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Neural Network on Photodegradation of Octylphenol using Natural and Artificial UV Radiation

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Abstract
The present paper comes up with an experimental design meant to point out the factors interfering in octylphenol's degradation in surface waters under solar radiation, underlining each factor's influence on the process observable (concentration of p-octylphenol). Multiple linear regression analysis and artificial neural network (Multi-Layer Perceptron type) were applied in order to obtain a mathematical model capable to explain the action of UV-light upon synthetic solutions of OP in ultra-pure water (MilliQ type). Neural network proves to be the most efficient method in predicting the evolution of OP concentration during photodegradation process. Thus, determination in neural network's case has almost double value versus the regression analysis.

Keywords: Octylphenol; Photodegradation; Regression analysis; Backward stepwise method; Neural network; Multilayer perceptron

Introduction

Alkylphenols (APs) and their compounds express a real threat towards aquatic biota, due to their toxic and estrogenic effects on the organisms [1]. APs are also low biodegradable [2], so permanent monitoring and removal solutions are necessary to be further developed.

The most potent alkylphenol compound was found to be octylphenol (OP) [3], which was active in many assays at 0.1 μM [4, 5] and was able to stimulate responses similar to those produced by estradiol at concentrations only 1000 times higher than those of estradiol [6]. Concerning fish reproduction, OP was investigated in a full life cycle test with zebra fish (D. rerio). OP caused significant reduction in juvenile growth and prolongation of the time until first reproduction at the highest test concentration of 38 μg/l [7]. At this concentration, egg-laying capacity of the females and fertility of the males were significantly affected. Increased incidence of endocrine-related diseases in humans [8], including declining male fertility, and more significantly, adverse physiological effects observed in wildlife, created concerns about the discharge of effluents from treatment facilities, likely to be a significant source of input of contaminants to many systems [9].

Octylphenol (OP) represents an important metabolite in the biodegradation of octylphenol ethoxylates (OPEs), which are released into the aquatic environment mainly via sewage treatment plant effluents. They are known to be taken up by organisms in the inland water system and to be stored in their fatty tissues [10, 11]. Due to its stable chemical structure does not easily biodegrade

[12]. Chronic exposure to those compounds can result in detrimental estrogenic effects on aquatic biota.

This paper uses data recorded in OP photodegradation experiments in the purpose of obtaining a neural network model to characterize the process.

Material and Method

Experiments pursuing degradation of octylphenol using real and artificial UV radiation were carried out according to experimental design presented in Figure 1 (OP solution prepared in ultra pure water). The irradiation procedures, along with all detailed experimental conditions, as well as the results obtained were previously reported [13].

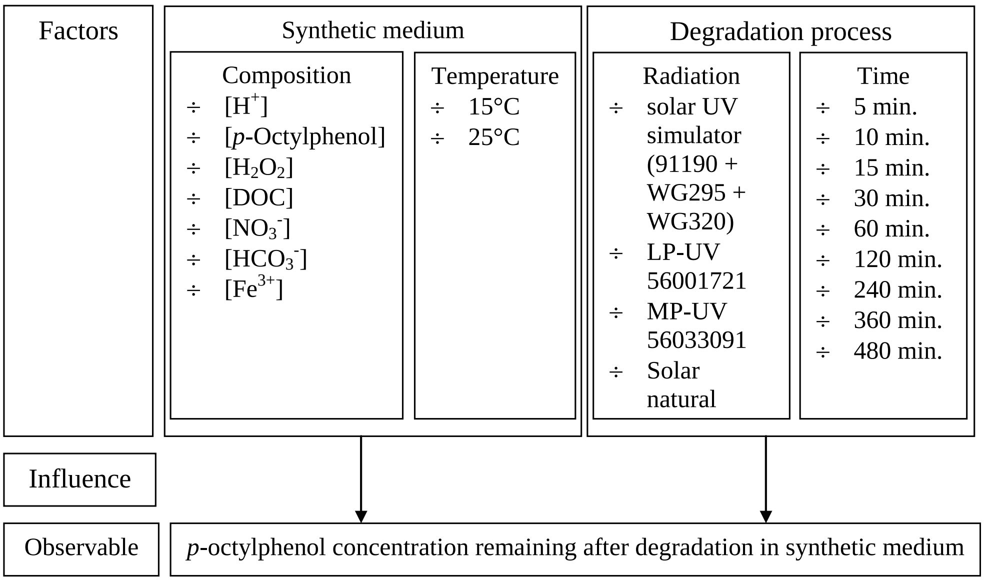

Figure 1. Experimental design for photochemical removal of OP in synthetic medium

Analysis of data resulted from irradiation experiments consisted in a multiple linear regression analysis and a neural network analysis, respectively (Figure 2).

