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Chance Constrained Programming to Handle Uncertainty in Nonlinear Process Models

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7.1 Introduction

The field of deterministic optimization has found many applications in the broad area of equipment design, the study of various engineering processes, managing supply chain operations, transportation and logistics from various domains like finance, energy, environment, telecommunications, drug delivery, molecular design, biological and agricultural sciences, automobile, engineering and technology, metals, chemicals, textile since the 1960s. A linear deterministic optimization problem is generally expressed as **Minimize** "objective" Cx, subjected to "constraints" Ax $\leq$ B, where x is the decision variable set, C and A are the set and matrix of coefficients appearing in the objective function and constraints respectively and B is a vector of terms of the constraints, which are independent of decision variable set. The constraints can assume the form of equality or inequality ($\leq$ or $\geq$) and the objective function can be of the "Minimize" or "Maximize" type. While solving the deterministic optimization problems, a general assumption is that the associated data as well as parameters (A, B and C), other than the decision variables (x), are certainly known and can be considered as fixed while carrying out optimization. However, during real-life problem solving, there may be flaws in assuming some or all of these parameters as constants because they may be exposed to uncertain situations and the results could be erroneous. Different sources of uncertainties that can change these A, B, Cs with time can

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be categorized as external (for example, fluctuating feed conditions to a process or changing market demands and prices of products), internal (precision errors during experiments), and others (for example, modeling errors arising from assumptions due to lack of process understanding). The conventional way of handling these uncertainties during design or operational stage is to overdesign equipment or overestimate operational parameters. Another popular approach is to solve the uncertain optimization problem in a deterministic fashion by representing the uncertain parameters by their nominal values. These approaches generally can lead to solutions that are costly, suboptimal and sometimes infeasible. The area of stochastic optimization or optimization under uncertainty has, therefore, emerged in the process systems engineering (PSE) literature with very strong contributions from various fields [1–6]. Stochastic optimization allows the uncertainty involved in data as well as parameters to be considered by appropriate methodologies from the field of statistics and optimization under uncertainty [7–10], which makes it more practical as compared to deterministic optimization.

7.2 Uncertainty Handling Techniques

There are different methodologies available in the literature for handling uncertainties [7]. Keeping the scope of this chapter in mind, only a few of them will be discussed here. Three such commonly used methodologies are stochastic programming (SP), fuzzy mathematical programming (FMP), and chance constrained programming (CCP) [7]. In this chapter, CCP will be discussed in details. However, SP and FMP are discussed very briefly in this section primarily to show the advantages and disadvantages of CCP over those techniques. Amongst various stochastic programming methodologies, a very popular method is the two-stage stochastic programming (TSSP) [11–24], where the decision variables are deployed into two stages. The decision variables in the first stage are to be decided before the uncertain parameters are realized. So, the decision variables that are independent of uncertain parameters come under this category. On the other hand, decision variables that are associated with uncertain parameters belong to the second stage variables, also known as recourse variables. These decision variables can assume different values for different realizations of uncertain parameters and can act as a buffer to combat infeasibility issues appearing because of a particular uncertain parameter realization [25]. Now, the objective function has both first- and second-stage cost components. Due to the association of second-stage variables with uncertain parameters, an expectation term appears in the objective function (second-stage cost component) to take care of different realizations of uncertain parameters. Moreover, penalty terms are associated with the recourse variable in the objective function. Minimization of all these cost components as well as penalty terms becomes the goal in TSSP by appropriately assigning the first stage variables. As the first stage variables are independent of uncertain parameters, they assume a fixed set of values as a solution whereas the second-stage variables assume a different set of values, each one corresponding to different realizations of uncertain parameters. This approach assumes that the information of variance for the uncertain parameters is available. Distribution of the uncertain parameters can be discrete or continuous. In case of discrete distribution, bounded uncertain parameters are divided into several intervals (scenarios) with some assumed probability of occurrence for each of them and the optimization formulation leads to a multiperiod optimization problem. However, the continuous distribution needs multivariate numerical integration to be performed (either approximate integration through sampling or direct numerical integration). As the numbers of uncertain parameters and scenarios increase, the problem size increases exponentially in this approach leading to unmanageable situations given the finite computational resources. Moreover, dealing with the recourse variables quite often leads to impractical issues. Sometimes it might not be easy to decompose the problem into two stage decision variables. On the other hand, FMP [26–29], proliferated by Zimmermann [30, 31], does not assume prior distribution information of the uncertain parameters. In this approach, a membership function is defined representing the extent of constraint violation where a value of 1 for membership function signifies no violation and a value of zero signifies maximum violation whereas the values for intermediate violations are linearly or nonlinearly interpolated in between the two extreme limits. The demand supply equation (supply $\leq$ demand) in a chemical engineering supply chain can be correlated to a situation where the right hand side (demand) is uncertain and more value of the uncertain parameter (i.e. meeting more demand) is desired from an enterprise profitability point of view. In this scenario, a decision maker wants to see whether improvement in the objective function can be achieved by allowing small level of constraint violation or not—whether more demand can be met by incurring more cost. Here objective functions are also converted into constraints by introducing auxiliary variables treated in a similar manner [27]. Incidentally, FMP has control over the problem size when the number of uncertain parameters increases. Here the challenge lies in utilizing the entire uncertainty space, which is often reported as only 50% utilization [26, 32].

Unlike SP, CCP [4, 33–37] requires that the constraints should be satisfied with a predefined value of probability, not necessarily for all occasions. The probability of constraint satisfaction can be linked with the reliability of the solution. To make this complicated probabilistic formulation more tractable, an equivalent deterministic formulation is derived that can be tackled using existing optimization techniques. The CCP approaches for tackling linear systems (uncertain parameters appear in constraints in linear fashion) are achieved by simple coordinate transformation [38, 39]. On the other hand, CCP approaches for nonlinear systems involve calculation of probability of the output constraints when uncertain parameters appear nonlinearly in the constraints. The use of simulation-based techniques [40] could be one of the ways to handle this nonlinear issue. Fortunately, CCP also has control over the problem size when the number of uncertain parameters increases. Generally, in scenario-based TSSP, a complicated tree structure emerges due to different assumed realizations of uncertain parameters and their mutual dependencies. This leads to combinatorial explosion in the number of realized scenarios as the number of uncertain parameter increases and thereby huge computation time is required to compute the expectation term. This problem of TSSP is overcome in CCP approach in general by representing uncertainty in a different manner and the problem size can be kept under control [39]. In a supply-chain planning problem [39], it has been shown that the problem cannot be solved using TSSP approach due to an increase in problem size while handling a large number of uncertain parameters ($\sim$1400) whereas the same problem can be solved using CCP. Emergence of applications of CCP in PSE literature is relatively recent as compared to its counterpart (TSSP) [24, 38, 39, 41–48].

In this chapter, several aspects of problem solving using CCP and the underlying theory will be briefly discussed. The basics of CCP and the treatment of uncertain formulations using CCP under different conditions are presented in section 7.3 with simplified examples. Next, an industrial case study has been presented to demonstrate how a deterministic formulation of industrial grinding can be adapted to an uncertain formulation to show the effect of variation in uncertain parameters on optimization results under a multi-objective scenario in section 7.4. Finally the summary of the work is presented and results are concluded.

7.3 Chance-Constrained Programming: Fundamentals

In CCP, it is required that the constraints should be satisfied with a predefined probability value, but not necessarily for all occasions. As uncertain parameters are present in constraints, there is no guarantee that the constraint will be satisfied all the time—based on the realization of uncertain parameters, there is a probability of these constraints being satisfied. So instead of assuming that the constraints will be satisfied under all realizations of uncertain parameters, which can be a very conservative approach, there is a certain probability with which these constraints will be satisfied. In this framework, a standard optimization formulation with uncertainty parameter vector ξ

$$\mathrm{Min}\,\{f(x)\,|h(x,\xi) \geq 0\} \tag{7.1}$$

can be expressed as

$$\mathrm{Min}\,\{f(x)\,|P(h_k(x,\xi) \geq 0) \geq p\} \qquad (k = 1, \ldots, u) \tag{7.2}$$

where f(x), x and ξ represent objective function, decision variable set and uncertain parameter set respectively. P is the measure of probability and $p \in (0,1]$ is the level of probability of constraint satisfaction. A higher p value ensures the system to be more reliable. The set of feasible x values is progressively reduced when the value of p approaches unity. Based on the requirements of several constraints being satisfied either individually or together, the methodology is called individual or joint chance constrained programming respectively. These two different concepts can be represented as Equations (7.2) and (7.3) respectively.

$$\mathrm{Min}\left\{f(x)\,\middle|P\left[(h_k(x,\xi) \geq 0) \qquad (k = 1, \ldots, u)\right] \geq p\right\} \tag{7.3}$$

It is seen that feasibility in the joint chance constrained case entails feasibility in the individual chance constrained case but the reverse is not true. In the joint chance constrained case, the deterministic equivalent form incorporates the quantile form on the multivariate probability distribution considering all the random parameters under consideration. Passing from joint to individual chance constraints may appear as a complication as that transforms single inequality into a multiple number (u) of inequalities. As the numerical treatment of probability functions involving high dimensional uncertain parameters is much more difficult than in one dimension, the increase in number of inequalities is more than compensated by a much simpler implementation.

