pressure, the higher energy required for the fluid handling. The latest aspect is of particular relevance in the calculation of *EC* reported in Figure 3. Moreover, transport mechanisms of solutes are definitely able to influence the degradation (additional simulations with different pollutants will give a deeper insight into the mentioned features).

In Figure 4, the effect of pollutant characteristics is shown. The experimental conditions have been fixed according to the ones reported in the work of Saharan et al. (2011), while, the input values of M_w, $logP_{ow}$ and T_{eb} are varied (for simulating different pollutant molecules).
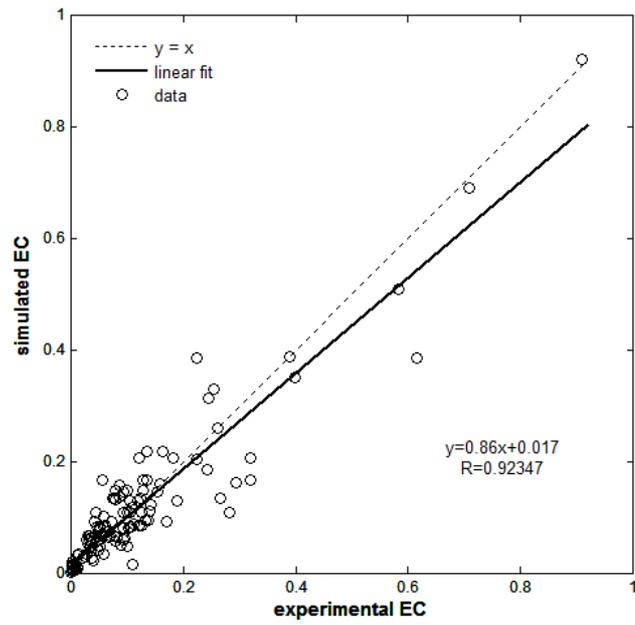
Figure 2: Parity diagram of the ANN: simulated versus experimental data
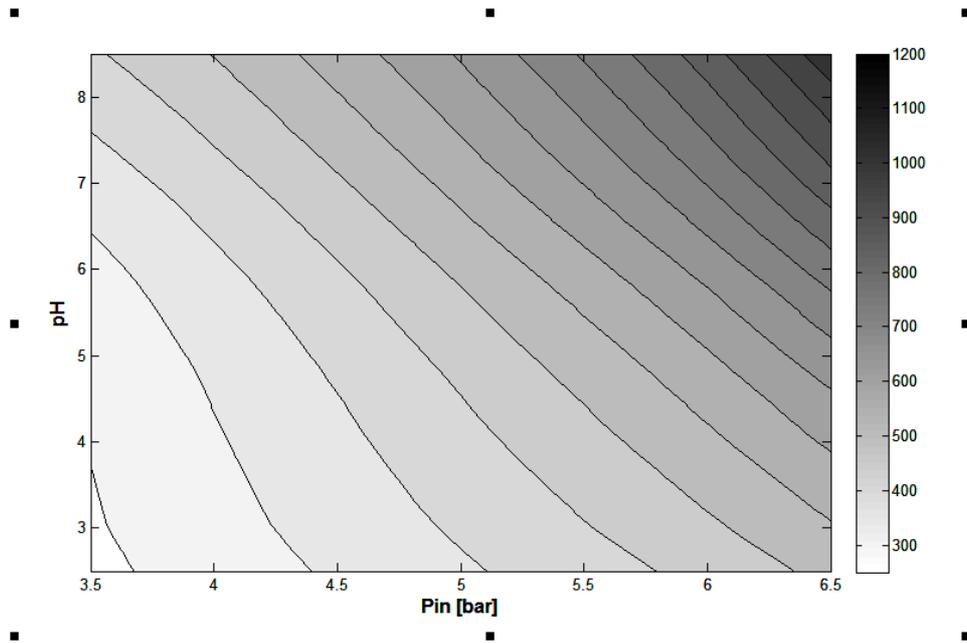
Figure 3: ANN Simulations of energy consumption EC (kJ/mg) for different values of pH and Pin. The other input variables are fixed according to the research of Gogate and Bhosale, 2013; (Orange Acid II); D=25mm; d/D=0.08, C_0= 20mg/L, T=20°C, V=4L