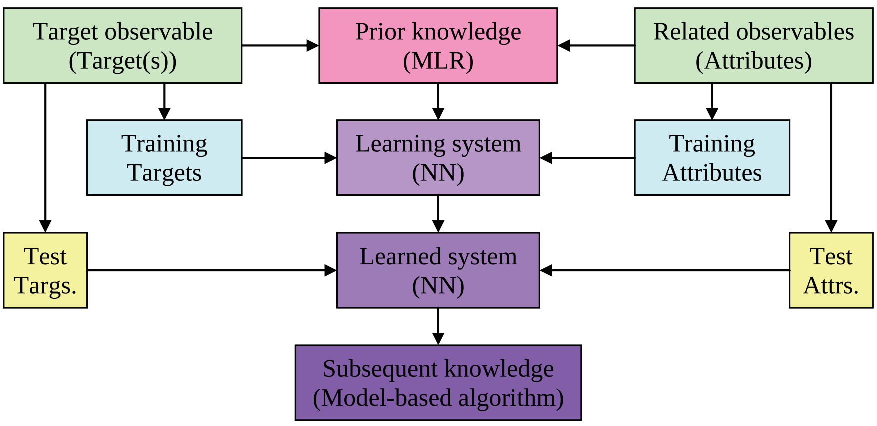

Figure 2. Experimental design for model-based learning

The neural network [14] is a sort of model-based learning [15] that uses prior knowledge (in this case coming from the multiple regression analysis [16], and being found in the selection of the model) to parameterize a model (to train the network). The parameterization of the model uses data from experiment (usually a part of it that is named "training set"). The result of the parameterization is a series of model parameters which can be further used to test the model (usually a part of the data from the experiment named "test set") or even used for making prediction of the outcome(s) when the attributes are known (see Figure 2).

Results and Discussions

For designing the experiment (Figure 1) each factor and its influence upon the observable of the process (*p*-octylphenol) was considered. All observations (137 records) about initial (before UV exposure) and final (after UV exposure) octylphenol concentration under different levels of environmental attributes (exposure time, pH, [H_2O_2], [NO_3^-], [HCO_3^-], [Fe^{3+}], exposure temperature, source of radiation) obtained using the experimental design from Figure 1 were included into the analysis, and fully presented in Table 1.

Table 1. Octylphenol degradation results under different exposure conditions

Source	[H_2O_2]	[NO_3^-]	[HCO_3^-]	[Fe^{3+}]	Temperature (°C)	pH	Time (h)	[OP]$_{initial}$	[OP]$_{final}$	[OP]$_{ratio}$
sUVs	0	0	0	0	10	8	0	2.05e-5	2.05e-5	1.000
sUVs	0	0	0	0	10	8	0.166	2.05e-5	1.86e-5	0.907
sUVs	0	0	0	0	10	8	0.333	2.05e-5	1.86e-5	0.906
sUVs	0	0	0	0	10	8	1	2.05e-5	1.81e-5	0.880
sUVs	0	0	0	0	10	8	2	2.05e-5	1.78e-5	0.866
sUVs	0	0	0	0	10	8	4	2.05e-5	1.72e-5	0.837
sUVs	0	0	0	0	10	8	8	2.05e-5	1.71e-5	0.833
sUVs	0	0	0	0	25	6.58	0	2.39e-5	2.39e-5	1.000
sUVs	0	0	0	0	25	6.58	0.166	2.39e-5	2.17e-5	0.907
sUVs	0	0	0	0	25	6.58	0.333	2.39e-5	2.14e-5	0.894
sUVs	0	0	0	0	25	6.58	1	2.39e-5	2.12e-5	0.885
sUVs	0	0	0	0	25	6.58	1.500	2.39e-5	2.11e-5	0.881
sUVs	0	0	0	0	25	6.58	2	2.39e-5	2.07e-5	0.864
sUVs	0	0	0	0	25	6.58	4	2.39e-5	2.01e-5	0.838
sUVs	0	0	0	0	25	6.58	6	2.39e-5	1.92e-5	0.800
sUVs	0	0	0	0	25	6.58	8	2.39e-5	1.69e-5	0.705
LPUV	0	0	0	0	15	6.58	0	1.96e-5	1.96e-5	1.000
LPUV	0	0	0	0	15	6.58	0.166	1.96e-5	1.76e-5	0.899
LPUV	0	0	0	0	15	6.58	0.250	1.96e-5	1.70e-5	0.867
LPUV	0	0	0	0	15	6.58	0.500	1.96e-5	1.44e-5	0.733
LPUV	0	0	0	0	15	6.58	1	1.96e-5	8.12e-6	0.415
LPUV	0	0	0	0	15	6.58	1.500	1.96e-5	6.51e-6	0.332
LPUV	0	0	0	0	15	6.58	2	1.96e-5	3.76e-6	0.192
LPUV	0	0	0	0	15	6.58	0	2.00e-5	2.00e-5	1.000
LPUV	0	0	0	0	15	6.58	0.500	2.00e-5	1.20e-5	0.601
LPUV	0	0	0	0	15	6.58	1	2.00e-5	7.59e-6	0.379
LPUV	0	0	0	0	15	6.58	1.500	2.00e-5	5.11e-6	0.255
LPUV	0	0	0	0	15	6.58	2	2.00e-5	3.69e-6	0.184
LPUV	0	0	0	0	15	6.58	4	2.00e-5	7.56e-7	0.038
LPUV	0	0	0	0	15	6.58	5	2.00e-5	1.79e-7	0.009
LPUV	0	0	0	0	15	6.58	6	2.00e-5	0.00e+0	0.000
Sun	0	0	0	0	15	6.58	0	2.00e-5	2.00e-5	1.000
Sun	0	0	0	0	15	6.58	0.166	2.00e-5	1.97e-5	0.984
Sun	0	0	0	0	15	6.58	0.333	2.00e-5	1.80e-5	0.902
Sun	0	0	0	0	15	6.58	0.500	2.00e-5	1.80e-5	0.901
Sun	0	0	0	0	15	6.58	1	2.00e-5	1.71e-5	0.854
Sun	0	0	0	0	15	6.58	1.500	2.00e-5	1.55e-5	0.775
Sun	0	0	0	0	15	6.58	2	2.00e-5	1.51e-5	0.756
Sun	0	0	0	0	15	6.58	4	2.00e-5	9.78e-6	0.489

