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PARAMETRIC SENSITIVITY THROUGH OPTIMIZATION UNDER UNCERTAINTY APPROACH

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Abstract

While mimicking a physical phenomenon in a computational framework, there are tuning parameters quite often present in a computational model. These parameters are generally tuned with the experimental data to capture the process behavior as close as possible. Any optimization study based on this model assumes the values of these tuning parameters as constant. However, it is known that these parameters are subjected to inherent source of uncertainties such as errors in measurement or model tuning etc. for which they are not tuned for. Assuming these parameters constant for rest of the optimization is, therefore, not realistic and one should ideally check the sensitivity of these parameters on the final results. In this study, we are going to use approach based on the paradigm of optimization under uncertainty that allows a decision maker to carry out such an analysis. Additionally, this study captures the tradeoff between solution quality and solution reliability that is captured here using non-dominated genetic algorithm II. The generic concept has been applied on a grinding process model and can be extended to any other process model.

Key words: optimization, uncertainty, parameter sensitivity, grinding, genetic algorithm, multi-objective optimization, Pareto

1. INTRODUCTION

Deterministic optimization problems can be presented in a generic form Maximize / Minimize objective function, $f(x, \Theta)$, subjected to constraints, $g(x, \Theta) \leq 0$, where x is a set of decision variables and Θ is a set of some parameters present in the model. These parameters can be tuning parameters in a model which are to be tuned with certain data set or they can be some thermodynamic or process system parameter (e.g. diffusivity or heat transfer coefficient). Irrespective of the type of parameters, they are generally kept constant during the entire course of optimization process. However, the assumption of these parameters do not change during optimization is unrealistic because these parameters are actually exposed to real life uncertainty, which we generally ignore to solve a relatively simplistic problem. For example, in case the parameters represent tuning handles in a model, a fixed value of these parameters might not be valid for the entire range of optimization search space because the tuning parameters, whatever best way they are calculated, are subjected to uncertainty related to experimental as well as regression errors. The general practice in optimization is to find the set of x using a fixed set of values of Θ and then see whether the set x gets influenced by little perturbation in the value of Θ. This approach is ad hoc in nature since there is no systematic procedure to carry out this operation. In this work, a systematic approach based on the paradigm of optimization under uncertainty (Sahinidis, 2004) has been adopted to show the efficacy of alternate approach to parametric sensitivity. An industrial grind-

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ing process has been chosen as an example here to show the feasibility of this approach.

2. PROCESS & MODEL DESCRIPTION

The industrial process considered here is taken from the domain of mineral processing. The purpose of this industry is to enrich the mineral content (e.g. from ~2-3% to ~50-60%) in the raw material (lead-zinc ore here) through various process operations called ore beneficiation. Ore beneficiation is primarily composed of grinding and flotation operation in this case. In the grinding process, the correct size of the material is achieved which is essential for the following flotation process where selective flotation of mineral occurs by means of several physical and chemical operations. In this work, we are concerned about the grinding part only. In the grinding process, the ore coming from crushing unit first passes through the Rod Mill kept in open circuit. The solid ore (S_1) is mixed with water to form the slurry that makes the flow of material easy within the beneficiation circuit. Ground ore slurry from Rod Mill is next collected in a tank, known as primary sump, where from it is fed to a primary classification unit, known as primary cyclone, to separate out the lighter and heavier part from it (based on a particular cut size). The lighter part (lower than cut size) is next collected in secondary sump and then fed to the secondary cyclone to get it classified for the second time. Underflows from both the cyclones are heavier material (higher than cut size) in the respective classification units that is fed to a Ball Mill. Ball Mill output is fed to the primary sump again and this material gets recirculated in the circuit. Water is additionally added in both the sumps (W_1 and W_2 to primary and secondary sumps, respectively) to maintain a particular specific gravity in the circuit. Overflow of the secondary cyclone is taken out as the final product of the grinding circuit which then goes to the following flotation circuit. A schematic diagram of the circuit is presented in figure 1.

