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Taguchi orthogonal array combined with Monte Carlo simulation in the optimization of wastewater treatment

Ana Paula Barbosa Rodrigues de Freitas[1, *], Leandro Valim de Freitas[1, 2], Carla Cristina Almeida Loures[1], Aneirson Francisco da Silva[1], Lúcio Gualiato Gonçalves[1], Messias Borges Silva[1, 3]

[1]Mechanical Engineering Department, Unesp, Guaratinguetá, Brazil
[2]Brazilian Petroleum S/A, São José dos Campos, Brazil
[3]Chemical Engineering Department, USP, Lorena, Brazil

Email address:

anapaulabrfreitas@gmail.com (A. P. B. R. Freitas), leandrovalimdefreitas@gmail.com (L. V. Freitas), ccaloures@hotmail.com (C. C. A. Loures), aneirson@yahoo.com.br (A. F. Silva), lucioseguranca2011@gmail.com (L. G. Gonçalves), messias.silva@feg.unesp.com.br (M. B. Silva), messias@dequi.eel.us.br (M. B. Silva)

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Abstract: In this work was performed a Monte Carlo Simulation for a mathematics model to experimental planning of Taguchi. The software has enabled an upgrading of the variables planning value of 54,26% of TOC, 53,28% of DQO and 6,58% of Total Phenols, that feature the importance of the method for the experimental optimizations, and thereafter reduction of experiments to be realized in the job first step.

Keywords: Monte Carlo Simulation, Taguchi, Multiobjective Optimization

1. Introduction

The environment degradation is consequence of industrial effluents sewage in a inadequate way, that has been bringing about serious problems of contamination on several world coutries [1].

The industrial process produces a large toxic molecules range that could foul the air and water, because result in negatives impacts for ecosystem and human being [2].

The phenols are toxic compound to microorganisms and can be hard to be removed for the system over biological treatment or by natural procedure in aquatic environment [3].

Phenol is one of the most ordinary organic compound and its found like effluent in many industries, such as oil refining, petrochemical, pharmaceutical products, dyes, textile industry, manufacture of organic chemicals and others [4].

According [5], believes that the necessary process at chemical area; chemical engineering specifically; will be achieved by multidisciplinary and a comprehensive approach, that it will be through constants scientific innovations and powerful computational tools.

According [6] increase the importance of shaping and simulation on chemical engineering development. These methods are critical technologies to reach the industrial purpose in process area.

This work consists on Monte Carlo simulation appliance at phenolic effluent treatment. It was used a comparative approach of simulation relative to orthogonal array of Taguchi for the environment variables, such as, Total Organic Carbon (TOC), phenols and Chemical Oxygen Demand (COD).

2. Literature Review

2.1. Operational Research

Human mistakes over an operation and consequent operational risk enlargement are the main concern for all sections. Besides, human reliability analysis with probabilistic risk analysis is a key element in reducing the operational risk. A prevision technique average of human error and risk of standardized plan and the reliability human methods has been used to quantify distinct human errors categories [7].

2.2. Monte Carlo Simulation

The Monte Carlo simulation is an associated method of use of random numbers and statistical probability [8].

According [9], Monte Carlo Simulationis applied in chemical process, being studied in kinetic behavior of hydrogenation of acetylene. The significant activation energy for this system shows the presence of carbon monoxide absorbed increase material selection, and activation energies obtained 16,7 and 56 KJ mol-1.

The Monte Carlo methodis conducted for model calibration used on incineration of waste in a landfill. Sensibility analysis also was realized to identify most sensible factors. At huge cities and metropolis with large creation of solids urban wastes, possibility of large scale construction incineration installations raise, while, for median and small cities, incineration of waste get down [10].

2.3. GeneticAlgorithms

Genetics Algorithms (AG) are an efficient technic of sweep the space of solutions and find close great values, being one of the several techniques of computational intelligence worthy of study [11].

Joint application of genetics algorithms and Monte Carlo simulation was realized for the study of determining the value of real options of several technical market uncertainties. The application obtained the goal of approach a great decision rule and determine the value of the real option in a way of having several investment in a project.[12].

According [13] genetic algorithms were applied in a electronics properties studies and optics of polymeric structures, in order of obtain a suitable copolymer for a given application. Evaluate the effect of polymer properties when subject to a system of electrical discontinuity when immersed in an optimal solution. Concluded by a binary model that polymers with increasing conduction band need better solutions and are dependents of greatest value.

3. Materials and Methods

3.1. Raw Material

Experimental data will be used at Laboratory of Environment Engineering School of Lorena (EEL / USP). At this step the phenolic effluents were treat over a design Experimental (Orthogonal array of Taguchi L_{16}) using advanced oxidation process. Obtained results were applied on Monte Carlo simulation.