Table 1. Octylphenol degradation results under different exposure conditions (continued)

Source	$[H_2O_2]$	$[NO_3^-]$	$[HCO_3^-]$	$[Fe^{3+}]$	Temperature (°C)	pH	Time (h)	$[OP]_{initial}$	$[OP]_{final}$	$[OP]_{ratio}$
Sun	0	0	0	0	15	6.58	6	2.00e-5	5.56e-6	0.279
Sun	0	0	0	0	15	6.58	8	2.00e-5	3.54e-6	0.177
MPUV	0	0	0	0	15	6.58	0	1.38e-5	1.38e-5	1.000
MPUV	0	0	0	0	15	6.58	1/12	1.38e-5	8.63e-6	0.627
MPUV	0	0	0	0	15	6.58	1/6	1.38e-5	6.89e-6	0.501
MPUV	0	0	0	0	15	6.58	1/4	1.38e-5	5.28e-6	0.384
MPUV	0	0	0	0	15	6.58	1/3	1.38e-5	3.62e-6	0.263
MPUV	0	0	0	0	15	6.58	5/12	1.38e-5	3.22e-6	0.234
MPUV	0	0	0	0	15	6.58	1/2	1.38e-5	2.31e-6	0.168
MPUV	0	0	0	0	15	6.58	1	1.38e-5	7.45e-7	0.054
sUVs	10	0	0	0	15	6.58	0	1.83e-5	1.83e-5	1.000
sUVs	10	0	0	0	15	6.58	1/6	1.83e-5	1.81e-5	0.994
sUVs	10	0	0	0	15	6.58	1/3	1.83e-5	1.69e-5	0.927
sUVs	10	0	0	0	15	6.58	4	1.83e-5	1.65e-5	0.903
sUVs	10	0	0	0	15	6.58	8	1.83e-5	1.35e-5	0.741
sUVs	50	0	0	0	15	6.58	0	2.03e-5	2.03e-5	1.000
sUVs	50	0	0	0	15	6.58	1/3	2.03e-5	1.58e-5	0.780
sUVs	50	0	0	0	15	6.58	1	2.03e-5	1.49e-5	0.737
sUVs	50	0	0	0	15	6.58	3/2	2.03e-5	1.32e-5	0.650
sUVs	50	0	0	0	15	6.58	2	2.03e-5	1.20e-5	0.593
sUVs	50	0	0	0	15	6.58	4	2.03e-5	1.02e-5	0.502
sUVs	50	0	0	0	15	6.58	6	2.03e-5	8.01e-6	0.395
sUVs	50	0	0	0	15	6.58	8	2.03e-5	3.92e-6	0.193
sUVs	0	0	0	100	15	6.58	0	1.91e-5	1.91e-5	1.000
sUVs	0	0	0	100	15	6.58	4	1.91e-5	1.77e-5	0.923
sUVs	0	0	0	100	15	6.58	6	1.91e-5	1.65e-5	0.861
sUVs	0	0	0	100	15	6.58	8	1.91e-5	1.60e-5	0.834
sUVs	0	0	0	0	15	6.58	0	1.54e-5	1.54e-5	1.000
sUVs	0	0	0	0	15	6.58	1/6	1.54e-5	1.48e-5	0.958
sUVs	0	0	0	0	15	6.58	1/2	1.54e-5	1.45e-5	0.940
sUVs	0	0	0	0	15	6.58	2	1.54e-5	1.41e-5	0.912
sUVs	0	0	0	0	15	6.58	4	1.54e-5	1.36e-5	0.885
sUVs	0	0	0	0	15	6.58	6	1.54e-5	1.35e-5	0.873
Sun	0	0	0	100	15	6.58	0	2.03e-5	2.03e-5	1.000
Sun	0	0	0	100	15	6.58	1/3	2.03e-5	1.94e-5	0.952
Sun	0	0	0	100	15	6.58	1/2	2.03e-5	1.87e-5	0.920
Sun	0	0	0	100	15	6.58	2	2.03e-5	1.52e-5	0.748
Sun	0	0	0	100	15	6.58	4	2.03e-5	1.17e-5	0.576
Sun	0	0	0	100	15	6.58	6	2.03e-5	7.74e-6	0.380
Sun	0	0	0	100	15	6.58	8	2.03e-5	3.41e-6	0.167
Sun	0	0	725	0	15	6.58	0	2.18e-5	2.18e-5	1.000
Sun	0	0	725	0	15	6.58	1/6	2.18e-5	2.15e-5	0.982
Sun	0	0	725	0	15	6.58	1/3	2.18e-5	2.09e-5	0.959
Sun	0	0	725	0	15	6.58	1/2	2.18e-5	2.02e-5	0.927
Sun	0	0	725	0	15	6.58	1	2.18e-5	1.96e-5	0.895
Sun	0	0	725	0	15	6.58	3/2	2.18e-5	1.92e-5	0.880
Sun	0	0	725	0	15	6.58	2	2.18e-5	1.89e-5	0.864
Sun	0	0	725	0	15	6.58	4	2.18e-5	1.46e-5	0.667
Sun	0	0	725	0	15	6.58	6	2.18e-5	9.68e-6	0.443
Sun	0	0	725	0	15	6.58	8	2.18e-5	4.80e-6	0.220
sUVs	0	0	725	0	15	6.58	0	2.10e-5	2.10e-5	1.000
sUVs	0	0	725	0	15	6.58	2	2.10e-5	2.00e-5	0.952