Assuming (i) a *normal distribution* for the uncertain parameters, ξ and (ii) uncertain parameters are *separable* from the decision variables, the constraints in Equation 7.2 can be transformed into an equivalent deterministic form:

$$\begin{aligned} & \mathrm{P}\left(\mathrm{h_k}\left(\mathrm{x}, \xi\right) \geq 0\right) \geq \mathrm{p} \Leftrightarrow \mathrm{P}\left(\tilde{\mathrm{h}}_{\mathrm{k}}\left(\mathrm{x}\right) \geq \xi_{\mathrm{k}}\right) \geq \mathrm{p} \\ & \Leftrightarrow \tilde{\mathrm{h}}_{\mathrm{k}}\left(\mathrm{x}\right) \geq \hat{\bar{\xi}}_{\mathrm{k}} := \bar{\xi}_{\mathrm{k}} + \mathrm{q_p}\sigma_{\xi_{\mathrm{k}}} \end{aligned} \tag{7.4}$$

where ξ_k is the random parameter associated with k^{th} constraint, $\bar{\xi}_k$ and σ_{ξ_k} are the mean and standard deviation values of the corresponding random parameters and q_p is the p-quantile of the standard normal distribution with zero mean and unit standard deviation (e.g. 97% probability corresponds to $q_p = q_{0.97} = 2.0$). The second term in the last equivalence form of Equation 7.4 (quantile value multiplied by standard deviation) corrects the nominal requirement, $\bar{\xi}_k$, and provides robustness of the generated optimal operating conditions under uncertain situations. If the random parameters are *not separable* from the decision variable vector x, meaning coefficients of the decision variable vector x in $h_k(x, \xi)$ are also uncertain, these uncertain parameters in Equation 7.4 should be treated in a similar way. In such a case, based on whether the uncertain terms are independent or dependent on each other, the corresponding mean and variance terms are incorporated into the equation in the same fashion and the deterministic equivalent form is derived. This deterministic equivalent generally becomes nonlinear as the computation of mean and variance of coefficients of decision variable leads to nonlinearity in terms of decision variables (see the appendix).

For handling probabilistic constraints efficiently, it is very crucial to have some insight into their analytical, geometrical and topological structure. Most results in this direction are concerned with the convexity issues of the resultant deterministic problem in chance constrained programming approach. It is known that if the individual constraints of the constraint set $h(x, \xi)$ is convex and ξ has such a probability density that the logarithm of which is concave, then $P(h(x, \xi) \geq 0)$ is concave and the corresponding probabilistic constraint may be convex [33, 34]. Otherwise, the resultant deterministic form may not be convex and issues related to this should be treated either with proper convexification approaches or with various global optimization techniques, conventional or evolutionary methods, for handling the resultant nonlinear programming problem (NLP) problems.

Now, we explain the concepts presented above in the form of a simple fleet design example taken from literature [30, 31]. While deciding on the size and structure of its truck fleet, a certain company wants to minimize cost while supplying all customers who have strong seasonally fluctuating demand considering the four trucks x_1, x_2, x_3, x_4 of different sizes. The corresponding linear programming problem (the deterministic version) in (**Min** Cx, Ax $\geq$ B) form is

$$\begin{aligned} & \text{Min} \quad 41400x_1 + 44300x_2 + 48100x_3 + 49100x_4 \\ & \text{s.t.} \\ & 0.84x_1 + 1.44x_2 + 2.16x_3 + 2.4x_4 \geq 170 \\ & 16x_1 + 16x_2 + 16x_3 + 16x_4 \geq 1300 \\ & x_1 \geq 6 \\ & x_2, x_3, x_4 \geq 0 \end{aligned} \tag{7.5}$$

Table 7.1 *Solution of the Zimmermann problem under uncertainty.*

Attribute	Deterministic *(a)*	Uncertainty in B vector *(b)*	Uncertainty in A, B, C vector *(c)*
q_p	0	1.0	1.3
x_1	0	0	4.99
x_2	24.54	26.99	0
x_3	6.0	6.6	62.78
x_4	50.71	55.78	0.81
w1, w2			0.5, 0.5
Constraint1	170	187	170
Constraint2	1300	1430	1300
Constraint3	6	6.6	6
Objective function	3865575	4252132.5	1784167

Solution of this deterministic problem is given in Table 7.1 (column a). Here we intend to show how the same problem can be formulated under CCP formulation paradigms. We consider first the right-hand side terms of the three constraints (i.e. vector B: $b_1 = 170$, $b_2 = 1300$ and $b_3 = 6$) are uncertain to depict the fact that the uncertain parameters are *separable* from the decision variables and uncertainty is present only in the constraints. Other parameters (vector C: $c_1 = 41400$, $c_2 = 44300$, $c_3 = 48100$, $c_4 = 49100$; matrix A: $a_{11} = 0.84$, $a_{12} = 1.44$, $a_{13} = 2.16$, $a_{14} = 2.4$; $a_{21} = a_{22} = a_{23} = a_{24} = 16$; $a_{31} = 1$, $a_{32} = a_{33} = a_{34} = 0$) are considered to be fixed in this case. We can write the uncertain version of equation 5 under CCP framework as

$$\begin{aligned}
&\text{Min} \quad 41400x_1 + 44300x_2 + 48100x_3 + 49100x_4 \\
&\text{s.t.} \\
&P(0.84x_1 + 1.44x_2 + 2.16x_3 + 2.4x_4 \geq 170) \geq p \\
&P(16x_1 + 16x_2 + 16x_3 + 16x_4 \geq 1300) \geq p \\
&P(x_1 \geq 6) \geq p \\
&x_2, x_3, x_4 \geq 0
\end{aligned} \tag{7.6}$$

The corresponding deterministic equivalent of Equation 7.6 can be written as

$$\begin{aligned}
&\text{Min} \quad 41400x_1 + 44300x_2 + 48100x_3 + 49100x_4 \\
&\text{s.t.} \\
&0.84x_1 + 1.44x_2 + 2.16x_3 + 2.4x_4 \geq \bar{b}_1 + q_p \times \sigma_{b_1} \\
&16x_1 + 16x_2 + 16x_3 + 16x_4 \geq \bar{b}_2 + q_p \times \sigma_{b_2} \\
&x_1 \geq \bar{b}_3 + q_p \times \sigma_{b_3} \\
&x_2, x_3, x_4 \geq 0
\end{aligned} \tag{7.7}$$

where $\bar{b}_1, \bar{b}_2, \bar{b}_3$ are the mean (170, 1300, 6) and $\sigma_{b_1}, \sigma_{b_2}, \sigma_{b_3}$ are standard deviation values (10% of corresponding mean values i.e. 17, 130, 0.6) for three uncertain parameters in vector B following *normal distribution*. Assuming a value for $q_p = 1$ (corresponding to 84% probability of getting those constraints satisfied, $p = 0.84$), we obtain the results presented in Table 7.1 (column b).