3.2. Methods

The Monte Carlo simulation associated to the genetic algorithm Metaheurística will do a scanning deterministic simulation of experimental design. It's a multiojective problem being realized an optimization using the CP function.

Simulation experiments will be held using a Minitab®, Crystal Ball® and Statistica® computational package.

4. Results and Discussions

4.1. Monte Carlo Simulation

In this work were performed a deterministic simulation of multiple TOC, COD and Phenols responses respectively represented by Y_1, Y_2 e Y_3according to table 1. This Table were obtained the target values of deterministic simulation realized, so we can compare the values obtained in the experimental planning. Target values showed huge relevance if compared to Taguchi. Mathematic model coefficients follows a distribution.

Table 1. *Monte Carlo Simulation the deterministic values*

	X1	**X2**	**X3**	**X4**	**X5**	**X6**										
Factors	0	0	0	0	0	0										
Response			Software target		Model Coefficients	B0	X1	X2	X1X2	X3	X2X3	X5	X1X5	X6	X1X6	X4	X1X4
Y1	21,57		33,27		Y1	21,6	3,4	1,4	-0,19	-2,6	-1,3	-0,1	-0,2	1,4	1,2	0,5	0,2
Y2	44,13		67,64		Y2	44,1	7,3	0,6	-1,3	1,4	-0,8	-0,3	-5,6	8,9	7,1	3,8	0,4
Y3	98,83		100		Y3	93,8	-6,0	-0,7	0,7	0,11	-0,3	3	-1,6	1,5	-2,6	2,4	-3,7

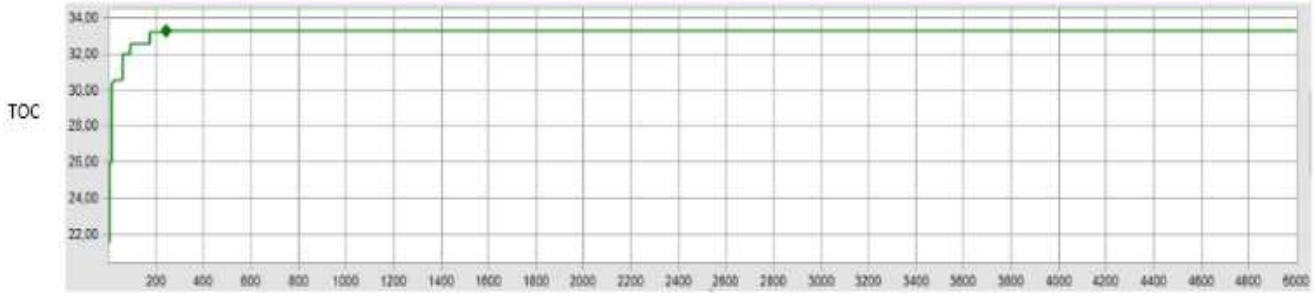

Figure 1. *Best solution with Monte Carlo simulation (% TOC)*

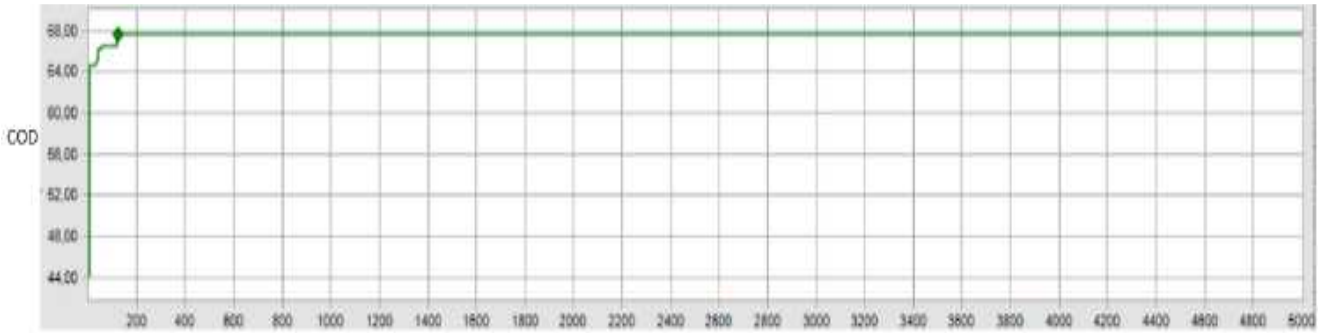

Figure 2. *Best solution with Monte Carlo simulation (% COD)*

On Monte Carlo simulation were realized 5000 interactions. In Figure 1, the percentage optimization of Total Organic Carbon (TOC) removal was realized, in which the optimization time was 1 minute and 04 seconds and, then, obtained a stabilization of the best solution. Software improved the outcome of 21,47 to 33,27, in other words, 54,26% was an improvement in the variable response.

