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Multivariate Normal Boundary Intersection based on rotated factor scores: A multiobjective optimization method for methyl orange treatment

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ABSTRACT

This paper presents the multiobjective optimization of methyl orange treatment with ozone using Normal Boundary Intersection and response surface models of rotated principal component factor scores for the expected value E[f(x)] and prediction variance Var[f(x)] of dye removal (Y_1) and chemical oxygen demand removal (Y_2). The innovation and the main contribution of this paper consists of building a 2-dimensional equispaced and convex Pareto Frontier for rotated factor scores representing the original multivariate set, reducing the number of objective functions without inverting the correlation among the original responses. Furthermore, this proposal provides a practical way to generate the narrowest possible prediction confidence intervals for a desired optima using the fuzzy membership function criterion in order to select the best compromise solution between E[f(x)] and Var[f(x)]. To illustrate the proposal's feasibility, a central composite design for the ozonation process of methyl orange solution with three factors (x_1 = pH, x_2 = air flow and x_3 = ozone dosage) was run. The optimization results showed a maximum dye removal of 94.1% ± 4.3 with a respective chemical oxygen demand removal of 88.4% ± 5.3 obtained at x^* = [9.5; 7.1 l.min-1; 18.4 g h^{-1}]. However, this point have presented the largest 95% prediction confidence interval. Based on the fuzzy membership of Pareto set it was possible to select the narrowest 95% confidence intervals with maximum removal rates (Y_1 = 90.5 ± 2.2 and Y_2 = 88.3 ± 2.7), obtained at x^* = [7.9, 5.6 l min^{-1}, 18.4 g h^{-1}]. Confirmation runs and comparisons among several optimization methods were done and indicated that the results fell within the respective confidence intervals for predictions, which corroborates the good adequacy of the proposal.

1. Introduction

Response surface methodology (RSM) has been extensively used in the modelling and optimization of industrial an urban wastewater treatments. Examples include the wastewater treatment of livestock (Tak et al., 2015), meat industry (Thirugnanasambandham et al., 2015), tobacco wastewater (Pi et al., 2015), leather industry (Boopathy and Sekaran, 2013), textile industry (Sheydaei et al., 2014), steel industry (Anouzla et al., 2009), petroleum refinery (Shahrezaei et al., 2012) among others. The most used RSM designs in wastewater treatment are the central composite design (CCD) (Asfaram et al., 2015a, 2015b; Li et al., 2015) and the Box-Behnken design (BBD) (Nair and Ahammed, 2015). Both designs are capable of generate nonlinear objective functions like full quadratic models (Montgomery, 2009). The central composite design (CCD) is a response surface array composed by three groups of points: a factorial design with 2^k experiments (where k is the number of controllable factors), $2k$ axial points and n center points. The

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distance between center and axial points are generally defined as $2^{(k/4)}$. Sometimes, the axial points produce a set of unfeasible experiments, since they represent extreme high or low conditions for the controllable factors (Myers and Montgomery, 2009). Then, if the chosen levels for the controllable factors lead to impracticable experiments, Box-Behnken design is more recommended since it is a design formed by combinations of factorial and center points without outside or extreme points. These designs have been used to build objective functions related to several characteristics of wastewater treatments like color removal (Tak et al., 2015), chemical oxygen demand (COD) (Nair and Ahammed, 2015), dye removal from aqueous solutions (Asfaram et al., 2015a), biological oxygen demand (BOD) (Lu et al., 2013), total organic carbon (TOC) (Arslan-Alaton et al., 2009), turbidity (Nair and Ahammed, 2015) and decolorization efficiency (DEC) (Sheydaei et al., 2014) among others. According to the objective of treatment these responses must be maximized, like in case of DEC or color removal or minimized, like in the case of COD. COD is one of the most important characteristics in wastewater treatments like is in the tanning process of leather industry (Dixit et al., 2015) which involves azo dyes (Orange II) and textile wastewater treatment based on advanced oxidation process (Asghar et al., 2015).

Box-Behnken Design (BBD) has been applied in several works. Šereš et al. (2016), for example, applied BBD in the treatment of vegetable oil refinery wastewater using alumina ceramic membrane. In it, two concave objective functions for the microfiltration process, permeate flux and COD, were fitted. Although the stationary points were not the same, no optimization routine was employed in this case. Other examples include the use of BBD in the biosorptive decolorization process by a green type sorbent (Akar et al., 2016), the ammonium nitrogen (NH_4—N) removal from ammoniacal waste (Kumar and Pal, 2013), a Polyaluminium chloride-based water treatment sludge (Nair and Ahammed, 2015), a livestock wastewater treatment based on electrocoagulation process (Tak et al., 2015), a meat industry wastewater by electrochemical treatment (Thirugnanasambandham et al., 2015) and in the Ca/MG/Al coagulation process of tobacco wastewater (Pi et al., 2015).