Each of these unit operations can be modeled using mass balance equations for that unit. In the Rod Mill and Ball Mill, where particle breakage is occurring, the particles are represented by certain number of size classes (coarse (CS), mid (MS) and fine (FS) sizes) and transition of particles among these classes are achieved by assuming certain breakage mechanism. Selection function, which determines the degree of separation to different size classes, can be assumed to be similar to chemical reactions of certain order where rate proportional constant (precisely known as grindability index) and order of the reaction has to be determined by the curve fitting exercise using industrial data. Similarly, the selection curves for primary and secondary cyclones, which determine the split of material fed to cyclone into overflow (smaller than cut size) and underflow (larger than cut size), are modeled using semi-empirical correlations available from the literature. A connectivity matrix that connect all units by means of a 1-0 entry (signifying connection exists and no connection, respectively) allows one to simulate the entire circuit when each of the unit operation models are ready with their individual equations. Dynamic model equations for each unit operation give rise to a set of differential algebraic equations which is solved here by a public domain solver (DASSL) (Petzold, 1983). By the overall simulation of the circuit, several properties (percent solid (*PS*), recirculation load (*RCL*)) of the flow streams can also be calculated. Interested people are referred to the work of Mitra and Gopinath (2004) to know more about the process as well as model.

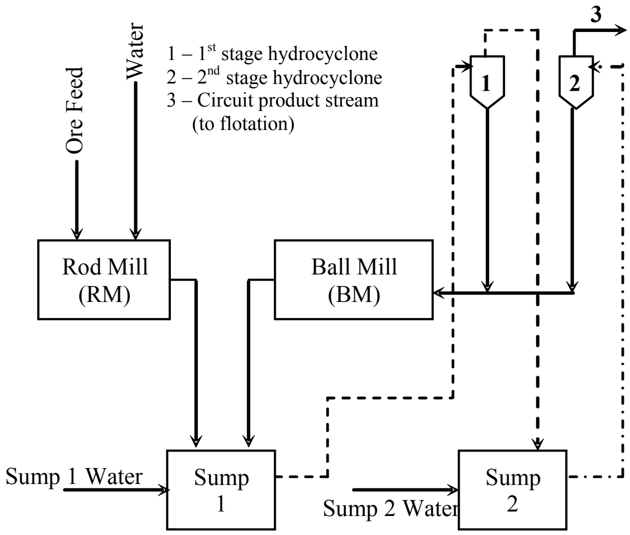

Fig. 1. *Schematic diagram of the industrial grinding circuit*

3. OPTIMIZATION FORMULATIONS

Productivity of any industrial operation (grinding unit here) is of utmost importance. However, this has to be achieved without compromising the product quality. Here, productivity is expressed in terms of throughput (*TP*) of the slurry coming out of the grinding circuit whereas the quality of grinding in expressed in terms of mid-size fraction (*MS*). Maximization of both of these helps to achieve the objective of the production unit where there is a conflicting relationship between them. This kind of scenario is best handled by solving it through the multi-objective optimization route. First, the deterministic formulation is presented.

Objectives

$$\underset{S,W_1,W_2}{Max} \quad TP \tag{1a}$$

$$\underset{S,W_1,W_2}{Max} \quad MS(\alpha,\beta) \tag{1b}$$

Subject to constraints

$$CS(\alpha,\beta) \le CS^U \tag{1c}$$

$$FS(\alpha,\beta) \le FS^U \tag{1d}$$

$$PS\ (\alpha,\beta) \le PS^U \tag{1e}$$

$$RCL(\alpha,\beta) \le RCL^U \tag{1f}$$

Other population and mass balance equations Decision Variables Bounds

$$S^L \le S \le S^U \tag{1g}$$

$$W_1^L \le W_1 \le W_1^U \tag{1h}$$

$$W_2^L \le W_2 \le W_2^U \tag{1i}$$

The decision variable handles are the solid flowrate and water flowrates (S, W_1, W_2). As described earlier, the selection functions of i^{th} size particle ($S(i)$) in ball mill or rod mill are assumed to follow Arrhenius type of chemical reaction representation ($S(i) = \alpha \times d(i)^{\beta}$), where $d(i)$ is that particular size class in micron. In this representation, α is generally known as the grindability index and β is known as the grindability exponent in selection function. They appear in both rod and ball mill models. Since, the ball mill operation is the most important as well as impactful in the circuit, we consider only α and β parameters for ball mill model. These parameters are conventionally found by the regression exercise of the steady state size class data collected from plant and analyzed through laboratory tests and thus are subjected to uncertainty due to experimental and regression errors. They are, therefore, assumed to be uncertain for the study of optimization under uncertainty which is presented next.