Table 1. Octylphenol degradation results under different exposure conditions (continued)

Source	$[H_2O_2]$	$[NO_3^-]$	$[HCO_3^-]$	$[Fe^{3+}]$	Temperature (°C)	pH	Time (h)	$[OP]_{initial}$	$[OP]_{final}$	$[OP]_{ratio}$
sUVs	0	0	725	0	15	6.58	4	2.10e-5	1.92e-5	0.916
sUVs	0	0	725	0	15	6.58	6	2.10e-5	1.77e-5	0.842
sUVs	0	0	725	0	15	6.58	8	2.10e-5	1.71e-5	0.813
Sun	0	61	0	0	15	6.58	0	2.13e-5	2.13e-5	1.000
Sun	0	61	0	0	15	6.58	1/6	2.13e-5	2.05e-5	0.960
Sun	0	61	0	0	15	6.58	1/2	2.13e-5	1.95e-5	0.913
Sun	0	61	0	0	15	6.58	1	2.13e-5	1.82e-5	0.853
Sun	0	61	0	0	15	6.58	3/2	2.13e-5	1.75e-5	0.821
Sun	0	61	0	0	15	6.58	2	2.13e-5	1.64e-5	0.767
Sun	0	61	0	0	15	6.58	4	2.13e-5	1.18e-5	0.554
Sun	0	61	0	0	15	6.58	6	2.13e-5	7.00e-6	0.328
Sun	0	61	0	0	15	6.58	8	2.13e-5	3.62e-6	0.170
sUVs	0	61	0	0	15	6.58	0	2.06e-5	2.06e-5	1.000
sUVs	0	61	0	0	15	6.58	1/3	2.06e-5	1.92e-5	0.934
sUVs	0	61	0	0	15	6.58	1/2	2.06e-5	1.88e-5	0.916
sUVs	0	61	0	0	15	6.58	1	2.06e-5	1.85e-5	0.898
sUVs	0	61	0	0	15	6.58	3/2	2.06e-5	1.80e-5	0.876
sUVs	0	61	0	0	15	6.58	2	2.06e-5	1.73e-5	0.841
sUVs	0	61	0	0	15	6.58	6	2.06e-5	1.66e-5	0.806
sUVs	0	61	0	0	15	6.58	8	2.06e-5	1.67e-5	0.809
sUVs	0	0	0	100	15	6.58	0	1.43e-5	1.43e-5	1.000
sUVs	0	0	0	100	15	6.58	1/6	1.43e-5	1.33e-5	0.926
sUVs	0	0	0	100	15	6.58	1/3	1.43e-5	1.26e-5	0.878
sUVs	0	0	0	100	15	6.58	4	1.43e-5	1.06e-5	0.738
sUVs	50	0	0	0	15	6.58	0	2.36e-5	2.36e-5	1.000
sUVs	50	0	0	0	15	6.58	1/2	2.36e-5	1.68e-5	0.713
sUVs	50	0	0	0	15	6.58	1	2.36e-5	1.51e-5	0.639
sUVs	50	0	0	0	15	6.58	4	2.36e-5	1.35e-5	0.574
sUVs	50	0	0	0	15	6.58	8	2.36e-5	1.19e-5	0.503
sUVs	50	0	0	0	15	6.58	72	2.36e-5	1.43e-7	0.006
sUVs	50	0	0	0	15	6.58	87	2.36e-5	1.24e-7	0.005
sUVs	0	61	0	0	15	6.58	0	2.17e-5	2.17e-5	1.000
sUVs	0	61	0	0	15	6.58	1/2	2.17e-5	1.99e-5	0.921
sUVs	0	61	0	0	15	6.58	1	2.17e-5	1.94e-5	0.898
sUVs	0	61	0	0	15	6.58	3/2	2.17e-5	1.74e-5	0.802
sUVs	0	61	0	0	15	6.58	2	2.17e-5	1.72e-5	0.795
sUVs	0	61	0	0	15	6.58	4	2.17e-5	1.61e-5	0.743
Sun	50	0	0	0	15	6.58	0	2.72e-5	2.72e-5	1.000
Sun	50	0	0	0	15	6.58	1/2	2.72e-5	2.08e-5	0.767
Sun	50	0	0	0	15	6.58	1	2.72e-5	1.96e-5	0.720
Sun	50	0	0	0	15	6.58	2	2.72e-5	1.86e-5	0.685
Sun	50	0	0	0	15	6.58	4	2.72e-5	1.17e-5	0.432
Sun	50	0	0	0	15	6.58	6	2.72e-5	4.51e-6	0.166
Sun	50	0	0	0	15	6.58	8	2.72e-5	3.01e-6	0.111

sUVs: Oriel Corp. Solar simulator; LPUV: 56001721 low pressure lamp; MPUV: 56033091 medium pressure lamp

The experimental data from Table 1 is structured as follows:

÷ 'Source' is of category based data type; it has four different values and can be binary encoded based at least on three, and no more than four binary (0/1) variables;

÷ $[H_2O_2]$, $[NO_3^-]$, $[HCO_3^-]$, $[Fe^{3+}]$ (concentrations, expressed in millimoles) and Temperature (°C) are of ordinal type due to the experimental design, and of continuous type by their nature;

÷ pH and Time (h) are of continuous type.

Construction of Multiple Linear Regression (MLR) model and of Multi-Layer Perceptron (MLP) Neural Network (NN) takes into account the data types.

The MLR model is of additive type [17] (did not consider possible interaction of factors) and is expected to explain less than the MLP-NN model which takes into account interactions of order two between factors. Nevertheless, obtaining an additive model that explains the observed concentration of octylphenol after the degradation process is the main argument for searching on a neural network explaining more of the octylphenol concentration observed variance.

Two additive models were obtained, in which the statistically insignificant parameters were eliminated using Backward Stepwise Method [18]. Both resulted regression equations, the one for absolute values of OP concentration (Eq1), and the one for relative value of OP concentration (Eq2), were able to explain about 50 % of the variance, which means that all factors come with a significant contribution, having an additive effect.

$$c_{final} = 0.495 \cdot c_{initial} - 2.84 \cdot 10^{-7} \cdot time - 7.07 \cdot 10^{-8} \cdot [H_2O_2] + 5.6 \cdot 10^{-6} \cdot [Sun?]_{0/1} + 8.61 \cdot 10^{-6} \cdot [sUVs?]_{0/1}$$
$$n = 137;\ s = 4 \cdot 10^{-6};\ r = 0.734;\ r^2_{adj.} = 0.517;\ t_{stat}(parameters) > 3;\ F = 31 \quad (1)$$

$$c_{ratio} = 0.456 + 0.304 \cdot [Sun?]_{0/1} + 0.467 \cdot [sUVs?]_{0/1} - 0.0038 \cdot [H_2O_2] - 0.01267 \cdot time$$
$$n = 137;\ s = 0.209;\ r = 0.708;\ r^2_{adj.} = 0.486;\ t_{stat}(parameters) > 3.5;\ F = 33 \quad (2)$$

Trying to explain the process evolution using neural network (Multi-Layer Perceptron (MLP) type), training was applied for 80 % randomly chosen (out of 137) observations, while testing was made for the rest of 20 %. The search started for different MLP-NN topologies, and a list of four topologies was selected for giving the topmost results in terms of training performances (Table 2).

