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Global sensitivity analysis for identifying critical process design decisions☆

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ABSTRACT

Process design is performed using deterministic values of input variables. However, these input variables may have uncertainties that can lead the designed process to unwanted conditions. This paper presents a methodology for determining critical variables to avoid unwanted responses in the designed process. The methodology proposed here consists of three stages: (1) deterministic process design, (2) elimination of non-influential input variables via the global sensitivity analysis method of Sobol', and (3) determination and regionalization of critical variables with Monte Carlo Filtering. The proposed methodology was applied to the design of a mineral concentration circuit and to the design of a desalination plant. The results show that the methodology could be helpful in analyzing whether a deterministic design works adequately under uncertainties, identifying critical variables in large models, and regionalizing operating conditions and design variables.

1. Introduction

The conceptual process design is an important stage because decisions made at this stage will affect future development stages in the life of a process. There are several methodologies for the design of processes, which are usually classified based on heuristics, optimization, and hybrid. Several reviews of the state of the art of the subject are available, and the reader can see the works of Li and Kraslawski (2004), Nikolopoulou and Ierapetritou (2012), and Sharifzadeh (2013a) for examples. The design is usually performed using deterministic variables considering mean values and expected values of the input variables.

However, the design of these processes may depend on several input variables that present uncertainty. This uncertainty can be epistemic (for lack of knowledge of the variable values under the design conditions) or stochastic (the variable presents random behavior). For example, the kinetic constants in flotation processes depend on the design conditions (e.g., equipment size, particle size) and its value must be determined experimentally. Then, it is not possible to know the exact value of the kinetic constants if the equipment size and particle size are variables in the conceptual process design problem. In contrast, product price, product demand, feed composition, and feed temperature are examples of stochastic uncertainty in the design of processes. Here, the definition of the input variables is wide, corresponding to any type of input variable that presents uncertainty. This uncertainty can be epistemic or stochastic. These variables can be related to flexibility, resiliency, or operability issues. However, without losing this generalization, the examples in this paper are related to flexibility issues (Grossmann et al., 2014; Sharifzadeh, 2013b). Several approaches have been proposed to formulate and solve optimization models with uncertain parameters (see Sahinidis, 2004). Particularly, two-stage stochastic programing is likely the most widespread approach to address

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optimization under uncertainty (Liu and Sahinidis, 1996). Two-stage stochastic formulations involve two types of decisions: first-stage decisions that must be made before the realization of the uncertain parameters, and second-stage decisions that are taken once the uncertainty is exposed. The goal is to choose the first-stage variables in a way that the expected value of the objective function is maximized or minimized over all the scenarios. However, these problems can be very challenging for process design because there may be several uncertain variables (and therefore a large number of scenarios) and the models can be complex MINLP. Robust optimization is an alternative approach to handle uncertainties that depend on the use of chance constraints. Herein, the original robust stochastic model is typically substituted by a deterministic formulation with several equations representing the probabilistic statements expressed through chance constraints (Li et al., 2008). The main disadvantage of this technique is that it does not include second-stage variables, that is, it does not quantify the effect of each uncertain outcome when it materializes. Fuzzy programing (Zimmermann, 1991) is another approach to address uncertainties, and it consists of modeling the random parameters as fuzzy numbers and treating the model constraints as fuzzy sets. However, the representation of uncertainty using fuzzy sets can be a difficult and costly task. The use of flexibility and resiliency concepts and indices has also been applied in the design of chemical processes with uncertainty (Grossmann et al., 2014; Pintarič and Kravanja, 2007).

Lucay et al. (2012) used local sensitivity analysis to identify critical variables in the design of a mineral concentration process to address the epistemic uncertainty of flotation stage recoveries. They derived explicit equations to identify critical stages in mineral concentrators. Sepúlveda et al. (2013) extended the previous work, applying global sensitivity analysis to identify critical stages in flotation circuits. They conclude that the method of Sobol' delivers optimal results in the analysis of such circuits. Later, from the identification of the critical variables, the flotation circuits were improved (Sepúlveda et al., 2014a).

