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Applications of ANNs on photocatalytic reactors: a brief overview

Stefano Curcio
Department of Computer Engineering, Modeling, Electronics and Systems, University of Calabria, Ponte P. Bucci, cubo 42/c, 87036 Rende (CS) – ITALY
E-mial: stefano.curcio@unical.it

Heterogeneous photocatalysis and neural model

Heterogeneous photocatalysis is a "green" technology with potential applications in various disciplines, such as chemical synthesis and environmental technologies. These processes use certain metal oxides those can generate hydroxyl radicals on the surfaces of particles when exposed to UV light. The anatase form of TiO_2 has low band-gap energy (approximately 3.2eV), which is almost equivalent to 400nm wavelength of light. Activation of semiconductor TiO_2 catalyst achieved through the absorption of photon of ultraviolet band gap energy, results in the formation of electron donor (reducing) and electron acceptor (oxidizing) sites. The photocatalytic activity of TiO_2 depends on the relative rates of generation and recombination of electron-hole pairs as well as the adsorption of radical-forming species on TiO_2 surfaces. Hydroxyl radicals (HO·) and superoxide ion are the principal agents responsible for the oxidation of aqueous organic contaminants [1]. The carbon containing pollutants are oxidized to carbon dioxide and water, while the other elements bonded to the organic compounds are converted to anions such as nitrate, sulphate or chloride. The purification of wastewater by heterogeneous photocatalysis is one of the most rapidly growing areas of interest to both research workers and water purification plants. Commercial application of the process is called advanced oxidation process (A.O.P).

Public Interest Statement

While many of the advances in materials science have been driven by breakthroughs in material design and fabrication, understanding the changes that occur in a material during its utilization or operation in devices is of immense importance for its successful integration. Considering these aspects and the continued growth in materials research, there is a clear need for new topical journals which can serve researchers to understand the phase transitions and exploit the phenomena to current, state-of-the-art research in the field of materials science, moreover with full accessibility.

In recent years, TiO_2 has been chosen as a photocatalyst for the destruction of polluting materials due to its efficiency, non-toxicity, high activity, photochemical inertness and low cost [2]. In some recent work, photocatalytic degradation of reactive black-5 (RB-5) dye using TiO_2 impregnated ZSM-5 has been investigated in a batch reactor [3].With some optimum formulation of supported catalyst, 98% degradation of 50mg/L RB-5 solutions was obtained in 90 minutes. Hosseinia et.al. [4] has synthesized nanosize TiO_2 particles and investigated photocatalytic degradation of different chromophores under visible light irradiation at different catalyst loading and different dye concentrations. In another work [5], phenol degradation had been examined with combined photocatalysts TiO_2 and ZnO under illumination of a 500W super high pressure mercury lamp mounted axially. The results revealed that, both TiO_2 and ZnO were effective, though the latter was much superior in terms of photocatalytic activity. Photocatalysis is particularly useful for cleaning biologically toxic or non-biodegradable materials such as aromatics, pesticides, petroleum constituents, dyes and volatile organic compounds in wastewater [6].

The effluents of various chemical and pharmaceutical industries, coal refineries, phenol manufacturing, pharmaceuticals, dying, petrochemical, pulp mill etc., include wide variety of organic chemicals like phenol and various substituted phenol. Phenol is one of the most prevalent chemical and pharmaceutical pollutants, due to its toxicity even at lower concentrations and formation of substituted compounds during oxidation and disinfection processes. Its direct effects on the environment include depletion of ozone layer, on the earth's heat balance, reduced visibility and adding acidic air pollutants to the atmosphere [7]. Phenol removal from the industrial wastewater is utmost necessary, as phenol concentration in wastewater inhibits or eliminates microorganisms thus strongly reduces biological biodegradation of other components. Accordingly, efforts are being given to reduce phenol concentration prior to the wastewater discharge, so as to decrease all these detrimental effects. Various methods have been suggested so far to degrade phenol effectively using A.O.P. [8,9]. The advantage of these processes is that they lead to the total mineralization of organic contaminants.