Table 2. Four topmost MLP-NN topologies and their scores

NN name	$r_{Training}$	r_{Test}	$s_{Training}$	s_{Test}	$4 \cdot s_{Test}$	$4 \cdot s_{Test}/s_{Training}$
MLP 12-4-1	0.943839	0.953258	0.002784	0.003032	0.012126	4.355342
MLP 12-12-1	0.982541	0.981220	0.000895	0.001260	0.005038	5.630745
MLP 12-9-1	0.976984	0.977468	0.001196	0.001616	0.006463	5.404035
MLP 12-6-1	0.973972	0.970469	0.001314	0.001919	0.007676	5.841192

Listing of MLP-NN topologies results in Table 2 was achieved based on $4 \cdot s_{Test}/s_{Training}$ ratio, being known that the quality of the learning for neural networks is always related to the size of the network [19-22]. The $4 \cdot s_{Test}/s_{Training}$ ratio is supposed to allow comparisons between networks expressing a measure for relative learning capability.

As can be seen in Table 2, all networks have 12 inputs expanded from Table 1: Source – four parameters ($[Sun?]_{0/1}$, $[sUVs?]_{0/1}$, $[LPUV?]_{0/1}$, and $[MPUV?]_{0/1}$), $[H_2O_2]$, $[NO_3^-]$, $[HCO_3^-]$, $[Fe^{3+}]$, Temperature (°C), pH, Time (h), and $[OP]_{initial}$ and one output ($[OP]_{final}$). Difference between networks consists from the number of hidden neurons, ranging from 4 to 12.

The NN-MLP-12-4-1 was chosen based on $4 \cdot s_{Test}/s_{Training}$ lowest ratio for further investigation. The comparison between the first three networks on test set is given in Figure 3.

There is to be noticed that the result generated by neural network (about 89 % determination coefficient) is distinctively significantly higher to the result of multiple regression analysis (about 50 % determination coefficient).

Based on the 57 connections established within NN-MLP-12-4-1 and on the training data (see all trained networks depicted in Figure 4) the weights were identified and given in Table 3.

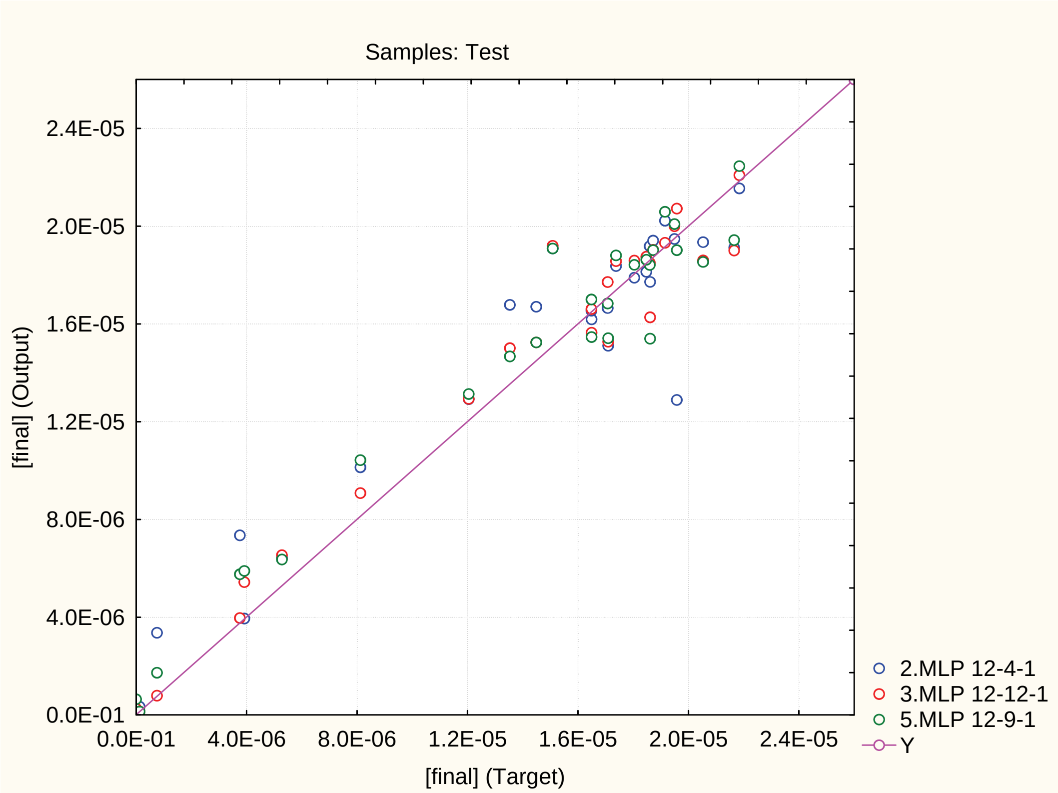

Figure 3. Output vs. target on test set for the first three networks in ascending order of $4 \cdot s_{Test}/s_{Training}$

