Computers and Chemical Engineering 63 (2014) 219–233

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

A comparison between two methods of stochastic optimization for a dynamic hydrogen consuming plant

D. Navia[a,*], D. Sarabia[b], G. Gutiérrez[b], F. Cubillos[c], C. de Prada[b]

[a] Departamento de Ingeniería Química y Ambiental, Universidad Técnica Federico Santa María, Vicuña Mackenna 3939, Santiago, Chile
[b] Systems Engineering and Automatic Control Department, University of Valladolid, c/ Real de Burgos s/n, Edif. Facultad de Ciencias, 47011 Valladolid, Spain
[c] Chemical Engineering Department, University of Santiago, P.O. Box 10233, Santiago, Chile

ARTICLE INFO

Article history:
Received 31 January 2012
Received in revised form 20 January 2014
Accepted 2 February 2014
Available online 10 February 2014

Keywords:
Two-stage stochastic optimization
Chance constrained optimization
Monte Carlo simulation
Economic dynamic optimization
Hydrodesulphurisation process

ABSTRACT

The following work shows the application of two methods of stochastic economic optimization in a hydrogen consuming plant: two-stage programming and chance constrained optimization. The system presents two main sources of uncertainty described with a binormal probability distribution function (PDF). Both methods are formulated in the continuous domain. For calculating the probabilistic constraints the inverse mapping method was written as a nested parameter estimation problem. On the other hand, to solve the two stage optimization, a discretization of the PDF in scenarios was applied with a scenario aggregation formulation to take into account the nonanticipativity constraints. Finally, a framework generalizing this solution based on interpolation was proposed. Both optimization methods, two-stage programming and chance constrained optimization, were tested using Monte Carlo simulation in terms of feasibility and optimality for the application considered. The main problem appears to be the large computation times associated.

1. Introduction

Uncertainty is always present in the operation of processes. Therefore, when optimal decisions have to be made, differences between the model and the reality must be considered in order to propose feasible actions. In this paper, two approaches have been used to deal with this problem for a hydrogen consumption process in a desulphurisation unit in which changes in the operating conditions take place.

In the classical approach of optimization, equations and parameters are considered totally known. However, when the computed solution is applied to the reality, frequently the value of the objective function is worse than expected and/or the constraints are violated (Birge & Louveaux, 1997; Rockafellar, 2001; Wendt, Li, & Wozny, 2002). These problems can be attributed to the uncertainty that affects the system (Wendt et al., 2002). Usually, the behaviour of the uncertain parameters can be described using random variables named ξ, that belong to a probability space with a given probability distribution function (PDF).

One of the first attempts to solve optimization problems explicitly considering the uncertainty in the processes, appears in the work of Grossmann and co-workers introducing the concept of flexibility (Grossmann, Halemane, & Swaney, 1983; Halemane & Grossmann, 1983). Also some works based on optimization under uncertainty using stages of decisions (Beale, 1955; Dantzig, 1955) were modified to be used in the process industry (Pistikopoulos & Ierapetritou, 1995; Rooney & Biegler, 1999, 2001, 2003). Additionally, this formulation has been used for discrete values of the random variables by means of the optimization over scenarios (Birge & Louveaux, 1997; Dupačová, Consigli, & Wallace, 2000). According to some authors, the idea behind methods with stages of decision is not very adequate for process control, because of the interaction between the decisions in different stages, and the compensative decisions that must be taken (Arellano-Garcia & Wozny, 2009; Li, Arellano-Garcia, & Wozny, 2008; Wendt et al., 2002). That's why these authors propose the chance constrained formulation to be used in process optimization. For further information, an extensive recompilation can be found in the work of Sahinidis (2004).

In this work, both methods, two-stage optimization and chance constrained optimization, have been used for solving the stochastic optimization of a hydrogen consumption problem in a typical plant of a petrol refinery. In contrast to other approaches that appear in the literature, the stochastic dynamic optimization problem has been solved in the continuous time domain using a sequential approach. To do this, a control vector parameterization was used, combining optimization methods and dynamic simulation. Two changes have been proposed in the stochastic methods according to the continuous formulation. In the implementation step of the

* Corresponding author. Tel.: +56 2 24326759.
E-mail addresses: daniel.navia@usm.cl, daniel.navia.lopez@gmail.com (D. Navia).

0098-1354/$ – see front matter © 2014 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.compchemeng.2014.02.004

two-stage one, an interpolation method is presented to face the loss of generalization that takes place when scenarios are used to describe the continuous PDF and an open loop policy must be applied. In the same way, in the chance constraint method, a new approach for calculating the limits of the probability integrals as the solution of a parameter estimation problem has been proposed. The optimization results obtained with these methods were tested and analyzed using Monte Carlo simulations.

The structure of this paper is as follows: Section 2 presents a brief introduction to the stochastic optimization methods. Section 3 presents the operation of the hydrodesulphurisation unit and the application of the stochastic optimization methods to its optimal management. Next, Section 4 shows the outcomes of the optimization and discusses the results using Monte Carlo simulations with the generalization method proposed. The paper ends with some conclusions and comments about future work.