In Figure 2, the optimization of removal percentage of Chemical Oxigen Demand (COD) was realized and, in a time of 1 minute and 18 seconds obtained a better stabilization solution. Software improved the outcome of 44,13 to 67,64, in other words, 53,28% was an improvement in the variable response.

In Figure 3, the optmization of removal percentage of total phenols was realizes and, in a time of 1 minute and 47 seconds obtained a better stabilization solution. Software improved the outcome of 93,83 to 100, in other words, 6,28% was an improvement in the variable response. Presented data showed a significant improvement ofvariable response percentage removal which proves the validity of the optimization method.

On Table 2, the individual values of each variable response were optimized by Compromise Programming (CP) function. The problem is multiobjective, and, therefore the optimization is performed in this way, in which the target value obtained is used and the weights assigned to each variable. The obtained value in CP function was 5,9, in other words, features a value of great importance, because the rejection rate was around 6,95%. This indicates a great quality of obtained data, because in experimental chemical problems the maximum allowed value must be less than 10%. In CP function was obtained weights for variable responses, in which the values are like 0,333; in other words, being also significant for the optimization process.

Table 2. *Simulation of CP function of variable response (Multiobjective)*

	X1	**X2**	**X3**	**X4**	**X5**	**X6**			**FCP Weights**	**0,3**	**0,3**	**0,3**	**1FCP**				
Factors	1	-1	-1	-0,6	1	1											
Response			Software target		Model Coefficients	B0	X_1	X_2	X_1X_2	X_3	X_1X3	X5	X1X5	X6	X1X6	X4	X1X4
Y1	30,46		33,27		Y1	21,6	3,4	1,4	-0,19	-2,6	-1,3	-0,1	-0,2	1,4	1,2	0,5	0,2
Y2	65,76		67,64		Y2	44,1	7,3	0,6	-1,3	1,4	-0,8	-0,3	-5,6	8,9	7,1	3,8	0,4
Y3	90,35		100		Y3	93,8	-6,0	-0,7	0,7	0,11	-0,3	3	-1,6	1,5	-2,6	2,4	-3,7
FCP	5,9		DPM	¨6,95%													

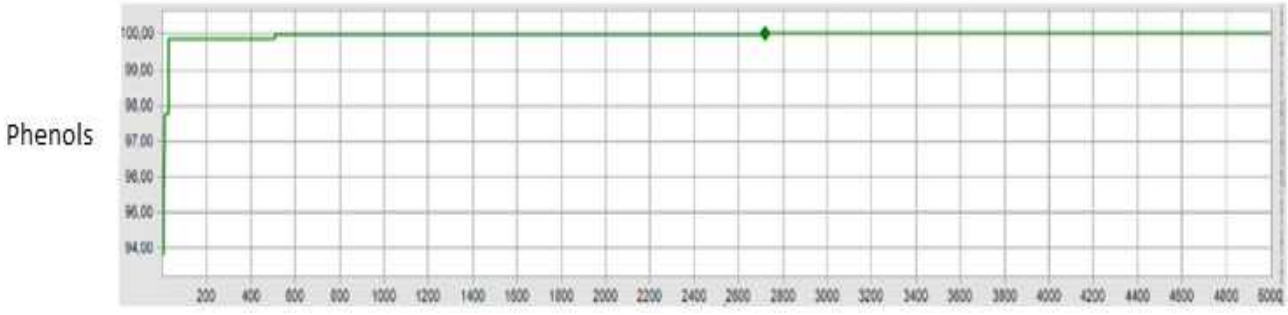

Figure 3. *Best solution with Monte Carlo simulation (% Total Phenols)*

4.2. Steps for Further Work

The next step to be realized will be the confirmation of laboratory experiments, and then,a stochastic planning data.

In this work will be comparatively evaluated using Monte Carlo method with the optimization approach of experiments planning in the study of phenolic effluents treatment by advanced oxidation processes. Thus, behavior of variable input and regression coefficients as stochastic variables will be studied, proposes to reduce the experimental number, as

well as the use of Metaheurísica genetic algorithm to solve Monte Carlo Simulation.

The proposal is to work with stochastic coefficients, so, witFh probability distribution associated.

5. Conclusion

In this work was realizedmultiobjective optimization of mathematical modeling obtained from experimental planning. Deterministic simulation was realized and improvements were obtained in 3 studied variable responses. Enhance responses were adjusted on CP function and obtained consistent values.

The software has enabled an upgrading of the variables planning value of 54,26% of TOC, 53,28% of DQO and 6,58% of Total Phenols, that feature the importance of the method for the experimental optimizations, and thereafter reduction of experiments to be realized in the job first step.

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