A Stochastic Optimization based on Sample Average Approximation for a Boiler Process

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Abstract: The goal of this study is to investigate stochastic optimal solutions for a boiler process in a pulp mill. The objective function is a steam generation while two pollutant emissions should be complied with their regulations. Support Vector Regression (SVR) is employed to build empirical models for representing a boiler process and air temperatures are considered as uncertainties. To make stochastic problems, Sample Average Approximation (SAA) based on Monte-Carlo sampling is introduced and Particle Swarm Optimization (PSO) technique is applied to investigate stochastic solutions. The results show that the stochastic optimal solutions can provide improved performances compared to the deterministic approach.

Keywords: Stochastic Optimization, SAA, PSO, SVM, Chemical recovery boiler, Pulp mill.

1. INTRODUCTION

In general, process modeling works are done based on mathematical models representing the first principle equations of chemical engineering such as mass and energy balances, reaction kinetics, and so on (Gustavo M. A. et al., 2019). Throughout satisfactory process models, various researches including process optimizations can be done. If process modeling works are unavailable due to the lack of understanding the process knowledge, it is very hard to find the optimal solutions indicating the best set points of a process. Even if process knowledge is available, modeling works are often very expensive. These reasons are more specifically for chemical recovery boilers in pulp mills. Moreover, emission modeling should be modeled with the lack of pure mathematical models (Rahat et al. (2018), Repo (2018)).

Ghaffari and Romagnoli (2003), Blasiak et al. (1997), and Leiviska (1996) performed the static or dynamic modelings of Kraft recovery boilers based the first principle equations and various assumptions regarding chemical reduction efficiency, smelt temperature, boiler efficiency, and so on. Therefore, model parameters such as the reaction kinetics should be tuned again and many studies have concerned on specific boiler subsystems.

To solve inherent difficulties of process modeling, data-driven methods have been widely used as an alternative. Maakala et al. (2018) employed simulated annealing, local polynomial regression, and computational fluid dynamics for geometry optimization of the superheaters to mimic the convective heat transfer section of a chemical recovery boiler. Safdarnejad et al. (2019) designed a model based on a recurrent neural network for the prediction of NOx and CO emissions in a boiler. Wang et al. (2018) applied a Gaussian process to reduce NOx emissions and Song et al. (2016) researched the combustion phenomena based on neural network and Gaussian adaptive resonance theory. Zhou et al. (2012) built a predictive model for NOx emissions in a power boiler using Support Vector Regression (SVR).

In this study, the SVR-based empirical model is employed for process modeling due to its many advantages for handling nonlinear processes. Vincent et al. (2018) showed that SVR is enough to predict variables of a reboiler process.

Unfortunately, in the SVR-based empirical models, traditional optimization approaches using the derivatives cannot investigate the optimal solutions. This study adopts a sample-based approach, which is a free-derivative one, to design a stochastic optimal problem. Realistic processes contain inherently uncertain variables. Thus, a deterministic optimal solution may be insufficient for realistic processes, and stochastic optimization approaches yield more realistic solutions (Lee et al. (2011), Yang et al. (2018)).

Many researchers have generated stochastic optimal problems to find more realistic solutions (Halemane and Grossmann, (1983), Maranas (1997), Tayal and Diwekar (2001), Shastri and Diwekar (2006), Lee et al. (2011), Yang et al., (2018)). In their studies, it is assumed that uncertain variables follow a specific probability functions and complex models are divided into a few linear systems. (Lee et al. (2011)). When it is hard to divide several linear systems, the sample-based approach can be used (Lee et al. (2011), Yang et al. (2018)). In this study, the optimal solutions, which provide the best results which have the maximum or minimum values in terms of averages on the objective function under the scenarios. And these scenarios are generated by the combinations of samples on uncertain variables.

In this study, SVR is employed to make empirical models of a boiler system and generate a stochastic problem based on the sample-based approach. In order to find the best optimal solutions, Particle Swarm Optimization (PSO) technique, which is gradient-free optimization, is used.

The paper is organized as follows. In sections 2 and 3, the basic model of the case study and its optimization problem are introduced. Section 4 explains how to generate the stochastic problem, and describes the PSO technique. In Section 5, the objective function and the stochastic optimization is described.