2. Optimization under uncertainty

In general, a problem of dynamic optimization under uncertainty can be summarized as:

$$\begin{aligned} & min_u f(x, u, \xi, t_f) \\ & s.t.: \\ & h(\dot{x}, x, u, \xi, t) = 0 \\ & g(\dot{x}, x, u, \xi, t) \le 0 \\ & x \in X, \quad u \in U, \quad \forall \xi \in \Xi, \quad t \in [t_0, t_f] \end{aligned} \tag{1}$$

Where x is the vector of states, u are the decision variables, t is time and ξ represent the uncertain variables that have a random behaviour which can be described using a certain probability distribution function (PDF), named Ξ. The process model is given by the set of equations h, and the cost function to be minimized is represented by f, while g denotes the constraints on the model variables that must be fulfilled for all the possible values that the random variable may have.

Many practical problems can be formulated as (1) due to the presence of unknown elements. The nature of the uncertainty can be very different, ranging from fairly constant but unknown values (e.g., compositions of a stream) to values that change continuously in a random way (e.g., wind). It is important to mention that the uncertain variables can affect the optimization problem in a general way, noting that these variables might be unknown parameters or independent variables that depend on other systems. In all the cases, it can be expected that the random behaviour will be propagated to the states and the output variables. With respect to the solution methods to cope with this uncertain behaviour, two approaches have been chosen considering the application target.

2.1. Two-stage formulation

In two-stage formulation the key idea is that we should take decisions at present time, taking into account that, after a certain period of time, more information will be available as measurements or known facts that will contribute to decrease the incertitude from that time on. So, when decisions have to be made over a time horizon, there are stages of decision that differ in the degree of knowledge of the uncertain variable: in the first one (stage 0) a choice must be made knowing the initial conditions of the system and without any certainty about the random variables except that they belong to a certain PDF. Then, in the second stage (stage 1), the decision variables can be chosen taking into account that the value of the random variable is available (measured or estimated) (Dantzig, 1955). If the subscripts denote the decision stages, the general problem can be formulated as (Rockafellar, 2001):

$$\begin{aligned} & min_u \, \mathbf{E}_\xi [f_0(u_0, x_0(\xi), \xi) + f_1(u_1(\xi), x_1(\xi), \xi)] \\ & s.t.: \\ & g_0(u_0, x_0(\xi), \xi) \le 0 \\ & g_1(u_1(\xi), x_1(\xi), \xi) \le 0 \\ & h_0(\dot{x}_0(\xi), x_0(\xi), u_0, \xi, t) = 0, \quad x_0(\xi, t_0) = x_{0,i}, t \in [t_0, t_1] \\ & h_1(\dot{x}_1(\xi), x_1(\xi), u_1(\xi), \xi, t) = 0, \quad x_{1,i}(\xi) \equiv x_1(\xi, t_1) = x_0(\xi, t_1), t \in [t_1, t_f] \\ & x_k \in X_k, \quad u_k \in U_k, \quad k = \{0, 1\} \\ & \forall \xi \in \Xi \end{aligned} \tag{2}$$

In Eq. (2), u_0 and $u_1(\xi)$ represent the decision variables applied in stages 0 and 1 respectively. Notice that these variables can take values according to a certain parameterization in each stage, but the notation has been shortened for simplicity. The initial states for both stages are represented as $x_{0,i}$ and $x_{1,i}(\xi)$ for stage 0 and 1 respectively, the second obtained as a result of the decision variables applied previously. It can be noted how the value of the uncertain parameter affects the evolution of the state variables in both stages. The functions that must be minimized are denoted as f_0 and f_1 for each decision stage. Due to the fact that these functions depend on the value of the random variables, their mean value ($\mathbf{E}_\xi$) must be used to group all these scenarios in a single objective function to be minimized. The model of the process and the inequality constraints are represented by $\{h_0, h_1\}$ and $\{g_0, g_1\}$ for both stages respectively.

In order to solve this problem for a continuous PDF, a nested numerical integration is required (Birge & Louveaux, 1997). Alternatively, it is possible to discretize the original PDF (D-PDF) producing a finite number of values for the random variable (scenarios) and then solve problem (2) using a weighted sum of the cost function (Birge & Louveaux, 1997; Dupačová et al., 2000; Ruszczynski & Shapiro, 2003; Sahinidis, 2004). The problem with the scenario approach is the loss of generalization in the optimization, because the solution is valid only for the discrete values considered, but it permits obtaining solutions that otherwise will not be available.

In this work, the scenario formulation was used with the two-stage approach described previously. From the point of view of the uncertain variable ξ, the situation can be represented in the schematic of Fig. 1(a), where in stage 0 we must consider that it

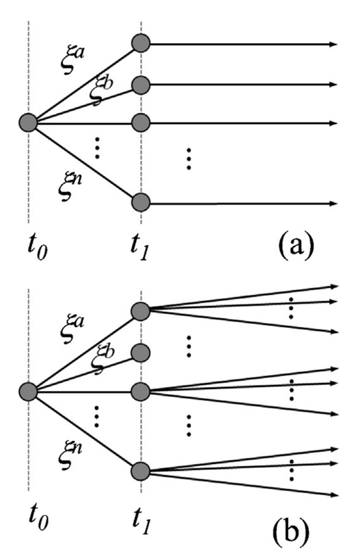

Fig. 1. Information about the stochastic variable in two-stage approach.