Evolutionary Optimization of Pulp Digester Process Using D-optimal DOE and RSM

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Abstract

Optimization of existing processes becomes more important than the past as environmental problems and concerns about energy savings stand out. When we can model a process mathematically, we can easily optimize it by using the model as constraints. However, modeling is very difficult for most chemical processes as they include numerous units together with their correlation and we can hardly obtain parameters. Therefore, optimization that is based on the process models is, in turn, hard to perform. Especially, for unknown processes, such as bioprocess or microelectronics materials process, optimization using mathematical model (first principle model) is nearly impossible, as we cannot understand the inside mechanism.

Consequently, we propose a new optimization method using empirical model evolutionarily instead of mathematical model. In this method, firstly, designing experiments is executed for removing unnecessary experiments. D-optimal DOE is the most developed one among DOEs. It calculates design points so as to minimize the parameters variances of empirical model. Experiments must be performed in order to see the causation between input variables and output variables as only correlation structure can be detected in historical data. And then, using data generated by experiments, empirical model, i.e. response surface is built by PLS or MLR. Now, as process model is constructed, it is used as objective function for optimization. As the optimum point is a local one, above procedures are repeated while moving to a new experiment region for finding the global optimum point.

As a result of application to the pulp digester benchmark model, kappa number that is an indication for impurity contents decreased to very low value, 3.0394 from 29.7091. From the result, we can see that the proposed methodology has sufficient good performance for optimization, and is also applicable to real processes.

1. Introduction

Optimizing the existing apparatuses becomes more important as operating costs increase. To optimize a certain process, first of all, a model that describes the process appropriately is needed. Process model is classified into two kinds, fundamental model and empirical model. For chemical processes, fundamental model has been mainly used for the accuracy of the optimization result and understanding of the inside system. However, fundamental model is very difficult to model, and even nearly impossible for unknown processes such as bioprocess and microelectronics materials process. On the other hand, empirical model is based on the data that passed through a system. Therefore, if we can obtain correct data that represent the causal relationship between input variables and output variables, we can easily model the process by multivariate statistical method, like partial least squares(PLS) or multivariate linear regression(MLR). But this modeling technique also has some defects. Empirical model has low prediction ability in the broad region and cannot extrapolate to the non-data region. In addition to these, we cannot understand the inside mechanism as this method takes black-box approach. In spite of all these defects, empirical modeling has many advantages in its applications as a good modeling technique since it is relatively easy and produces fairly good results if we complement some properties.

Statistical optimization methodology using empirical model has been developed mainly with design of experiments(DOE) and response surface methodology(RSM). As for DOE and RSM, many application cases have been published, but statistical optimization based on DOE and RSM has been rarely applied to large-scale chemical processes since the number of variables is large as well as it is somewhat risky for experiments to be performed to the real processes. After Box suggested a new methodology, EVOP, in 1957(Box, 1957), the industrial world paid a lot of attention to it. However, due to the development of fundamental modeling technique and the difficulty of EVOP for which we must perform many experiments on a real process especially when the number of independent variables is large, application cases rarely exist except some bioprocesses(Banerjee and Bhattacharyya, 1993; Tunga *et. al.*, 1999) and materials processes(Saad, 1994). Nevertheless, the possibility of EVOP is unlimited as an excellent optimization methodology at this moment when fundamental modeling becomes more difficult as new and more complex processes are developed, as long as close cooperation with industrial operators can be achieved.

In this paper, we propose a new methodology of EVOP by modifying some of its demerits, and test the efficiency by applying it to a dynamic model describing a real process. The disadvantages of EVOP is that we cannot use it in irregular experimental region because of the use of factorial design, and the direction of process improvement may be ambiguous with only estimating main effects and changes in mean when many independent variables exist. Consequently, we introduced D-optimal design instead of conventional factorial design and RSM instead of effect estimation. D-optimal design reduces the number of experiments compared to the factorial design as well as handles the irregularity of experimental region, and RSM makes us find the optimum point more quickly and clearly relative to effect estimation. This modification of EVOP makes it more valuable and applicable as an optimization methodology. By combination of EVOP and RSM, statistical optimization using empirical model can give reliable results since EVOP takes experimental region narrowly, which increases the accuracy of empirical model, and makes a process move to the more improved operating condition gradually. We applied the proposed methodology to the pulp digester benchmark model to prove its utility.

2. Theoretical Background

Design of experiments(DOE) and D-optimal design

For some systems, to understand the obvious causal