We now assume that uncertainty exists in all parameters (right-hand side and decision variable coefficients in constraints and objective function) and investigate the effect of uncertainty in final quality of the solution. Following is the formulation using CCP approach assuming the uncertain parameters are *independent* of each other and follow *normal distribution*:

$$
\begin{aligned}
&\text{Min} \quad w_1 \times (\bar{c}_1 x_1 + \bar{c}_2 x_2 + \bar{c}_3 x_3 + \bar{c}_4 x_4) + w_2 \times \sqrt{\left(\sigma_{C_1}^2 x_1^2 + \sigma_{C_2}^2 x_2^2 + \sigma_{C_3}^2 x_3^2 + \sigma_{C_4}^2 x_4^2\right)} \\
&\text{s.t.} \\
&\bar{a}_{11} x_1 + \bar{a}_{12} x_2 + \bar{a}_{13} x_3 + \bar{a}_{14} x_4 - \bar{b}_1 + q_p \sqrt{\left(\sigma_{a_{11}}^2 x_1^2 + \sigma_{a_{12}}^2 x_2^2 + \sigma_{a_{13}}^2 x_3^2 + \sigma_{a_{14}}^2 x_4^2 + \sigma_{b_1}^2\right)} \geq 0 \\
&\bar{a}_{21} x_1 + \bar{a}_{22} x_2 + \bar{a}_{23} x_3 + \bar{a}_{24} x_4 - \bar{b}_2 + q_p \sqrt{\left(\sigma_{a_{21}}^2 x_1^2 + \sigma_{a_{22}}^2 x_2^2 + \sigma_{a_{23}}^2 x_3^2 + \sigma_{a_{24}}^2 x_4^2 + \sigma_{b_2}^2\right)} \geq 0 \\
&\bar{a}_{31} x_1 - \bar{b}_3 + q_p \sqrt{\left(\sigma_{a_{31}}^2 x_1^2 + \sigma_{b_3}^2\right)} \geq 0 \\
&x_1, x_2, x_3, x_4 \geq 0
\end{aligned}
\tag{7.8}
$$

where

$$
\begin{aligned}
\bar{c}_1 &= 41400.0; \;\; \bar{c}_2 = 44300.0; \;\; \bar{c}_3 = 48100.0; \;\; \bar{c}_4 = 49100.0 \\
\bar{a}_{11} &= 0.84; \;\; \bar{a}_{12} = 1.44; \;\; \bar{a}_{13} = 2.16; \;\; \bar{a}_{14} = 2.4 \\
\bar{a}_{21} &= 16.0; \;\; \bar{a}_{22} = 16.0; \;\; \bar{a}_{23} = 16.0; \;\; \bar{a}_{24} = 16.0 \\
\bar{a}_{31} &= 1 \\
\bar{b}_1 &= 170.0; \;\; \bar{b}_2 = 1300.0; \;\; \bar{b}_3 = 6.0 \\
\sigma_{C_1} &= 4140.0; \;\; \sigma_{C_2} = 4430.0; \;\; \sigma_{C_3} = 4810.0; \;\; \sigma_{C_4} = 4910.0 \\
\sigma_{a_{11}} &= 0.084; \;\; \sigma_{a_{12}} = 0.144; \;\; \sigma_{a_{13}} = 0.216; \;\; \sigma_{a_{14}} = 0.24 \\
\sigma_{a_{21}} &= 1.6; \;\; \sigma_{a_{22}} = 1.6; \;\; \sigma_{a_{23}} = 1.6; \;\; \sigma_{a_{24}} = 1.6 \\
\sigma_{a_{31}} &= 0.1 \\
\sigma_{b_1} &= 17.0; \;\; \sigma_{b_2} = 130.0; \;\; \sigma_{b_3} = 0.6
\end{aligned}
$$

The objective function now has two terms, first one is the corresponding mean and second one is the corresponding standard deviation of the uncertain parameters which is a *linear* combination of four *normally distributed* random variables (c_1–c_4), connected by two weights (w_1, w_2) signifying the weightages on mean and standard deviation terms. The choice of these weightages depends on how the decision maker's interest in considering the effect of the mean and standard-deviation terms in the objective function. For example, a weight of $w_1 = 0$ signifies that mean terms are not going to be considered in the objective function, only the effect of variance is minimized. Similarly, $w_2 = 0$ signifies that the decision maker does not want to consider the variance terms in the objective function. Next, the constraints are also modified where probability of constraint satisfaction defines the nature of equation (see the appendix) assuming uncertain parameters are *independent* of each other. Terms with bar signifies the mean value of the uncertain parameters whereas σ signifies their standard deviation values. Although Equation 7.5 is a linear system, the uncertainty formulation of the same leads to different deterministic equivalents of a linear (Equation 7.7) and nonlinear (Equation 7.8) nature under the CCP paradigm based on whether uncertain parameters are *separable* from the decision variables or not. Both the equations in Equations 7.7 and 7.8 are convex in nature (see the appendix) and can be solved by any standard convex optimization techniques. The solution of this problem is given in Table 7.1 (column c).

Next, we investigate the effect of q_p and σ on the solution of the problem. First we change the values for q_p. As we increase this quantile value, probability of constraints in Equation 7.7 being satisfied increases, which in turn says solution reliability increases with increase in the values for q_p. The values for q_p have been increased from 1 to 2 which is an indication for increase in solution reliability to the extent of 84% to 97% respectively. The values for $\bar{b}_1$, $\bar{b}_2$, $\bar{b}_3$ are kept at the same (i.e. 170, 1300, 6) and σ_{b_1}, σ_{b_2}, σ_{b_3} are kept at 10% of their corresponding mean values i.e. 17, 130, 0.6 for uncertain parameters in vector B. We assume the parameters follow normal distribution and can see the results in Table 7.2(a). Similarly we can generate the results in Table 7.2(b) by varying q_p values from 1 to 2 assuming standard deviation values (σ_{b_1}, σ_{b_2}, σ_{b_3}) are 20% of their corresponding mean values i.e. 34, 260, 1.2 for three uncertain parameters in vector B. We can observe two important findings here: (i) solution reliability has a tradeoff relationship with solution optimality—in the problem involving Equation 7.7, we want to minimize the objective function whereas objective value increases as we increase the value of q_p in search of a more reliable solution; this also shows that, with more loosening of constraint satisfaction, optimal solution quality improves at the cost of solution reliability; (ii) with an increase in variation in the process, the optimizer becomes more conservative to combat uncertainty and provide solution of inferior (higher in this case) objective value. The results of an uncertain case can be compared with those of a deterministic case (Table 7.2(a), first column) as well. These trends are presented in Figure 7.1.

The significant difference between the deterministic and stochastic optimization formulation is that the latter has some uncertain component in it. Once the deterministic equivalent of the stochastic formulation is known to us, the main difficulty in the problem is probably over unless the challenge is to find a global solution for a non-convex formulation, which is present anyway in any non-convex optimization problem. Leaving the problem of finding a global solution for an optimization problem, a primary challenge in stochastic optimization problem is to find the corresponding deterministic equivalent. However, this process is usually hard to perform and only successful for some special cases, as mentioned above. For example, if the uncertain parameters are related in nonlinear fashion, propagation of that uncertainty to the constraints cannot be achieved in a straight forward manner. One of the ways might be using Taylor series expansion of the nonlinear function around the mean value and calculate mean and standard deviation of the combined function considering only the few (say linear) terms in the Taylor series (see the appendix). This approach is generally

Table 7.2 *Effect of q_p on the Zimmermann problem under uncertainty.*

(a)

Attribute	Deterministic	Uncertainty in B vector (σ = 10% of mean values)					
q_p	0	1	1.2	1.4	1.6	1.8	2
x_1	0	0	0	0	0	0	0
x_2	24.54	26.99	27.49	27.98	28.47	28.96	29.45
x_3	6	6.6	6.72	6.84	6.96	7.08	7.2
x_4	50.71	55.78	56.79	57.81	58.82	59.84	60.85
Constraint1	170	187	190.4	193.8	197.2	200.6	204
Constraint2	1300	1430	1456	1482	1508	1534	1560
Constraint3	6	6.6	6.72	6.84	6.96	7.08	7.2
Objective function	3865575	4252132.5	4329444	4406756	4484067	4561378.5	4638690

(b)

Attribute	Deterministic	Uncertainty in B vector (σ = 20% of mean values)					
q_p	0	1	1.2	1.4	1.6	1.8	2
x_1	0	0	0	0	0	0	0
x_2	24.54	29.45	30.43	31.41	32.4	33.38	34.36
x_3	6	7.2	7.44	7.68	7.92	8.16	8.4
x_4	50.71	60.85	62.88	64.91	66.94	68.96	70.99
Constraint1	170	204	210.8	217.6	224.4	231.2	238
Constraint2	1300	1560	1612	1664	1716	1768	1820
Constraint3	6	7.2	7.44	7.68	7.92	8.16	8.4
Objective function	3865575	4638690	4793313	4947936	5102559	5257182	5411805