In this paper, a methodology is proposed to identify the critical variables of a process to avoid unwanted process output under the uncertainty of the input variables. The proposal involves Sobol' and Monte Carlo Filtering (MCF) global sensitivity methods. While both methods are used to identify critical variables, the first has the disadvantage of not indicating how to move into the uncertainty intervals of the critical variables to avoid bad results. The second, in contrast, identifies regions based on the critical variables in which the output of the model has a certain behavior. However, practice has shown that MCF exhibits a lack of statistical power for large models (Saltelli et al., 2004). The proposed methodology consists of three stages: (1) conceptual process design, (2) elimination of non-influential input variables based on a ranking built on the Sobol' method, and (3) determination and regionalization of critical variables using MCF. This methodology is illustrated by the mineral flotation circuit design and by the conceptual design of a reverse-osmosis desalination plant.

2. Methodology for determining critical variables

As indicated above, the methodology consists of three stages: (1) conceptual process design, (2) elimination of non-influential input variables, and (3) determination and regionalization of critical variables. These stages are described below:

2.1. *Conceptual process design*

In the literature, there are a number of procedures for process design, and here it is assumed that any procedure can be used if the results are adequate. For designing mineral concentration plants, there are the procedures of Hu et al. (2013) based on genetic algorithms, Cisternas et al. (2014) based on mathematical programing, and Sepúlveda et al. (2014b) based on group contribution, among several others. For the design of reverse-osmosis desalination plants, there exist graphical procedures (Evangelista, 1986) and those based on mathematical programing (Sassi and Mujtaba, 2012). The review of these methods is beyond the scope of this paper; readers interested in design mineral flotation plants can see the review of Mendez et al. (2009), and those interested in reverse osmosis desalination plant design can see the introduction given by Sassi and Mujtaba (2012).

2.2. *Elimination of non-influential input variables*

As discussed later, MCF works best if the model has fewer variables with uncertainty. For this reason, in this second stage, we apply a method of reducing the number of variables with uncertainty. Based on Sepúlveda et al. (2014a), the Sobol' and Morris methods can identify input variables that most affect the uncertainty of the output variable, and therefore both methods can be applied. In this work the Sobol' method is used. In the Sobol' (1993) method, the variance of the model output can be decomposed in terms of increasing dimensions, called partial variances, which represent the contribution of the inputs (i.e., single inputs, pairs of inputs, etc.) to the overall uncertainty in the model output. Statistical estimators of partial variances are available to quantify the sensitivities of all the inputs and of groups of inputs through multi-dimensional integrals. The partitioning of the total variance of the model output V(Y), considering that the model has the form $Y = f(x_1, x_2, \ldots x_n)$, where Y is a scalar and x_i is a model factor, can be represented by the following equation (Confalonieri et al., 2010):

$$V(Y) = \sum_{i=1}^{n} D_i + \sum_{i\leq j\leq n}^{n} D_{ij} + \ldots + \sum_{i\leq\ldots n}^{n} D_{i\ldots n} \quad (1)$$

where, D_i represents the first-order effect for each factor x_i $(D_i = V[E(Y|x_i)])$ and D_{ij} $\left(D_{ij} = V\left[E\left(Y|x_i, x_j\right)\right] - D_i - D_j\right)$ to $D_{1\ldots n}$ the interactions among n factors. The variance of the conditional expectation $(V[E(Y|x_i)])$ is sometime called the main effect and is used as an indicator of the significance of x_i.

The calculation of all partial variances of input groups has a high computational cost, which is the reason Homma and Saltelli (1996) introduced the concept of a total sensitivity index. The total sensitivity index indicates the overall effect of a given input by considering all the possible interactions of the respective input with all the other inputs.

In this paper, the Sobol' method and the improved formulas of Jansen (1999) and Saltelli et al. (2010) for the Sobol' method were applied. The Sobol'–Jansen method allows for the