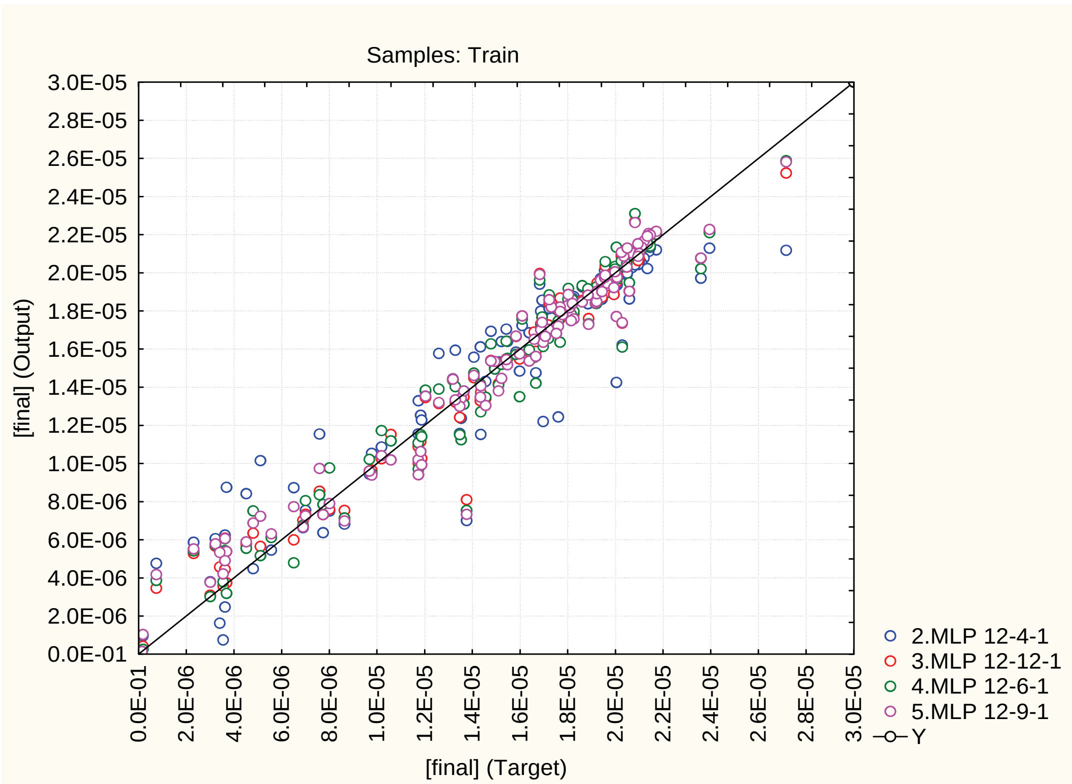

Figure 4. Output vs. target on training set for the selected networks

Table 3. Connections and connection weights in NN-MLP-12-4-1

No	Connection	Weight	No	Connection	Weight
1	time[h] --> hidden neuron 1	-3.6661	**30**	temp[°C] --> hidden neuron 2	-0.4550
2	time[h] --> hidden neuron 2	0.1970	**31**	temp[°C] --> hidden neuron 3	-0.4132
3	time[h] --> hidden neuron 3	1.4840	**32**	temp[°C] --> hidden neuron 4	0.4053
4	time[h] --> hidden neuron 4	-0.6107	**33**	Source(LP-UV) --> hidden neuron 1	-0.3938
5	pH --> hidden neuron 1	0.0125	**34**	Source(LP-UV) --> hidden neuron 2	-1.6106
6	pH --> hidden neuron 2	0.1723	**35**	Source(LP-UV) --> hidden neuron 3	0.2807
7	pH --> hidden neuron 3	0.0008	**36**	Source(LP-UV) --> hidden neuron 4	0.0014
8	pH --> hidden neuron 4	1.3709	**37**	Source(MP-UV) --> hidden neuron 1	-12.8633
9	[init] --> hidden neuron 1	-0.0705	**38**	Source(MP-UV) --> hidden neuron 2	0.6212
10	[init] --> hidden neuron 2	0.2041	**39**	Source(MP-UV) --> hidden neuron 3	3.8856
11	[init] --> hidden neuron 3	-0.4036	**40**	Source(MP-UV) --> hidden neuron 4	-2.3275
12	[init] --> hidden neuron 4	0.9644	**41**	Source(Sun) --> hidden neuron 1	0.0848
13	[H_2O_2] --> hidden neuron 1	-12.0043	**42**	Source(Sun) --> hidden neuron 2	-0.3214
14	[H_2O_2] --> hidden neuron 2	0.0260	**43**	Source(Sun) --> hidden neuron 3	-0.3454
15	[H_2O_2] --> hidden neuron 3	1.7898	**44**	Source(Sun) --> hidden neuron 4	2.5572
16	[H_2O_2] --> hidden neuron 4	-0.8007	**45**	Source(sUVs) --> hidden neuron 1	-2.1825
17	[NO_3^-]- --> hidden neuron 1	-0.0576	**46**	Source(sUVs) --> hidden neuron 2	-0.2371
18	[NO_3^-]- --> hidden neuron 2	-0.0755	**47**	Source(sUVs) --> hidden neuron 3	-0.6989
19	[NO_3^-]- --> hidden neuron 3	0.1519	**48**	Source(sUVs) --> hidden neuron 4	2.0548
20	[NO_3^-]- --> hidden neuron 4	0.2291	**49**	input bias --> hidden neuron 1	0.7258
21	[HCO_3^-]- --> hidden neuron 1	0.2488	**50**	input bias --> hidden neuron 2	-1.7384
22	[HCO_3^-]- --> hidden neuron 2	-0.3295	**51**	input bias --> hidden neuron 3	-1.9500
23	[HCO_3^-]- --> hidden neuron 3	-0.0741	**52**	input bias --> hidden neuron 4	-1.2934
24	[HCO_3^-]- --> hidden neuron 4	-1.3380	**53**	hidden neuron 1 --> [output]	-0.7469
25	[Fe_3^+] --> hidden neuron 1	-0.6289	**54**	hidden neuron 2 --> [output]	2.1047
26	[Fe_3^+] --> hidden neuron 2	0.3437	**55**	hidden neuron 3 --> [output]	-1.4564
27	[Fe_3^+] --> hidden neuron 3	0.0255	**56**	hidden neuron 4 --> [output]	1.5273