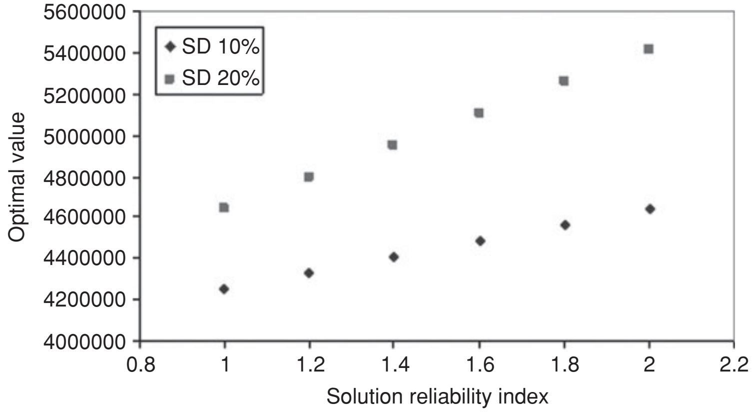

Figure 7.1 *Solution optimality and reliability tradeoff in CCP formulation.*

adopted for most of the practical problems, to simplify the computation involved though it has limitation in terms of order of accuracy due to consideration of limited number of terms in the Taylor series. Moreover, this technique requires the derivatives to be calculated, which might be time consuming for complex problems. Simulation-based approaches provide an alternative for calculating the probability of constraint satisfaction where no such assumption is needed. Most importantly, simulation-based approach can take care of the case of different inputs following different distributions. A simulation based scheme for computing a probabilistic constraint is presented below.

7.3.1 Calculation of $P(h_k(x, \xi) \geq 0) \geq p \quad (k = 1, \ldots, u)$

1. If N_{samp} represents the number of entire sampling set and N' represents the number of successful constraint satisfaction cases for different instances of uncertain parameter realization, set $N' = 0$ initially.
2. Following given individual variance information, generate an instance of uncertain parameter realization (denoted as ξ').
3. If the associated constraint is satisfied, i.e. $(h_k(x, \xi) \geq 0) \quad (k = 1, \ldots, u)$, $N' \leftarrow N' + 1$.
4. Repeat steps 2 and 3 for N_{samp} times.
5. $P = N'/N_{samp}$.

If uncertain parameters also affect the objective functions in simulation-based approaches, the optimization problem can be written by introducing an auxiliary variable [40] $\tilde{f}$ as

$$\begin{aligned}
&\underset{x}{\text{Max}} \quad [\underset{\tilde{f}}{\max}\, \tilde{f}] \\
&\text{subject to} \\
&P\left\{\xi \,\middle|\, f(x,\xi) \geq \tilde{f}\right\} \geq \delta \\
&P\{\xi \,|\, g_i(x,\xi) \leq 0\} \geq \beta_i \qquad i = 1, 2, \ldots, n
\end{aligned} \tag{7.9}$$

Here, another probability level $\delta \in (0, 1]$ is defined in the similar fashion as β_i. Similarly, this case can be extended [40] for a multi-objective optimization formulation (with j as the index for objective functions and $\delta_j \in (0, 1]$) as

$$\begin{aligned}
&\underset{x}{\text{Max}} \quad \left[\max_{\tilde{f}_1} \tilde{f}_1, \max_{\tilde{f}_2} \tilde{f}_2, \ldots, \max_{\tilde{f}_m} \tilde{f}_m \right] \\
&\text{subject to} \\
&P\left\{\xi \left| f_j(x, \xi) \geq \tilde{f}_j \right.\right\} \geq \delta_j \qquad j = 1, 2, \ldots, m \\
&P\left\{\xi \left| g_i(x, \xi) \leq 0 \right.\right\} \geq \beta_i \qquad i = 1, 2, \ldots, n
\end{aligned} \tag{7.10}$$

This can be applied for cases where even some of the multiple objectives may be subjected to uncertainty. The following scheme can be used for handling uncertainty in parameters in the objective function.

7.3.2 Calculation of $\max\left\{\tilde{f} \left| P\left\{f(x, \xi) \geq \tilde{f}\right\} \geq \alpha \right.\right\}$

1. Assume N_{samp} represents the number of entire sampling set.
2. Following given individual variance information, generate an instance of uncertain parameter realization (denoted as ξ').
3. Compute new value of objective function (f') for ξ'.
4. Repeat above two steps for N_{samp} times.
5. $N' = \text{Integer}(\alpha N_{samp})$.
6. Return the N' th largest element from the set of values calculated in step 4.

Thus simulation based approaches can be extremely useful for solving general nonlinear and complicated CCP constraints without many assumptions. However, this increases the computational cost required for carrying out the simulation exercises. One should remember that this might not be a great limitation when we have access to modern age computing resources and techniques (e.g. parallel processing ability, or function approximation techniques such as artificial neural network) to expedite computation. In the next section, we are going to use some of the techniques discussed above for the uncertainty analysis of a complex nonlinear process model.

7.4 Industrial Case Study: Grinding

7.4.1 Grinding Process and Modeling

The industrial grinding circuit under consideration has the following units, which are connected by different flow streams: rod mill, ball mill, hydrocyclones and water sumps. Raw ore is fed to the rod mill from the crushing unit and water is added. The resultant slurry is collected in a sump called the primary sump. The outlet stream of the primary sump is fed to a bank of hydrocyclones – primary hydrocyclones. The underflow of the primary hydrocyclones is fed to the ball mill whereas the overflow is taken in another sump called a secondary sump. The outlet of the ball mill is collected in the primary sump. The secondary sump feeds to another bank of hydrocyclones, namely secondary hydrocyclones. The overflow from the secondary hydrocyclone is taken as the final product whereas the underflow is fed back to the ball mill for further grinding. Water is also added in the two

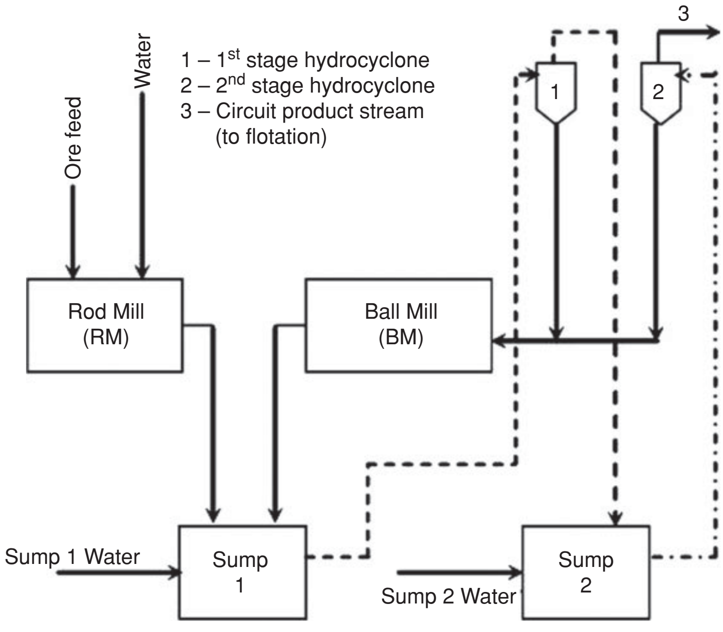

Figure 7.2 *Industrial grinding circuit schematic. Reprinted with permissions from Modeling of an industrial wet grinding operation using data-driven techniques by K. Mitra and M. Ghivari, Computers & Chemical Engineering, 30, 3, 508–520 Copyright (2006) Elsevier Ltd.*

sumps to ensure smooth flow of slurry in the circuit. A schematic diagram of the process can be seen in Figure 7.2.

Each of the unit operations described above is modeled separately using a hybrid approach of population balance and empirical correlations. The connection among various units has been established for the whole circuit with the help of a square connectivity matrix where each of the unit operations is written in rows and columns and connectivity among various units is expressed in terms of 0 and 1 (0 denoting no connection and 1 denoting connection exists). The population balance approach is used for a general material balance across all unit operations whereas empirical correlations are used for calculating breakage functions in the rod and the ball mill and sharpness index, and so forth, in hydrocyclones. The complete set of equations led to a solution of the differential algebraic equations (DAE) system [49], which is solved here using DASSL [50], a public-domain software. The model is nonlinear in nature having exponential (e^x type) as well as power term (x^y type) nonlinearity present in it [48, 49].