CCD has been wider used in the wastewater treatment. Sheydaei et al. (2014), for example, optimized a photo-Fenton decolorization process of Orange 29 applied to textile wastewater using CCD; Li et al. (2015) studied the photo-Fenton decolorization of Orange II. Lu et al. (2011) used this design for Photo-Fenton pretreatment of carbofuran; Wang et al. (2014), used it in the coagulation-flocculation process of tobacco slice wastewater; Studies of Asfaram et al. (2015a, 2015b, 2015c), Asfaram et al. (2015d), Dastkhoon et al. (2015), Bagheri et al. (2016), Dil et al. (2016, 2017), Asfaram et al. (2016, 2017) used CCD for optimize the removal of dyes by adsorption processes. Torrades and Garcia Montano (2014) employed CCD in the Fenton and photo-Fenton degradation of real dye wastewater; Saeed et al. (2014) studied the palm oil mil effluent wastewater treatment by fenton using CCD; the same design was employed by Boopathy and Sekaran (2013) in the leather industry wastewater treated by electrochemical process. A face centered CCD was used by Muhamad et al. (2013) for optimization of COD, NH3—N and 2.4-DCP removal from recycled paper wastewater. It can also be cited the use of CCD in a petroleum refinery wastewater treatment by photocatalytic oxidation and mineralization using TiO2 nanoparticles (Shahrezaei et al., 2012), coagulation of highly concentrated industrial grade leather dye (Khayet et al., 2011), the electrochemical treatment of dairy industry wastewater using iron electrodes (Kushwaha et al., 2010), Fenton oxidation pretreatment of wastewater sludge (Pham et al., 2010), advanced oxidation process of Terasil Red R dye using H2O2/pyridine/Cu(II) (Lim et al., 2009), disperse azo dyes by coagulation-flocculation in the steel industrial wastewater treatment (Anouzla et al., 2009), photo-fentom-like advanced oxidation process of azo dye production wastewaters (Arslan-Alaton et al., 2009) and the advanced oxidation process by Fenton's peroxidation of olive oil mil wastewater (Ahmadi et al., 2005).

Second order surface models are generally used to build objective functions of explain the relationship between input ($\mathbf{x}$) and output (y) variables. After modelling, objective functions may be used to optimize the dependent variable (y). The simplest way to optimize a process is to find the stationary point of the objective function, taking its first partial derivative. Depending on the convexity of the second order surface model, the stationary point will be a minimum, maximum or saddle point. For example, in Pi et al. (2015) the response surface model for DEC is concave and therefore, the stationary point is a maximum. The same result may be seen in the paper of Li et al. (2015), with a saddle point for DEC in the photo-fenton decolorization of Orange II. Sheydaei et al. (2014) also modelled DEC in textile wastewater and obtained a surface model that is neither convex nor concave. The same kind of surface models are observed in the adsorption ultrasound-assisted simultaneous removal of Pb^{2+} ion and malachite green (MG) dyes in the work of Dil et al. (2017). In such cases, the stationary point is a saddle point.

The convexity of any function may be determined assessing the eigenvalues of hessian matrix (a second partial derivatives of the objective function). If the eigenvalues of the hessian are all positive then the function is convex and the stationary point is a minimum. If the eigenvalues are all negatives, function is concave and the stationary point is a maximum. If the eigenvalues are simultaneously positives and negatives then the function is neither convex nor concave and the stationary point is a saddle point (Rao, 2009). It is worth mentioning that the reduced models produced when the no significative terms are removed will imply in response surface that will be neither convex nor concave, which is very common in the wastewater treatment. Examples of such models may be seen in several works like Dastkhoon et al. (2015), Asfaram et al. (2015a).

If a convex objective function needs to be maximized, it will be necessary to add a constraint to close the solution region. In this case, the solution will fall far from the center point and the prediction variance will be the largest. Therefore, when the convexity of objective functions is not compatible with the optimization direction, it will be necessary to use a constraint function like $g(\mathbf{x}) = \mathbf{x}^\mathbf{T}\mathbf{x} \le \rho^2$, which represents a hypersphere outlined by the CCD design (Myers and Montgomery, 2009). According to the classical theory of DOE (Design of Experiments), the variance of prediction is a minimum in the vicinity of center points (design center) and increases in the direction of axial point (extreme points in CCD designs) (Myers and Montgomery, 2009). Therefore, every time the convexity of response surface is contrary to the optimization direction, the solution of the optimization problem will be an external point with poor predictability. This means that the (1-α)% confidence interval for the optimum will be as large as possible, and the predicted value for the optimization will be unreliable. The problem increases if more than one response is considered for optimization.

If the stationary point is a saddle point, the aforementioned constraint will be always required since the response surfaces will be neither convex nor concave. Saddle points have been extensively observed in the literature, like the response surface for COD of a photocatalytic oxidation of petroleum refinery wastewater (Shahrezaei et al., 2012), COD of dairy industry wastewater (Kushwaha et al., 2010), COD in the textile wastewater treatment by iron electrode (Lim et al., 2009) and the response surface for dye removal in the leather industry wastewater (Khayet et al., 2011).