2. A RECOVERY BOILER

In this study, a chemical recovery boiler of a Kraft pulp mill in Brazil would be tested. In a pulp mill, the recovery of specific sodium-based compounds for reuse as cooking chemicals in the cooking stage of the wood chips, from which the cellulose pulp is obtained for papermaking (Gustavo et. al. (2020)). A recovery boiler produces high-pressure steam for electric power generation and heat exchange operations in the mill. Its fuel is a residual liquor, which is the byproduct of the cooking stage and aqueous solutions containing organic and inorganic compounds. Fig. 1 shows the brief steps of Kraft pulp mills with an emphasis on the boiler (Vakkilainen (2005), Gullichsen and Fogelholm (1999)).

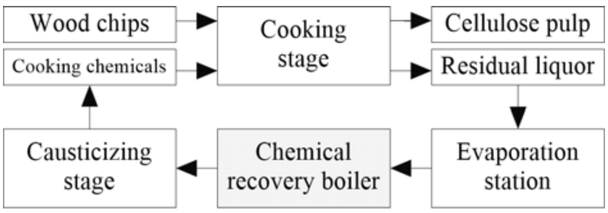

Figure 1. Main stages of Kraft pulp mills.

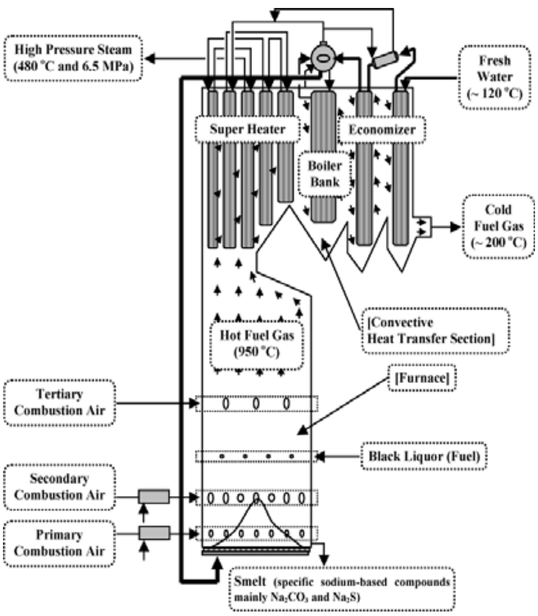

Figure 2. Scheme of the chemical recovery boiler of the case study

This boiler has two main sections; a furnace and a convective heat transfer section (Gustavo et. al. (2020)). In a furnace, the combustion and the recovery of the inorganic compounds occur. And there are three air injections. In a convective heat transfer section, a fresh water is transformed into high-pressure steam approximately (480°C and 6.5MPa). Fig. 2 shows the chemical recovery boiler.

In collected data sets, there are nineteen process variables (Table 1). These data set composes of fifteen input variables, one intermediate variable, and three output variables. These data sets are hourly average data and contain four months of operations. Thus, the measurements of each variable are 2,928 and it is confirmed that the operating conditions are normal.

Table 1.Process variables of a boiler process

Number	Variable	Unit
1	Fuel flow rate(residual liquor)	*ton/h*
2	Fuel temperate	℃
3	Fuel pressure(walls 2 and 4)	mmH_2O
4	Fuel pressure(walls 1 and 3)	mmH_2O
5	Dry solids content(measure 1)	*%*
6	Dry solids content(measure 2)	*%*
7	Primary air flow rate	*ton/h*
8	Primary air temperature	℃
9	Primary air pressure	mmH_2O
10	Secondary air flow rate	*ton/h*
11	Secondary air temperature	℃
12	Secondary air pressure	mmH_2O
13	Tertiary air flow rate	*ton/h*
14	Tertiary air temperature	℃
15	Tertiary air pressure	mmH_2O
16	Boiler drum pressure	kg/cm^2
17	H_2S emissions	ppm
18	SO_2 emissions	ppm
19	Steam flow rate	*ton/h*

3. STOCHASTIC PROBLEMS FOR A BOILER

3.1 The SVR-based Modeling of a Boiler Process

To build empirical models for representing steam generation of the boiler, four discrete-time dynamical models containing process variables are described by (1), where x(t), u(t) and Y(t) represent the input vector, manipulated variables, and the output vector. BP (t) is the boiler drum pressure.

$$
\begin{aligned}
BP\ (t+1) &= g(x(t), u(t), BP(t)) \\
Y_{Steam}(t+1) &= h_1(x(t), u(t), BP(t+1)) \\
Y_{SO_2}(t+1) &= h_2(x(t), u(t), BP(t+1)) \\
Y_{H_2S}(t+1) &= h_3(x(t), u(t), BP(t+1)) \quad (1)
\end{aligned}
$$

Y_{steam} is the steam flow rate and Y_{SO2} and Y_{H2S} indicate the amount of chemical compounds emissions. These relationships are based on the prior process knowledge and the functions g and h should be trained via SVR.