In this case study, we consider the uncertainty in (i) model parameters, (ii) constraints bounds and (iii) objective functions, and explore the merits of the simulation-based CCP approach in analyzing their impact on the multi-objective optimization of the grinding system. The need for nonlinear propagation of the uncertain parameters to the output constraints build the rationale for adopting the simulation based CCP approach. Two mutually conflicting objectives considered for this study are simultaneous maximization of throughput and maximization of percent passing of medium-size particles. The deterministic multi-objective grinding model of Mitra and Gopinath [49] forms the basis of this work on which various impacts of uncertainty have been analyzed. An uncertain version of non-dominated sorting genetic algorithm, CCPNSGA II, has been proposed for solving the multi-objective optimization under uncertainty. Apart from many other advantages, one of the reasons for using derivative free optimization method in this case is to avoid the computation of derivative of probabilistic constraints, which otherwise could have made the optimization formulation even more computationally expensive.

7.4.2 Optimization Formulation

7.4.2.1 Deterministic and Stochastic Formulation

Two important goals of the industrial grinding operation are the maximization of productivity and maximization of the quality of the grinding product. As the grinding circuit's final product slurry goes directly to the following flotation circuit, the quality of the grinding can be measured primarily by the grinding size distribution of the final product stream, which determines the particle floatability in the flotation circuit. Through laboratory experiments, it has been established that correct flotation dynamics can be achieved in the following flotation circuit by supplying grinding product consistently around the mid-size fraction for the given ore mineralogy and flotation reagent used. The mid-size fraction of a grinding product is therefore maximized to maintain a quality check on the grinding product whereas productivity maximization can be directly achieved by maximizing the circuit throughput. However, there is a tradeoff between these two objectives that is known from our previous work [49]. Simultaneous maximization of these two objectives, therefore, builds an ideal platform for deterministic multi-objective optimization. Size distribution (percentage passing of coarse- and fine-size classes, S_C, S_F, respectively), percentage solids (P_S), and circulation load (C_L) are to be treated as upper bound constraints. Raw ore feed flowrate to rod mill (F_{RM}), flowrate of water to primary sump (W_{PS}) and secondary sump (W_{SS}) can be manipulated within their respective upper and lower bounds during optimization to achieve this task. Other water additions to the grinding circuit are considered as fixed due to practical limitations. Keeping circulation load within certain upper bound indicates an effort towards energy saving, whereas keeping the size distribution and percent solids under bounds indicate correct mineral liberation in the next unit operation. With all justifications, the deterministic multi-objective optimization formulation mentioned above can be expressed as follows.

Objectives:

$$\underset{F_{RM}, W_{PS}, W_{SS}}{\text{Max}} \quad T$$

$$\underset{F_{RM}, W_{PS}, W_{SS}}{\text{Max}} \quad S_M\left(G_{RM}, G_{BM}, S_{PS}, S_{SS}\right)$$

Subject to control variable bounds:

$$S_C\left(G_{RM}, G_{BM}, S_{PS}, S_{SS}\right) \le S_C^U$$
$$S_F\left(G_{RM}, G_{BM}, S_{PS}, S_{SS}\right) \le S_F^U$$
$$P_S\left(G_{RM}, G_{BM}, S_{PS}, S_{SS}\right) \le P_S^U$$
$$C_L\left(G_{RM}, G_{BM}, S_{PS}, S_{SS}\right) \le C_L^U$$

Other model equations

Decision variables bounds:

$$\begin{aligned} F_{RM}^{L} &\le F_{RM} \le F_{RM}^{U} \\ W_{PS}^{L} &\le W_{PS} \le W_{PS}^{U} \\ W_{SS}^{L} &\le W_{SS} \le W_{SS}^{U} \end{aligned} \tag{7.11}$$

where G_{RM}, G_{BM}, S_{PS} and S_{SS} are parameters that are assumed to be known with certainty for the deterministic optimization formulation and considered as uncertain parameters for the stochastic optimization formulation (presented later). G_{RM} and G_{BM} are the grindability indices for the rod mill and ball mill, and S_{PS} and S_{SS} are sharpness indices for primary and secondary hydrocyclones, respectively. These parameters were initially calculated 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 and hence are assumed to be uncertain for the stochastic optimization study. In this study, we assume that the variance information of the uncertain parameters are available from the experiments and treat the stochastic optimization formulation using the simulation based CCP approach.

In the stochastic formulation, we consider different types of uncertainty:

(i) Uncertain parameters present in the left-hand side of the constraint (four parameters that are considered uncertain are $\hat{G}_{RM}$, $\hat{G}_{BM}$, $\hat{S}_{PS}$ and $\hat{S}_{SS}$).
(ii) Uncertain parameters present in the right hand side of the constraint (upper bounds for control variables $\hat{S}_C^U$, $\hat{S}_F^U$, $\hat{P}_S^U$ and $\hat{C}_L^U$)
(iii) Uncertainty in the objective function (one of the objective functions considered for this multi-objective optimization study under uncertainty, e.g. percent passing of mid size classes, $\hat{S}_M$, is exposed to uncertainty due to the uncertainty present in the parameters $\hat{G}_{RM}$, $\hat{G}_{BM}$, $\hat{S}_{PS}$ and $\hat{S}_{SS}$).

Uncertain parameters presented in (ii) above have linear relationship with the constraints whereas uncertainty presented in (i) and (iii) above are nonlinear in nature. Based on the description of the CCP, the stochastic multi-objective grinding optimization problem is described below.

Objectives:

$$\max_{F_{RM}, W_{PS}, W_{SS}} \quad T$$

$$\max_{F_{RM}, W_{PS}, W_{SS}} \quad \tilde{S}_M$$

Subject to control variable bounds:

$$\begin{aligned} &P\left(\hat{S}_M\left(\hat{G}_{RM}, \hat{G}_{BM}, \hat{S}_{PS}, \hat{S}_{SS}\right) \ge \tilde{S}_M\right) \ge \delta_1 \\ &P\left(\hat{S}_C\left(\hat{G}_{RM}, \hat{G}_{BM}, \hat{S}_{PS}, \hat{S}_{SS}\right) \le \hat{S}_C^U\right) \ge \beta_1 \\ &P\left(\hat{S}_F\left(\hat{G}_{RM}, \hat{G}_{BM}, \hat{S}_{PS}, \hat{S}_{SS}\right) \le \hat{S}_F^U\right) \ge \beta_2 \\ &P\left(\hat{P}_S\left(\hat{G}_{RM}, \hat{G}_{BM}, \hat{S}_{PS}, \hat{S}_{SS}\right) \le \hat{P}_S^U\right) \ge \beta_3 \\ &P\left(\hat{C}_L\left(\hat{G}_{RM}, \hat{G}_{BM}, \hat{S}_{PS}, \hat{S}_{SS}\right) \le \hat{C}_L^U\right) \ge \beta_4 \end{aligned}$$

All model equations

Decision variables bounds:

$$\begin{aligned} F_{RM}^{L} &\leq F_{RM} \leq F_{RM}^{U} \\ W_{PS}^{L} &\leq W_{PS} \leq W_{PS}^{U} \\ W_{SS}^{L} &\leq W_{SS} \leq W_{SS}^{U} \end{aligned} \tag{7.12}$$

where $\tilde{S}_M$ is the auxiliary variable introduced to handle uncertainty in the second objective function and β_i, δ_i are the predefined confidence level of getting corresponding constraints and objective satisfied, respectively.

7.4.2.2 Chance Constrained Programming Simulation

As the uncertain parameters bear a nonlinear relationship with the constraints, the probability of constraint satisfaction is calculated by a simulation process. Two cases are going to be discussed: (i) How to calculate the probability of constraint satisfaction and (ii) how to calculate the probability measure in the objective function term.