A number of photocatalytic reactors have been patented in recent years but none has so far been developed in pilot scale. In the light of the above discussion, photocatalytic degradation of phenol in aqueous using TiO_2 is summarized in combination of Artificial Neural Network (ANN) model.

Mathematical modeling represents a useful support to the design, optimization, and control of chemical processes. In the case of heterogeneous photocatalytic reactions, a comprehensive kinetic analysis aimed at describing the real behavior of a photoreactor is usually difficult to be achieved since many parallel-serial reactions could be involved. In addition, the process efficiency may be strongly affected both by mass transfer limitations, which determine a significant worsening of reactor performance, and by the presence of contaminants, which may interfere with the catalyst during the reaction progress. Different approaches, e.g. theoretical, empirical, semi-empirical, were proposed in the literature to develop reliable models aimed at investigating how the responses of photocatalytic processes change, with time, under the influence of both external disturbances and manipulated variables [10]. Fundamental or theoretical modeling is based on well-established conservation principles, whose exploitation allows formulating rather accurate kinetic/ transport models describing the time evolutions of some characteristic parameters, as a function of process operating conditions [11]. An exhaustive analysis of all the complex phenomena occurring in a photoreactor, however, is difficult to be accomplished. The huge number of chemical reactions occurring in the reactor, together with a series of not-completely-understood phenomena related to the actual reaction pathways involved in the process, determines a significant level of uncertainness, which generally does not allow a rigorous model formalization by proper mathematical relationships. On the other hand, a model based on Artificial Neural Networks (ANNs) does not make use of any kinetic or transport equation, which could help to determine, on the basis of fundamental principles, the mutual relationships existing between the inputs and the outputs [12]. ANNs are composed of several simple interconnected computational elements called neurons, which operate in parallel. The simplest kind of neuron is characterized by a scalar input (i), actually multiplied by a scalar weight (w); the weighted input (i*w) is summed to a second scalar, known as the bias (b). The resulting neuron input (n = i*w + b) is then fed to a transfer function (F), which eventually produces a scalar output (o). Both w and b can be adjusted, during the so-called training step, so as to allow the network performing a particular task or exhibiting a desired behavior. A single neuron may also receive P different inputs (i[1], i[2], ….., i[P]) each of them multiplied by the corresponding weights so to get a multiple input neuron, which is characterized, as in the previous case, by a net input (n), given by sum between the bias b and the dot product of the row vector, w, and the column vector, i, a transfer function (F) and an output (o). The perceptron is a particular type of ANN created by Rosenblatt. One of the simplest forms of perceptron is represented by a single layer network whose weights and biases are continuously adjusted during neural network training so to obtain a correct target vector when presented with the corresponding input vector. Due to its intrinsic limitations, single layer networks are generally replaced by multi-layer ANNs in which the input signal is propagated forward through different processing layers before the network output is calculated. A multilayer perceptron (MLP) network is a supervised network consisting of, at least, three layers: two or more hidden layers (the first one is sometimes called the input layer) and an output layer which produces the final output(s) of the network. Each layer is composed by one or more nodes; each node has input connections only with the nodes of the previous layer and the node's output is transmitted only to the neurons belonging to the next layer. Each node has an associated weight vector and, usually, a bias, both transforming its input vector, and a transfer function which allows obtaining the neuron's non-linear response. The weights and the biases, therefore, represent the ANN model parameters which are to be adjusted to allow the network producing the desired outputs. This feature makes ANN a parametric model. The final output of the network is compared with a target vector, generally represented by a set of available experimental data; the difference, known as error, between the network output and the desired target is used to update the weights and biases during network training by means of a proper learning algorithm aimed at minimizing the error (13). Actually, two or more of such multiple input neurons may be combined in a layer and a specific network might contain one or more such layers. In a multilayer network the layer which produces the network output(s) is called the output layer; all the other layers are, instead, called hidden layers. ANNs are a data-driven method capable to learn from examples capturing the functional relationships existing between the input(s) and the output(s). Even if the prediction of each single neuron could be imperfect and bias-affected, the outcome of the interconnection(s) among neurons is a computational tool capable to learn from examples and to provide accurate predictions even with examples never seen before [13]. This feature makes ANNs a particularly useful tool when the behavior of complex systems is to be described, since no a priori knowledge of system dynamics is actually required. A neural model, however, can be rather complicated, since it requires a large number of connections and, therefore, a great number of parameters that are to be estimated. The neural network architecture, i.e. the definition of the number of layers composing the network, of the number of neurons and the types of transfer function in each layer, strongly affects the reliability of ANN predictions and the computational effort required to train the network with a given set of experimental data.