SVR is one of the most effective regression techniques for handling nonlinear information (Vapnik (1995)). SVR has the advantage of high predictive capabilities by minimizing model complexities (Nandi et al. (2004)). In (2), w is the weight vector and x is the input data. Φ and b are the kernel function and the bias.

$$f(x, w) = w^T \Phi(x) + b \quad (2)$$

The parameter estimation is given by minimizing (3), in which $\|w\|^2$ is the model complexity, ξ is the error tolerance, and C is a scalar value, to control the trade-off between both of them (Vapnik (1995)). In this study, the ϵ-insensitive loss function is adopted (an error ξ greater than ϵ is penalized).

$$\min_{w,b,\xi_i} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi_i, \quad \text{subject to}$$

$$\xi_i = \begin{cases} |y_i - f(x_i, w)| - \epsilon, if |y_i - f(x_i, w)| \geq \epsilon \\ 0, \qquad\qquad otherwise \end{cases} \quad (3)$$

This work used the radial basis function (RBF) as the kernel function, where σ is a free parameter in (4) and all parameters (C, s, and σ) are optimized by the PSO technique. Detailed concepts and equations regarding SVR may be found in the study of Vapnik (1995).

$$K(x_i, x_j) = \left(\phi(x_i) \cdot \phi(x_j)\right) = exp\left(-\frac{\|x - x'\|}{2\sigma^2}\right) \quad (4)$$

Fig. 3 shows the predictive performances of four regression models. Their all parameters are optimized by PSO. These models can be applied to find the stochastic optimal design variables. In the SO2 model, there are sensor faults. Except these, most estimates are really close to real measurements.

3.2 Sensitive analysis

A sensitive analysis was done to identify the importance of process variables. At first, all variables should be normalized. And, the sampling points of each variable were selected according to the same intervals from their nominal values. In this study, the changes in the objective function were evaluated according to changes of the standard deviations on decision variables (−σ, −0.8σ, −0.6σ, −0.4σ, −0.2σ, 0.2σ, 0.4σ, 0.6σ, 0.8σ, and σ). The only one variable was changed while fixed other variables on their nominal values. Table 2 shows the results of a sensitivity analysis study. The next section describes how to generate a stochastic optimization problem.

4. SAMPLE AVERAGE APPROXIMATIONS AND PARICLE SWARM OPTIMIZATION

4.1 Sample average approximations

The aim of stochastic optimization problem is to investigate a robust optimal values of decision variables under uncertain variables. Stochastic optimization may provide more realistic solutions than deterministic optimization depending on the strength of the impact of the random components (Lee et al. (2011), Yang et al. (2018)).