$$\underset{S,W_1,W_2}{Max} \quad T\,P \tag{2a}$$

$$\underset{S,W_1,W_2}{Max} \quad MS' \tag{2b}$$

Subject to control variable bounds

$$\Pr\left[MS(\alpha,\beta) \ge MS'\right] \ge \gamma_1 \tag{2c}$$

$$\Pr\left[CS(\alpha,\beta) \le CS^U\right] \ge \gamma_2 \tag{2d}$$

$$\Pr\left[FS(\alpha,\beta) \le FS^U\right] \ge \gamma_3 \tag{2e}$$

$$\Pr\left[PS(\alpha,\beta) \le PS^U\right] \ge \gamma_4 \tag{2f}$$

$$\Pr\left[RCL(\alpha,\beta) \le RCL^U\right] \ge \gamma_5 \tag{2g}$$

Other population and mass balance equations Decision Variables Bounds

$$S^L \le S \le S^U \tag{2h}$$

$$W_1^L \le W_1 \le W_1^U \tag{2i}$$

$$W_2^L \le W_2 \le W_2^U \tag{2j}$$

where "Pr" is the probability associated with objective function and constraints and individual γ values are the measure of such probabilities lying between 0 and 1. This formulation is known as chance constrained programming (CCP) (Charnes & Cooper, 1959) where constraints are not satisfied for all instances of uncertain parameter realizations e.g. α, β etc. Hence a probability term is associated with each of the constraints where uncertain terms are present. The objective function can also be converted into a constraint, as done above, by introducing an auxiliary variable, MS′, and treating it as constraint. In case the uncertain terms appear in the equation linearly, their deterministic equivalent can be achieved by simple coordinate transformation, which is then can easily be solved using deterministic optimization methods. For example, if the uncertain terms in the equations follow normal distributions, the deterministic equivalent of the uncertain formulation can be achieved by replacing those uncertain terms by the sum of their means and quantile times standard deviations. However, if the uncertain terms appear nonlinearly in the constraint equations, one of the ways of calculation of probability of constraint satisfaction is achieved by simulation based methods. In this approach, several instances of realization of uncertain parameters is generated based on a sampling size of uncertain parameters and based on feasibility of the constraint for those uncertain parameter realizations, overall probability of the constraint satisfaction is determined. For example, if a sample size of (N) 50 has been chosen, 50 instances of α_i

and β_i can be generated first. Now for each one of these α_i, β_i combinations, it is observed whether a constraint is getting satisfied or not. Counting all the instances for feasible constraint cases (say, N_f), the probability of constraint satisfaction can be computed as (N_f /N). One of the prerequisites of this technique is that the variance information of the uncertain parameters should be available. Assuming that α and β both follow normal distribution and their individual variance information are known, we solve the above uncertain formulation using simulation based CCP approach. Here we should remember that the uncertain parameters appear in the constraint equation in nonlinear fashion. This uncertain formulation is a multi-objective optimization problem which is solved here using real coded Nondominated Sorting Genetic algorithm II (NSGA II), a well-established algorithm. When the aforementioned CCP simulation block is amalgamated with the multi-objective optimization algorithm, called as CCPNSGA II, the simulation block gets executed for each of the values of decision variables. The function evaluation part in original NSGA II has, therefore, to be replaced by the simulation block where instead of deterministic function evaluation, probabilistic function evaluation takes place to calculate the probabilistic objective and constraints. The following parameters are used for this study in real coded CCPNSGA II: Maximum number of generations = 50; Number of population = 50; crossover probability = 0.9; mutation probability = 0.0; SBX distribution index = 0.01; polynomial mutation distribution index = 0.01; sampling size in CCP simulation = 300. The probability computation with 300 simulations was reported to be sufficient for this case. Details on NSGA II have not been included in this paper for the sake of brevity as the same can be referred from the literature (Deb et al., 2002).