From the results reported in Figure 4, it is clear that M_w has a negative effect on the degradation efficiency: the energy consumption is higher for heavier molecules. This behavior can be addressed to the low diffusivity of bigger molecules which results in lower availability at the bubble-liquid interface for reaction with hydroxyl radicals (Xiao et al., 2013). The hydrophobicity affects the repartition of pollutant in the different reaction regions as bubble core or gas-liquid interface (Braeutigan et al., 2010) and is related to the time scale of bubble growth and collapse. Thus, the effect of $logP_{ow}$ is more complex and is related to bubble dynamics and consequently to the other operating conditions (P_{in}, D, d/D). Additional simulations (with the tested ANN) will be extremely useful in order to discuss the interaction between $logP_{ow}$ and operating parameters (the ANN model also allow for the estimation of correlation and relative importance of parameters). Moreover, it will be of a great interest to evaluate the combined effect of other parameters and to include additional variables into the model (solubility, volatility of compounds as well as cavitation recovery pressure).
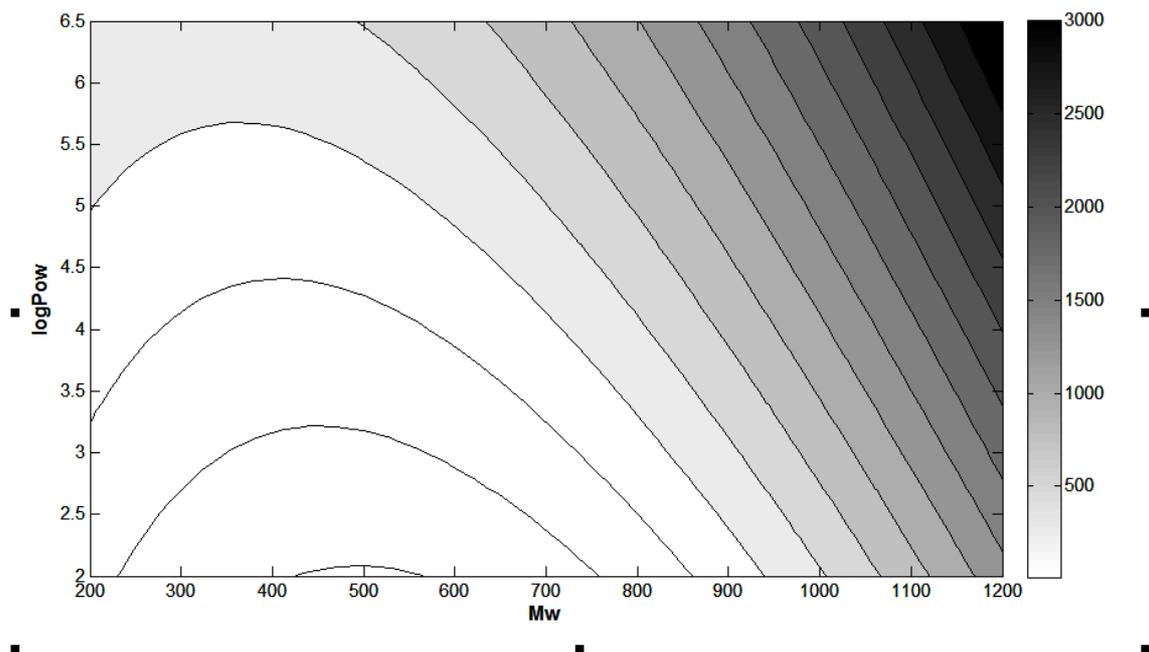
Figure 4: ANN Simulations of energy consumption EC (kJ/mg) for different values of logPow and Mw. The other input variables are fixed according to the research of Saharan et al., 2011; D=17mm; d/D=0.08, C₀= 40mg/L, T=30°C, V=15L, Pin=5bar; Cv=0.15; pH=2

4. Conclusions

In this work, an artificial neural network has been created and implemented for the evaluation of HC as an advanced oxidation process. The main novelty of the model consists of considering both the influence of operating parameters and pollutant characteristics as fundamental modelling variables. This effort of abstraction, allows the creation of a valid tool for predicting the treatment feasibility, for designing an experimental campaign for emerging compounds and ideating new *ad hoc* cavitating geometries. During the treatment the ANN can be used also for an intelligent real-time process control.

The ANN was able to reproduce a set of experimental results reported in literature. The tool created has been used for evaluating the effect of operating parameters, finding a good theoretical explanation in accordance with the pertinent literature (*i.g.* preliminary results confirmed the positive influence of operating at low pH). The importance of quantifying the energy consumption, in dependence of a set of variables, is extremely useful in controlling and optimizing the process (even in real time).

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