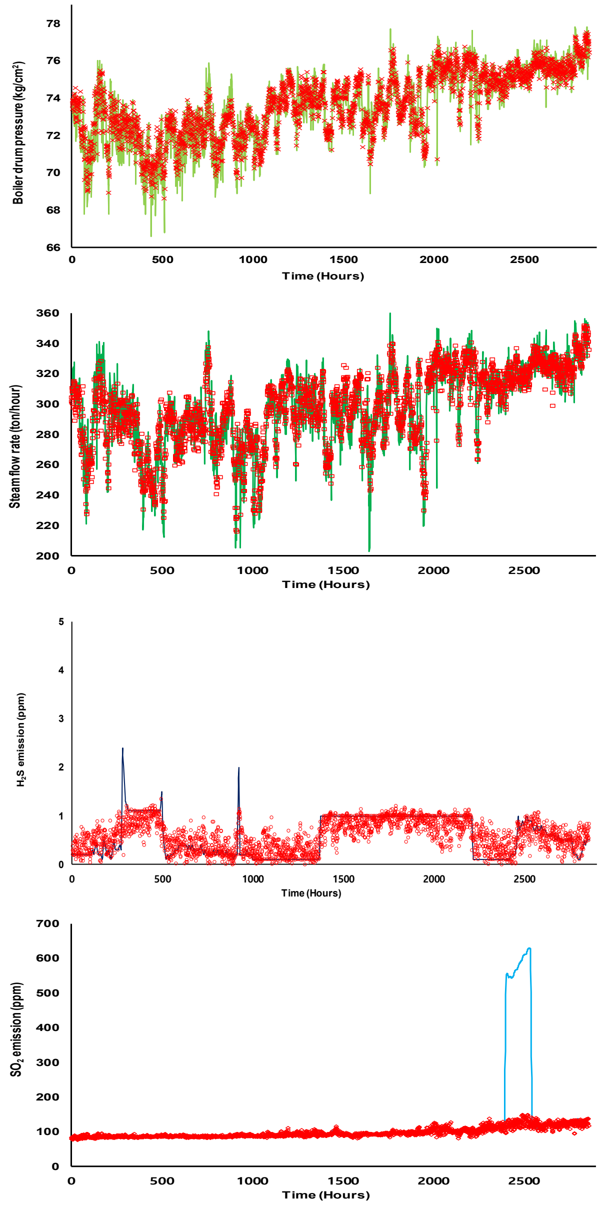

Figure 3. Comparisons between measurements (a soild line) and model estimates (points) (boiler pressure drum, steam flow rate, SO2 and H2S emissions).

In this study, the SVR-based empirical models, which are a kind of models, are built. To solve this problem, Monte Carlo sampling-based Sample Average Approximation (SAA) is used. In this approach, huge scenarios are generated by the combination of the sampling points of uncertain variables and the optimal solutions, which provides the best performance of the objective function, on average, under generated scenarios, are investigated (Lee et al. (2011), Yang et al. (2018)). The advantage of this approach is to find the optimal solution without differentiability of process models. However, this may suffer from a huge amount of computational works and the number of scenarios grow exponentially. SAA is formulated in (5).

$$\hat{f}_N(Q) = \frac{1}{N}\sum_{k=1}^{N} f(Q, \varepsilon_k) \quad (5)$$

In (5), f and Q are the objective function and the set of design variables with all possible scenarios, ε_k. N is the total number of scenarios. The goal is to find the best Q solution.

In this study, because the objective function is based on empirical models, PSO, a gradient-free optimization solver, is employed to find the best Q. This solver can easily handle empirical black box or highly nonlinear models.

Based on the sensitivity analysis, the significant variables are identified. To reduce the number of scenarios, the sampling points of negligible variables were controlled.

Table 2. The results of a sensitivity analysis

Random variable	Absolute average slope [ton/(hour · σ)]	Rank
Fuel flow rate	1.50	1
Dry solids content(Measure 2)	0.53	2
Dry solids content(Measure 1)	0.34	3
Primary air pressure	0.23	4
Boiler drum pressure	0.17	5
Secondary air pressure	0.13	6
Fuel pressure (Wall 2&4)	0.11	7
Tertiary air pressure	0.10	8
Fuel pressure (Wall 1&3)	0.05	9

4.2 Particle Swarm Optimization

The PSO, which is a population-based heuristic optimization technique, is employed without the need of explicit derivatives. (Kennedy and Eberhart (1995)). A population of particles is randomly generated on a search space and their position and velocity are then updated according to the historical best solutions (Kennedy and Eberhart (1995)). At the end, the particles are centered and converged around the best optimal solution. The PSO can be used to black-box models. More detailed algorithms and its concepts can be found in the study of Schwaab et al. (2008).

5. The OBJECTIVE FUNCTION AND STOCHATSTIC OPTIMAL SOLUTIONS

5.1 The objective function

In this study, the stochastic optimal solution under generated scenarios provides the maximization of the expected values on an objective function. The objective function (*F*) is described by (6).

$$max_u \mathbb{E}[\mathrm{F}(\mathrm{x(t)}, \mathrm{u}, \varepsilon)]$$

subject to

$$C_i \begin{cases} Y_i\big(x(t), u, BP(t+1)\big) - R_i, & if\ Y_i - R_i \geq 0 \\ 0, & otherwise \end{cases}$$

$$\mathrm{F}\big(\mathrm{x(t)}, \mathrm{u}, \mathrm{BP(t+1)}\big) = \mathrm{Y1} - W_{SO_2} \cdot C_{H_2S} - W_{H_2S} \cdot C_{H_2S}$$

$$\mathbb{E}[\mathrm{F}(\mathrm{x(t)}, \mathrm{u}, \varepsilon)] = \frac{1}{N}\sum_{t=1}^{T}\sum_{k=1}^{N} F(x(t), u, \epsilon_k) \quad (6)$$

