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Quality costs and robustness criteria in chemical process design optimization

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Abstract

The identification and incorporation of quality costs and robustness criteria is becoming a critical issue while addressing chemical process design problems under uncertainty. This article presents a systematic design framework that includes Taguchi loss functions and other robustness criteria within a single-level stochastic optimization formulation, with expected values in the presence of uncertainty being estimated by an efficient cubature technique. The solution obtained defines an optimal design, together with a robust operating policy that maximizes average process performance. Two process engineering examples (synthesis and design of a separation system and design of a reactor and heat exchanger plant) illustrate the potential of the proposed design framework. Different quality cost models and robustness criteria are considered, and their influence in the nature and location of best designs systematically studied. This analysis reinforces the need for carefully considering/addressing process quality and robustness related criteria while performing chemical process plant design. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

At the design stage of a process system, decisions have to be made in the presence of high uncertainty level. For instance, equipment configuration and dimensions, and their operating conditions have to be decided on the basis of an available process model, whose parameters may be uncertain, and on external information, which commonly exhibits a random behavior.

Taguchi (1986) approach to quality engineering provides a robust design strategy aimed at determining nominal settings for the design variables (parameter design) and their associated tolerance limits (tolerance design), in order to reduce process sensitivity to uncertainty. The traditional Taguchi methodology, which is based on running statistically designed experiments on a process prototype, is not, however, directly applicable to early process system design. On the other hand, process design and optimization under uncertainty (Pistikopoulos, 1995) offers a systematic optimization-based vehicle to address process system design issues in the presence of uncertainty. However, in most such optimization studies, robustness issues are not explicitly considered, although attempts to link robustness/quality engineering aspects to stochastic process design optimization have begun to appear in the literature (Straub & Grossmann, 1993; Diwekar & Rubin, 1994; Bernardo & Saraiva, 1998; Samsatli, Papageorgiou & Shah, 1998; Georgiadis & Pistikopoulos, 1999).

In this article, we introduce a systematic design framework for process quality that embeds Taguchi's method and other robustness criteria within a stochastic optimization formulation. Quality related constraints are relaxed and process robustness is guaranteed through the explicit incorporation of robustness criteria in the optimization formulation, such as penalty terms in the objective function and/or limits on the variance of quality variables. With the relaxation strategy mentioned above, feasibility tests are not required, and thus the objective function expected value is obtained through integration over the entire uncer-

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tainty space. As a consequence, the original two-stage optimization problem was transformed into a single-level stochastic optimization formulation.

The computation of multiple integrals over the uncertainty space is a critical numerical issue in stochastic process design. Integration techniques applied so far to this kind of problems include Gaussian quadrature and stratified sampling techniques. In the first case, the number of points where the integrand function need to be evaluated increases exponentially with the integral dimension (the number of uncertain parameters), making the problem untreatable for a reasonably large number of uncertain parameters (Pistikopoulos & Ierapetritou, 1995). On the other hand, sampling techniques may be computationally more attractive, since the number of points required does not necessarily increase with the number of uncertain parameters. However, even the most efficient sampling techniques, such as the Hammersley sequence sampling (HSS) introduced by Diwekar and Kalagnanam (1997a,b) require some hundreds of points to achieve a reasonable accuracy.

At the numerical level, the present work employs a cubature technique (Stroud, 1971) to compute the multiple integrals involved in the stochastic problem formulation. When all uncertain parameters are normally distributed, a specialized cubature formula is applied, reducing significantly the number of points needed when compared with other integration strategies, such as product Gauss rules or efficient sampling techniques (Bernardo & Saraiva, 1998).

The remaining parts of this paper are structured as follows. First, the proposed mathematical problem formulation, addressing process quality, is developed, based upon a two-stage stochastic optimization framework. Next, robustness criteria and their implementation are described in more detail. Finally, the proposed formulation is illustrated through two chemical process design examples (synthesis and design of a separation system and design of a reactor and heat exchanger system).

2. Stochastic formulation for process quality

The problem of process design under uncertainty can be represented mathematically according to the following general formulation:

$$\begin{aligned}
&\max_{d,z,x,y} f(d, z, x, \theta) \\
&\text{s.t.} \quad h(d, z, x, \theta) = 0 \\
&g(d, z, x, \theta) \le 0 \\
&g_{\mathrm{q}}(y, y^*) \le 0 \\
&d \in D, \quad z \in Z, \quad x \in X, \quad y \in Y, \quad \theta \in \Theta \qquad (1)
\end{aligned}$$

where d, z and x are the vectors of design, control and state variables, respectively; y stands for the vector of quality-related variables (usually a simple function of state and control variables), with desired values y^*, and θ represents the vector of uncertain parameters over the domain Θ. The performance metric to be optimized is defined by the scalar function f, the model equalities h refer to process model equations (heat and mass balances, equilibrium relationships, etc.), the inequalities g_{q} reflect quality constraints and the inequalities g other types of constraints.

Several approaches have been suggested to formulate and solve problem (Eq. (1)), differing in how uncertainty is handled, how an operating policy is selected in the face of uncertainty and also in the design objective considered. In the following paragraphs, we will briefly discuss some of these different approaches, while at the same time trying to clarify the assumptions that lie behind our approach.

2.1. Uncertainty formulation

With respect to the way uncertainty is handled, three different approaches can be stated, (i) scenario-based approach (Grossmann & Sargent, 1978; Halemane & Grossmann, 1983; Varvarezos, Grossmann & Biegler, 1992; Ahmed & Sahinidis, 1998); (ii) stochastic approach (among others, Pistikopoulos & Ierapetritou, 1995; Bernardo & Saraiva, 1998) and (iii) parametric approach (Acevedo & Pistikopoulos, 1996, 1997; Pertsinidis, Grossmann & McRae, 1998).

In the scenario-based approach, the uncertainty domain Θ was approximated by a set of discrete scenarios (periods) with a given probability and, as a result, the original problem (Eq. (1)) was transformed into a multiperiod optimization problem. In the stochastic approach, uncertain parameters were assumed to follow a given joint probability density function (PDF) and an expected average criterion was optimized via a stochastic optimization strategy. In the parametric approach, no assumption was made about the uncertainty model and problem (Eq. (1)) was solved parametrically in the space of the uncertain parameters. The resulting solution was itself a function of the uncertain parameters realizations, providing a full map of the optimal decisions over the uncertainty domain considered. The formulation presented in this article follows a *stochastic approach*, defining the uncertainty domain Θ as a probabilistic space of the form $\Theta = \{\theta : \theta \in j(\theta)\}$, where j is a joint PDF for the random vector of uncertain parameters θ, which may be related or mutually independent.

2.2. Operating policy

The selection of an operating policy in the presence of uncertainty is another issue to be considered when