28	[Fe_3^+] --> hidden neuron 4	-1.5460	**57**	hidden bias --> [output]	0.1364
29	temp[°C] --> hidden neuron 1	0.4554			

Table 3 provides useful knowledge about the influence of the degradation conditions on the concentration of octylphenol. Thus, the highest positive weight on output comes from the hidden neuron no. 2 (2.1047) – variables contributing to this neuron are the most influents on the increase of octylphenol quantity after the degradation process. Based on the same reasoning, variables contributing to the value of hidden neuron no. 3 (-1.4564) are most influents on the decrease of octylphenol quantity after the degradation process.

The exposing time contributes unfavourably in a small weight (0.1970) to hidden neuron no. 2 and favourably in a significantly larger weight (1.4840) to hidden neuron no. 3.

The pH contributes favourably in a small weight (0.0008) to hidden neuron no. 3 and unfavourably in a significantly larger weight (0.1723) to hidden neuron no. 2.

As expected, the initial concentration of octylphenol contributes unfavourably in a positive weight (0.2041) to hidden neuron no. 2 and unfavourably (again) in a negative weight (-0.4036) to hidden neuron no. 3.

The oxygenated water contributes unfavourably in a small weight (0.0260) to hidden neuron no. 2 and favourable in a significantly larger weight (1.7898) to hidden neuron no. 3.

The nitro ion contributes favourably in a negative weight (-0.0755) to hidden neuron no. 2 and favourably in a positive weight (0.1519) to hidden neuron no. 3.

The acid carbonate ion contributes favourably in a negative weight (-0.3295) to hidden neuron no. 2 and unfavourably in a smaller negative weight (-0.0741) to hidden neuron no. 3.

The Fe^{3+} ion contributes unfavourably in a larger weight (0.3437) to hidden neuron no. 2 than it contributes favourably in weight (0.0255) to hidden neuron no. 3.

Conclusions

Based on the knowledge provided by the most influential hidden neurons of the NN-MLP-12-4-1 designed network (able to explain about 90 % of the observed variance in octylphenol concentration), the octylphenol in the water under radiation exposure is diminished when pH is less acid. Oxygenated water contributes favourably to octylphenol decomposition. Acid carbonate ion contributes favourably but in a less decisive measure than nitro ion does. The presence of the ferric ion inhibits the decomposition of octylphenol in water under radiation exposure.

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