R_i is the upper emission limit value of chemical compound *i*. C_i indicates the penalty in case the predictive emission for *i* is larger than its upper emission limit. W is the weighting parameter to penalize the emission limit and ε_k is a scenario generated by the combination of sampling points. In (6), there are *N* scenarios and *u(t)* is the set of decision variables; and $\mathbb{E}[F(u, \varepsilon)]$ is the expected value of the objective function under scenarios. In this study, three hundred populations on decision variables are randomly generated and stochastic solutions are investigated by PSO.

5.2 Results and discussions

Throughout a sensitivity analysis results, the importance of decision variables was identified. To make the number of scenarios proper, the number of sampling points on significant variables was increased and the sampling points of negligible ones were reduced.

It was assumed that all uncertain variables follow the Gaussian probability distribution. Five sampling points were randomly selected on the significant variables (the fuel flow rate, dry solid contents (measures 1 and 2), and primary air pressure), and three samples were randomly selected on the negligible variables. The total number of scenarios was $5^4 \times 3^5$. In case of 300 population sets, $5^4 \times 3^5 \times 300$ calculations should be performed at each calculation. The drawback of SAA is that a global stochastic solution cannot be investigated. To overcome this disadvantage, twenty computers containing an AMD Athlon 2.9 GHz were operated.

To verify the efficacy of the stochastic optimization, the comparison between stochastic and deterministic solutions were compared each other. In case of a deterministic problem, it is assumed that all variables are fixed at their nominal values. Table 3 shows the stochastic and the deterministic optimal solutions. Fig. 4 shows that most differences of a steam flow rate between the stochastic and the deterministic solutions are positive values and it means that the stochastic optimal solution provided better performances. At least, 1.914% steam production under a stochastic solution can be increased.

Table 3 A comparison of decision variables between the stochastic and deterministic optimizations

Design variable	Stochastic solutions	Deterministic solutions
Fuel temperature	125.47 ℃	125.46 ℃
Primary air flow rate	147.49 *ton/h*	146.94 *ton/h*
Primary air temperature	148.16 ℃	148.08 ℃
Secondary air flow rate	205.36 *ton/h*	208.47 *ton/h*
Secondary air temperature	163.10 ℃	163.06 ℃
Tertiary air flow rate	51.08 *ton/h*	51.47 *ton/h*
Tertiary air temperature	34.34 ℃	34.47 ℃

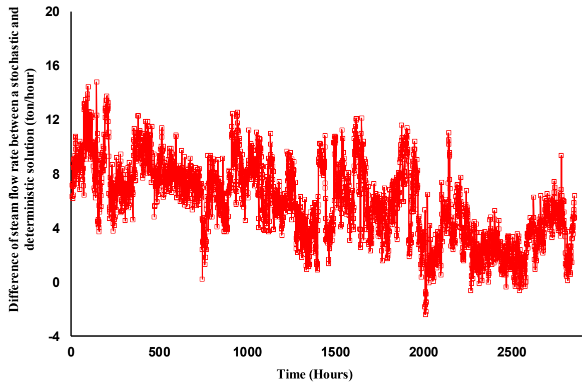

Figure 4. Differences between the stochastic and the deterministic optimal solutions on a steam flow rate.

6. CONCLUSIONS

Since there are many unknown phenomena and conventional simulators cannot be employed for a reboiler process, SVR was selected to build four empirical models in this study. The goal of a stochastic optimization is to maximize the steam generation while avoiding the violation of pollutant emissions. Throughout a sensitivity analysis, the impacts of process variables are identified and the stochastic problem is generated by SAA based on Monte Carlo sampling. Due to the difficulties of using the derivatives of the empirical models, a gradient-free based PSO technique was introduced. The results show that a stochastic optimal solution provides better results than a deterministic solution. Overall, the proposed method is based on SVR, which is a black box model, and PSO, which is a gradient-free technique. Therefore, the proposed strategy can be easily applied to various problems including uncertain variables.

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