Generally, a larger number of neurons results in a more powerful network, but also in a higher computational effort. It is worthwhile remarking, however, that the exploitation of too many hidden neurons may determine the so-called over-fitting, i.e. the incapability of the network to generalize to new situations different from the examples memorized during the training [8]. The identification of the number of layers and of the neurons belonging to each layer is, therefore, the result of an optimization process. Even if several methods were proposed to achieve the final network architecture, a general procedure is not yet available and the network structure is usually determined according to heuristic guidelines and to trial-and-error procedures [11]. The development of an artificial neural network model consists of several steps. During the training phase, the network learns how to correlate the input to the output variables. More specifically, the network is submitted to a certain number of input and output data, generally collected from experimental measurements; according to an error minimization algorithm, the weights characterizing each of the neurons are continuously updated. Only a certain number of the available experimental points are exploited during the training phase. The remaining data are used during a post-training analysis, namely the network test, during which the neural network is called to predict the output values corresponding to an input combination never seen before. The test phase does indeed play a fundamental role in ANN definition since the convergence of the above-mentioned trial-and-error procedure is usually considered achieved with reference to a performance index based on test points. The neural network test is performed in the definition domain in which ANN training was carried out. As a matter of fact, the forecasting capability of the neural networks outside this definition range cannot be guaranteed; due to the intrinsic black-box nature of neural networks models, the validity domain does indeed strictly depends on the range of data used in model definition [13]. Another kind of post-training analysis is the so-called validation phase. Similarly to the test phase, the network is called to predict the experimental points excluded from both the training and the test sets; unlike test phase, the evaluation of model prediction reliability does not influence the definition of neural network architecture.

A reasonable trade-off between theoretical and neural network approach is represented by hybrid neural modeling, leading to a so-called “grey-box” model capable of good performance in terms of data interpolation and extrapolation [13]. Hybrid neural model (HNM) predictions are given as a combination of both a theoretical and a “pure” neural network approach, together concurring at the obtainment of system responses. The main advantage of hybrid neural modeling regards the possibility of describing some well-assessed phenomena by means of a theoretical approach, leaving the analysis of other aspects, very difficult to interpret and describe in a fundamental way, to rather simple “cause-effect” models [14]. The main advantage of a hybrid system is the possibility of describing some well-assessed phenomena by as simpler as possible theoretical relationships, leaving the analysis of other aspects, generally difficult to interpret, to rather straightforward neural models. The neural network ability to properly manage unreliable or noisy data is strongly improved when it is inserted in a hybrid structure. This is due to the theoretical part of the model that, among all the other tasks it is called to accomplish, may perform as a filtering function that limits the error propagation throughout the system even when its inputs are perturbed. When ANNs are utilized in a hybrid model, it is first necessary to identify the respective domain of exploitation pertaining to either theoretical or empirical models in such a way as to decide which aspects of the process are to be described by the black-box model and which ones by the fundamental relationships. Two kinds of HNMs can be generally defined depending on the interactions existing between the neural and the theoretical blocks. In a model based on a parallel architecture the inaccuracy in the predicted value from the fundamental part is minimized by the addition of the residuals calculated by the neural network. In a model based on a serial architecture one (or more) process variable, which is difficult to measure, is estimated by a neural network and, then, fed to the theoretical block as an input. Finally, the outputs coming out from the fundamental part is checked with the experimental values for convergence. The interest of scientific and academic community towards the applications of ANNs to photocatalytic reactors is progressively increasing.

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