7.4.2.2.1 Calculation of $\mathbf{P}\left(\hat{\mathbf{S}}_{\mathbf{C}}\left(\hat{\mathbf{G}}_{\mathbf{RM}}, \hat{\mathbf{G}}_{\mathbf{BM}}, \hat{\mathbf{S}}_{\mathbf{PS}}, \hat{\mathbf{S}}_{\mathbf{SS}}\right) \leq \hat{\mathbf{S}}_{\mathbf{C}}^{\mathbf{U}}\right) \geq \beta_{\mathbf{1}}$

1. If N_{samp} represents the number of entire sampling set and N' represents the number of successful constraint satisfaction cases for different instances of uncertain parameter realization, set $N' = 0$ initially.
2. Following given individual variance information, generate an instance of uncertain parameter realization (denoted as $G'_{RM}, G'_{BM}, S'_{PS}, S'_{SS}, S'^{U}_{C}$).
3. If the associated constraint is satisfied, i.e. $S_C\left(G'_{RM}, G'_{BM}, S'_{PS}, S'_{SS}\right) \leq S'^{U}_{C}$, $N' \leftarrow N' + 1$.
4. Repeat step 2 and step 3 for N_{samp} times.
5. $P = N'/N_{samp}$

7.4.2.2.2 Calculation of $\max\left\{\tilde{\mathbf{S}}_{\mathbf{M}} \middle| \mathbf{P}\left(\hat{\mathbf{S}}_{\mathbf{M}}\left(\hat{\mathbf{G}}_{\mathbf{RM}}, \hat{\mathbf{G}}_{\mathbf{BM}}, \hat{\mathbf{S}}_{\mathbf{PS}}, \hat{\mathbf{S}}_{\mathbf{SS}}\right) \geq \tilde{\mathbf{S}}_{\mathbf{M}}\right) \geq \delta_{\mathbf{1}}\right\}$

1. Assume N_{samp} represents the number of entire sampling set.
2. Following given individual variance information, generate an instance of uncertain parameter realization (denoted as $G'_{RM}, G'_{BM}, S'_{PS}, S'_{SS}$).
3. Compute new value of S'_M for $(G'_{RM}, G'_{BM}, S'_{PS}, S'_{SS})$.
4. Repeat above two steps for N_{samp} times
5. $N' = \text{Integer}(\delta_1 N_{samp})$
6. Return the N'^{th} largest element from the set of values calculated in step 4.

7.4.2.3 Multivariate Probability Space Sampling

The next step after the uncertain parameters are assigned to their individual probability distribution functions is to sample the multivariate probability space using effective sampling techniques that help propagate the uncertainty effects from uncertainty parameters to the corresponding constraints and objective functions through model simulation. The propagation of uncertainty effects from uncertainty parameters to the corresponding constraints and objective functions can also be achieved by means of coordinate transformation which is only limited to some special results for linear systems [40]. A relatively new quasi-random

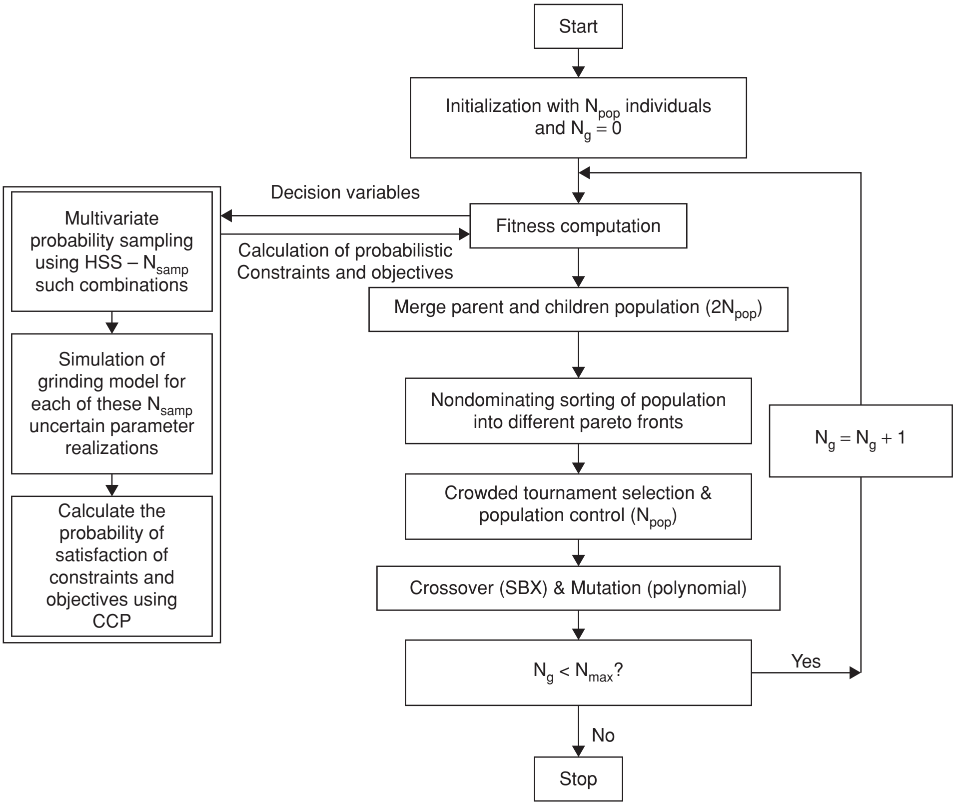

Figure 7.3 *Working principle of NSGA II amalgamated with simulation based chance constrained programming.*

sampling technique based on Hammersley sequence sampling (HSS) proposed by Diwekar and Kalagnanam [51] is used here for multivariate probability space sampling. As compared to many other popular sampling techniques, HSS shows 3–100 times faster convergence while determining various statistical properties and therefore requires less number of sample points [51]. For these reasons, HSS has been our choice for sampling the multivariable probability space. We assume each of the uncertain parameter is going to follow normal distribution. If N_{samp} numbers of combinations for eight uncertain parameters are generated by the HSS based sampling method, an inverse transformation over the cumulative probability distribution acted upon each of these eight uncertain parameters is going to provide the specific values for each uncertain parameter. These values of uncertain parameters are going to be used to create specific instances of uncertain parameters for CCP simulation.

7.4.2.4 Simulation Based CCP Amalgamated NSGA II (CCPNSGA II)

A block diagram of the complete real coded NSGA II algorithm amalgamated with the simulation based CCP approach (CCPNSGA II) is presented in Figure 7.3 and described here. The primary difference of CCPNSGA II with actual NSGA II is the presence of a simulation-based CCP block that calculates the probability associated with a constraint and objective function. Like many other population-based multi-objective evolutionary algorithms, CCPNSGA II starts the search process with N_{pop} number of initial candidate solutions (called population) each having different values of decision variables. For each of these N_{pop} solutions, probability measures for constraint and objectives are calculated using the simulation-based CCP block across N_{samp} instances of random uncertainty realizations. Here the HSS based multivariate probability space sampling method is used for creating N_{samp} number of samples each having eight uncertain parameters. Once the fitness and constraints values are computed for all population members (parent population), the entire population is sorted using the principles of non-dominated sorting and different Pareto fronts are identified [52]. A better Pareto front receives a smaller ranking as compared to its inferior counterpart. Within each Pareto front, different solutions are tagged with different values of crowding distance signifying how populated that solution is with respect to its neighbors. A greater value of the crowding distance parameter for a particular solution signifies that the nearest neighbors of that solution are further away from it. Now a crowding tournament selection scheme is going to be applied, where two solutions are picked at random and (i) if both of them are infeasible, the one with less infeasibility wins; (ii) if both of them are feasible, one with better rank wins and if they are from the same rank the one with more crowding metric wins; (iii) if one of them is feasible and the other is infeasible, the feasible solution wins. This builds a selection pressure to find better Pareto-optimal (PO) solutions with good spread. Next, these selected solutions are allowed to mate with each other at random to create new solutions (child population) using genetic operators such as crossover and mutation. This completes a single iteration (N_g) of CCPNSGA II and this continues until the iteration counter reaches the maximum number of iteration (N_{max}) specified in the beginning. As NSGA II is an elitist approach, merging of parent and child population before carrying out non-dominated sorting ($2N_{pop}$) and then controlling the population during selection (N_{pop}) is a regular feature in CCPNSGA II [53]. The following parameters are used for this study: $N_{max} = 50$; $N_{pop} = 50$; crossover and mutation probabilities of 0.9 and 0.01 respectively; 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 enough for this case. Different sampling sizes were tried and finally it is kept at 300. This sampling size could have been increased to some number higher than 300. However, it is observed that it has increased the computational burden further without significantly contributing towards accuracy of the results.