4. RESULTS AND DISCUSSION

The industrial grinding example discussed here has been extracted from a leading vertically integrated lead-zinc multinational company. So, the results will be expressed in normalized fashion to honor the nondisclosure agreement signed during the research program. In this work, it is assumed that the uncertainty in α and β can be described reasonably well by the normal distribution. Setting that the standard deviation value is 5% of its nominal value, the uncertain formulation given in equation (2) can be solved and Pareto optimal (PO) solutions can be generated for several values of probabilities as presented in figure 2. When the probability value is chosen as 0.95 (= $\gamma_1 = \gamma_2 = \gamma_3 = \gamma_4 = \gamma_5$), it assumed that out of 300 simulations, 285 instances of uncertain parameter realizations are going to be feasible. Certainly this condition is going to be stringent as compared to another case where the probability of constraint satisfaction is relatively less e.g. 0.65 or 0.45 i.e. PO front of probability value 0.45 is superior as compared to the same corresponding to probability value 0.95. This is clearly depicted from the figure 2 as we can see better PO fronts are generated under these relaxed conditions. However, under CCP formulation, the probability measure is related to the reliability of the solution. As we relax the probability of constraint satisfaction, we obtain less reliable solutions as compared to the deterministic formulation presented in equation (1). So, in that way, the results presented in figure 2 not only provide solution to the two-objective problem presented in equation (2), but also present the case of three-objective optimization problem where throughput, mid-size fraction and solution reliability of the solution are simultaneously maximized (here these objectives are mutually conflicting to one another). Practically, first it is to be quantified whether any scope of improvement in the PO front exists by sacrificing the reliability of the solution and then decide from the higher level business experience which level of reliability is best suitable for a particular plant scenario.

Similarly, the other PO solutions can also be found assuming the standard deviations of uncertain parameters are 10% of their nominal values. These results are not presented here. Instead a comparison of 5 and 10% standard deviation cases is presented in figure 3. As the standard deviation value is increased, more variation in the values of the uncertain parameters is considered which can only be tackled by going for higher production options. This leads to marginally better PO front keeping the reliability of the solutions at the same level. So these two uncertain situations (5 and 10% standard deviation) are different and should be tackled differently. A common practice in industry is to tackle these situations in the same fashion e.g. providing solutions using the nominal values of uncertain parameters for all cases. However, if different realizations of uncertain parameters are handled in similar fashion using nominal values of the uncertain parameters, there will be cases where either the system will underperform (when realized uncertain condition is more than nominal value) and not be able to extract best out of the situation or over perform to pile unnecessary inventory (when realized uncertain condition is less than nominal value). As compared to ad hoc sensitivity analysis mentioned in the introduction, this methodology provides a systematic way of carrying out the sensitivity analysis of various parameters present in the model by controlling the extent of constraint violations by assigning the associated probabilities for those constraints correctly.

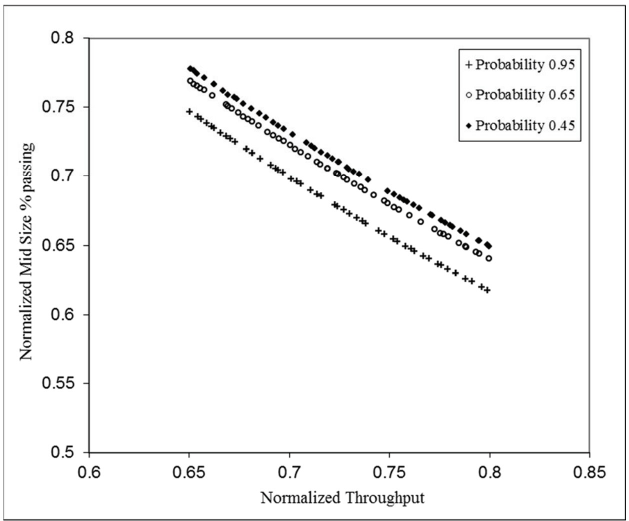

Fig. 2. *Pareto optimal front expressed in terms of normalized objective functions for 5% standard deviation case*

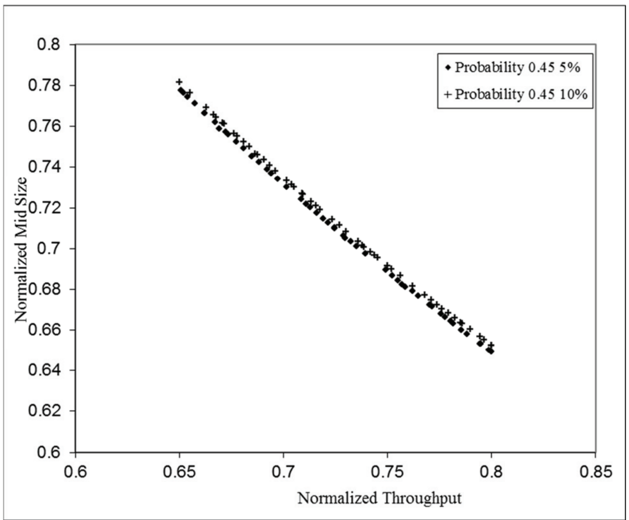

Fig. 3. *Effect of change in standard deviation value of uncertain parameters on the Pareto optimal front for probability of constraint satisfaction value of 0.45*