7.4.3 Results and Discussion

The industrial grinding example discussed here has been extracted from a leading vertically integrated lead-zinc multinational company. First the grinding circuit model is validated against steady-state industrial data taken from several representative operating regimes covering the entire span of operation. Interested readers can find these validation results elsewhere [49]. Four out of the eight uncertain parameters ($\hat{G}_{RM}$, $\hat{G}_{BM}$, $\hat{S}_{PS}$ and $\hat{S}_{SS}$) represent the parametric uncertainty whereas the remaining parameters ($\hat{S}_C^U$, $\hat{S}_F^U$, $\hat{P}_S^U$ and $\hat{C}_L^U$) represent the decision maker's choice to present them in an uncertain way. Assuming that the uncertainty in all these parameters can be described reasonably well by the normal

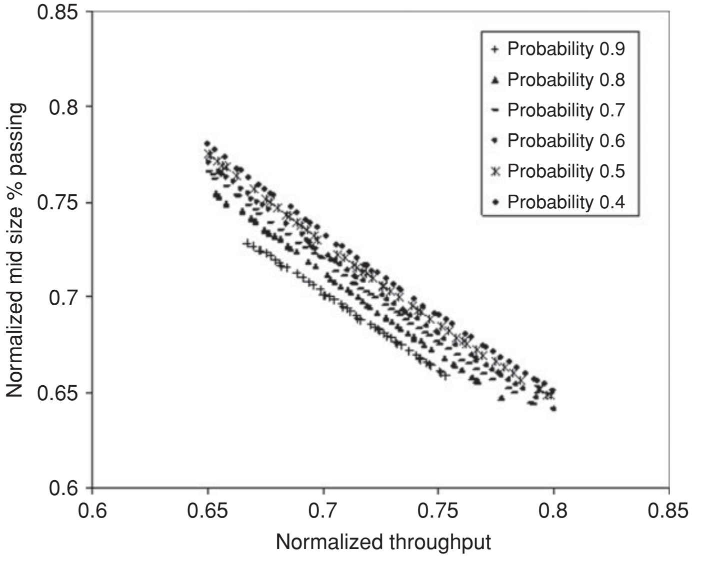

Figure 7.4 *PO points between normalized objectives as a function of probabilities of constraint satisfaction.*

distribution, we assume normal distribution for all uncertain parameters with standard deviation value 5% of its nominal value and nominal values of these parameters are kept same as our earlier work of deterministic formulation [49]. The value of extent of uncertainty was chosen from the experience of the plant practitioners. All the parameters are varied simultaneously and the results are investigated. The multi-objective PO fronts for the stochastic formulation described earlier are presented in Figure 7.4 where tradeoffs between two objectives (throughput and mid-size percentage passing) are shown at a normalized scale for different extents of constraint satisfaction probabilities. Effects of different extents of constraint satisfaction on Pareto front were shown by assuming different probability levels of constraint satisfaction. Here they were selected based on some measure of reliability associated with the chosen probability extent (in case of normal distribution, probability measure of 0.9 gives the reliability of that constraint being satisfied to the extent of 90%, etc.). The primary purpose was to establish and quantify the improvement in the PO front by sacrificing the reliability of the solution first and then decide from the higher level business experience where to draw the line between the two. Single-chance constraints were considered because the joint probability distribution information of the uncertain parameters was very difficult to make available in this case. More stringent requirements come with an increase in value of probability measures for constraint satisfaction leaving relatively fewer alternative solutions. The recommended solutions for higher probability values (0.9 in this case) are most reliable as well as conservative compared to the solutions of lesser probability values. The span of the PO fronts increases on both sides as the probability value decreases and it is at its minimum for the probability value 0.9. Probability of constraint satisfaction can be linked with the reliability of the obtained solution [39]. Figure 7.4 also shows that better PO fronts can be achieved by compromising on the reliability of

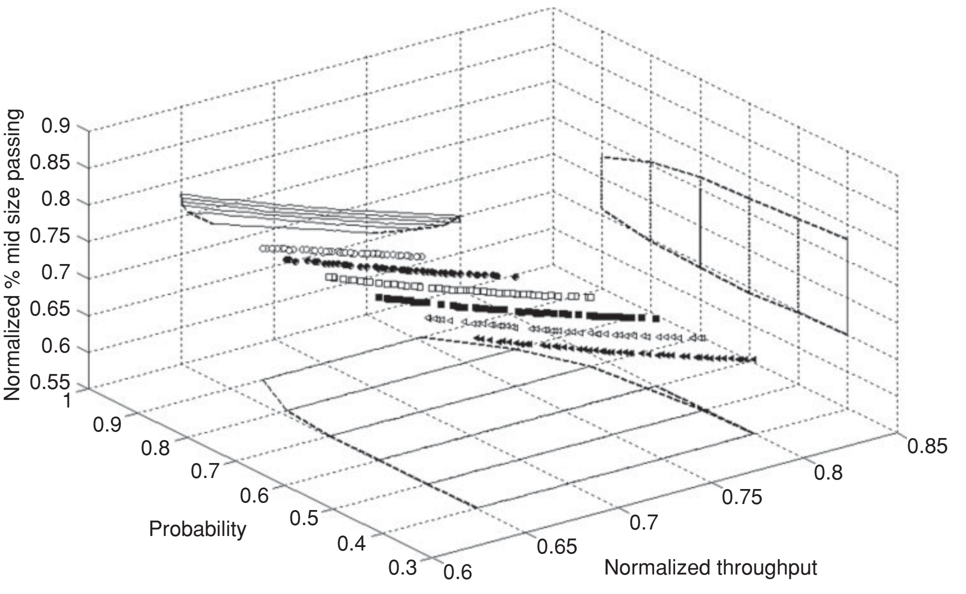

Figure 7.5 *Three dimensional PO points between normalized objectives as a function of probabilities of constraint satisfaction.*

the solution. This means that any point chosen from the PO front corresponding to the probability value 0.4 can lead to better throughput as well as quality of grinding product compared to a solution from the PO front corresponding to the probability value 0.9; however, running a plant with the former solution may not always be optimal (or sometimes infeasible with certain realization of uncertain parameters) as the reliability associated with this solution is much less compared to the latter solution. There is therefore a tradeoff among two objectives and reliability of the solution obtained (Figure 7.5). The span of increase in PO front with the decrease in probability value is clearly visible in Figure 7.5 (look at the bounded search space in the probability-normalized throughput plane). The effect of change of standard deviation can be seen in Figure 7.6 where the standard deviation value is changed from 5% to 10% for probability of constraint satisfaction value of 0.4. As the standard deviation value is increased, more variation in the values of the uncertain parameters is considered, leading to marginally better PO front keeping the reliability of the solutions at the same level. The hypothesis is verified with the PO solutions of other reliability levels as well. This shows that if different realizations of uncertain parameters are handled in similar fashion, using nominal values of the uncertain parameters where each of these realizations can be tackled by different optimal conditions, there will be ample cases where either the system will not be able to extract the best out of the situation (it will underperform) or it will overperform to pile unnecessary inventory. As compared to tedious deterministic sensitivity analysis, this methodology provides a systematic way of carrying out the sensitivity analysis by controlling the constraint violations through defining probability of constraint satisfaction for those constraints and allowing variations in different uncertain parameters.

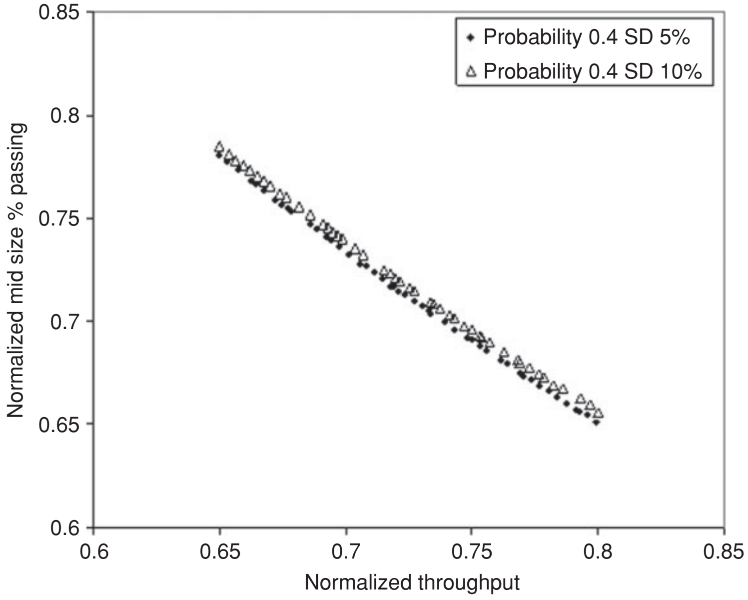

Figure 7.6 *Effect of change of standard deviation for uncertain parameters on the final PO front.*