So far, uncertain parameters α and β are considered together. Next, they are considered one by one. First it is assumed that α is the only uncertain parameter and the value of β is kept at its nominal value. For a probability value of 0.45, PO solutions are generated for a 10% standard deviation case as presented in figure 4 as "Prob 0.45 SD 10% Grind Indx". Similarly, PO solutions for the other case, where β is varied and α is kept constant for identical probability and standard deviation case, are generated and presented in figure 4 as "Prob 0.45 SD 10% Grind Expo". We can clearly see how the impact of grindability index is more as compared to grindability exponent. This is also another way of conducting sensitivity analysis for individual parameters.

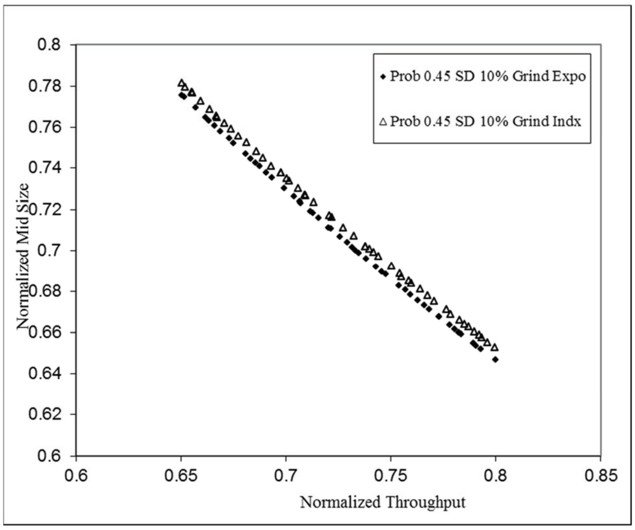

Fig. 4. *Parametric sensitivity of uncertain parameters considered individually*

5. CONCLUSIONS

An alternative approach of sensitivity analysis based on the idea of optimization under uncertainty has been proposed in this work. An industrial case study of beneficiation process is taken into consideration to show the efficacy of the approach. Chance constrained programming based NSGA II (CCPNSGA II) has been utilized to solve the multi-objective optimization problem. It is shown that this approach is more systematic as compared to conventional unsystematic way of doing the same.

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PARAMETRYCZNA ANALIZA WRAŻLIWOŚCI I OPTYMALIZACJA Z WYKORZYSTANIEM ANALIZY NIEPEWNOŚCI POMIARÓW

Streszczenie

Modelowanie zjawisk fizycznych metodami numerycznymi często wymaga określenia wartości parametrów charakteryzujących modelowany proces w taki sposób, tak aby jak najdokładniej uchwycić przebieg zjawiska fizycznego. Proces optymalizacji wykorzystujący tak zdefiniowany model przyjmuje wartości dopasowanych parametrów jako stałe. Jednocześnie wiadomo, że parametry te zależą od źródeł niepewności związanych z błędami pomiaru lub samą regulacją modelu, i dla innych danych pomiarowych model z wcześniej dopasowanymi parametrami może nie dawać wystarczająco dokładnej odpowiedzi. Przyjęcie stałych wartość tych parametrów w optymalizacji jest zatem nierzeczywiste i należałoby sprawdzić wrażliwość odpowiedzi modelu względem tych parametrów. W niniejszej pracy zastosowano metodę opartą na optymalizacji z wykorzystaniem analizy niepewności pomiarów, która umożliwia przeprowadzenie tego typu analizy wrażliwości. Ponadto w optymalizacji za istotne uznano utrzymanie równowagi pomiędzy jakością rozwiązania i jego wiarygodnością, co było możliwe dzięki zastosowaniu niezdominowanego algorytmu genetycznego II (ang. NSGA II). Ogólną koncepcję rozwiązania zastosowano w modelu procesu szlifowania, ale może ona być rozszerzona na każdy inny rodzaj modelu procesu.

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