Each of the PO solutions shown so far carries information about the decision variables concerned. The Fritz–John conditions for multi-objective optimization [52] say that PO solutions must obey certain mathematical conditions. So, if the solutions obtained are near to the true PO solutions, Fritz–John necessary conditions would be applicable to them and some similarity or dissimilarity among the solutions would be visible as they all obey the necessary conditions. It was therefore decided to search for such properties in the present real-world application problem [54, 55]. Considering the PO points for probability 0.9 in Figure 7.4, manipulated variables are plotted in ascending order of throughput with the purpose of finding trends in the decision variables. Three different trends are found out (see Figure 7.7): (i) raw ore feed flowrate to rod mill (F_{RM}) shows a monotonically increasing trend within its given range; (ii) water flowrate to primary sump (W_{PS}) gradually increases from its lower bound to upper bound (0.2–0.4 in the normalized scale), and (iii) flowrate of water to the secondary sump (W_{SS}) is found to be very close to the middle of the given bound (0.2–0.4 in the normalized scale). Relatively different trends are found for probability 0.4 PO points for gradually increasing values for throughput (see Figure 7.8): (i) F_{RM} shows a monotonically increasing trend within its given range, however, this curve is relatively more stiff, (ii) W_{PS} hovers around the upper bound of the given range (0.2–0.4 in the normalized scale), and (iii) W_{SS} is found to be varying between the lower to the medium values of the given bound (0.2–0.4 in the normalized scale). This kind of mapping information between PO points and decision variables that is derived here as a result of the analysis of a multi-objective optimization problem under uncertainty can clearly guide a plant operator to improve the grinding operation as per requirement, which can only be achieved otherwise through an extensive as well as prolonged expertise over the process.

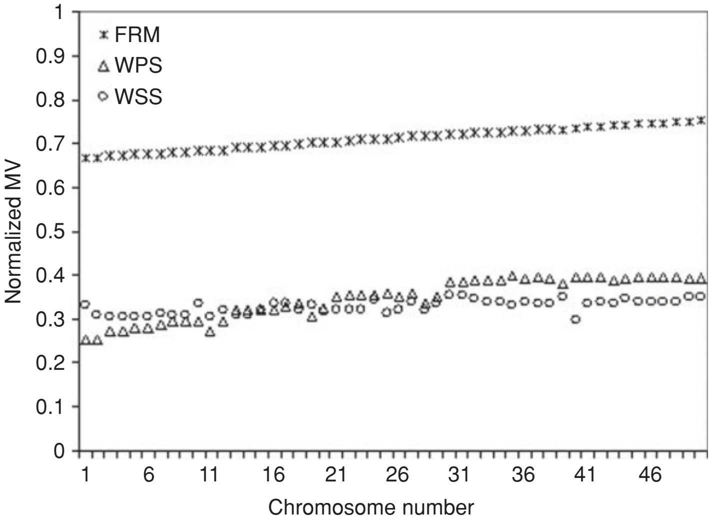

Figure 7.7 Manipulated variable trends corresponding to PO points for probability value 0.9 in Figure 7.4.

Many other instances of deterministic multi-objective optimization studies such as design of gearbox and truss-structure [54, 55], grinding [49], sintering [56], continuous casting [57], polymerization of epoxy [58, 59], Poly-propylene Terepthalate (PPT) [60], iron-ore induration [61] shown similar trends. Control variable values corresponding to the PO solutions of probability 0.9 and 0.4 are presented in Figures 7.9 and 7.10, respectively. As

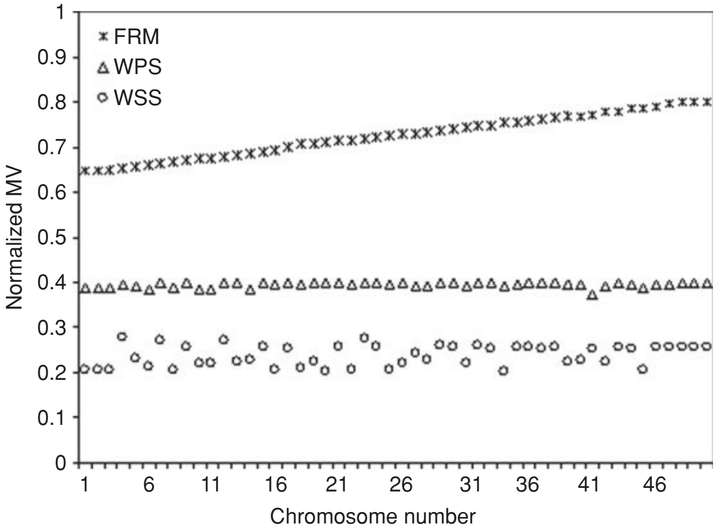

Figure 7.8 Manipulated variable trends corresponding to PO points for probability value 0.4 in Figure 7.4.

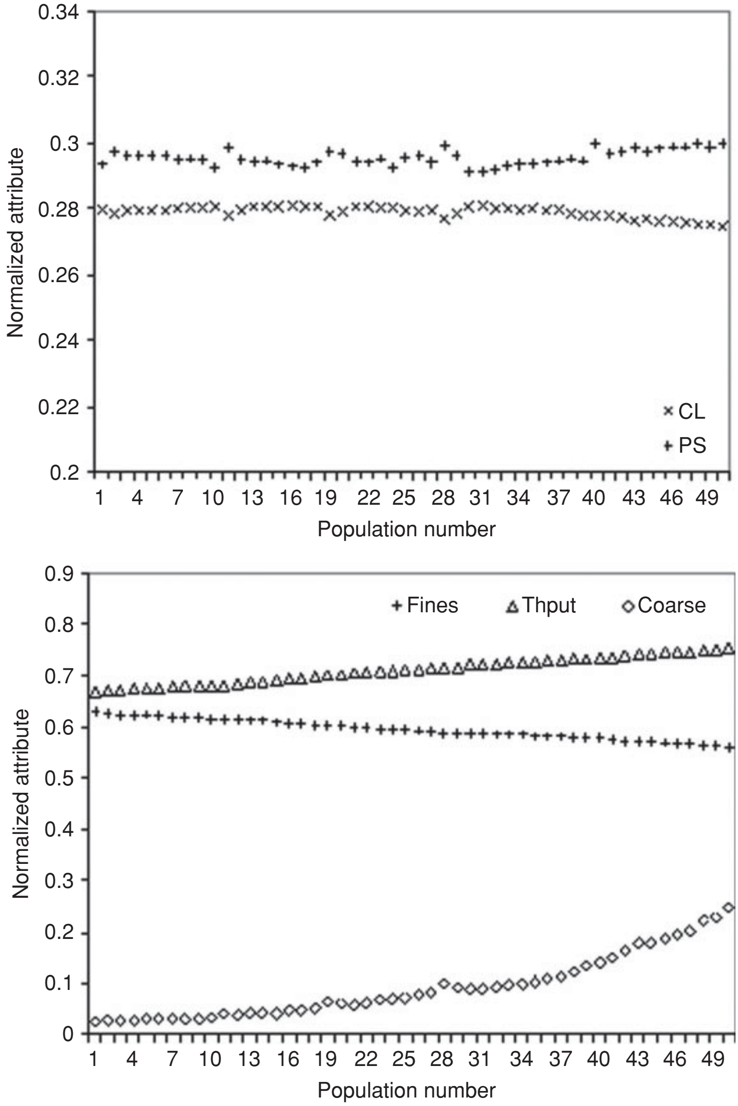

Figure 7.9 *Control variable trends corresponding to PO points for probability value 0.9 in Figure 7.4.*

the value of reliability is allowed to be reduced, a greater degree of freedom is available in the decision variable space leading to a better variety of control variable values. As is evident from Figures 7.9 and 7.10, more variations in alternative solutions with broader range of control variable values (circulation load, percent solids, percent passing coarse size etc.) is available for PO solutions of probability value 0.4.

Some important streams that are constantly monitored for consistent operation of grinding circuit are ball-mill discharge (BMD), rod-mill discharge (RMD), primary cyclone overflow

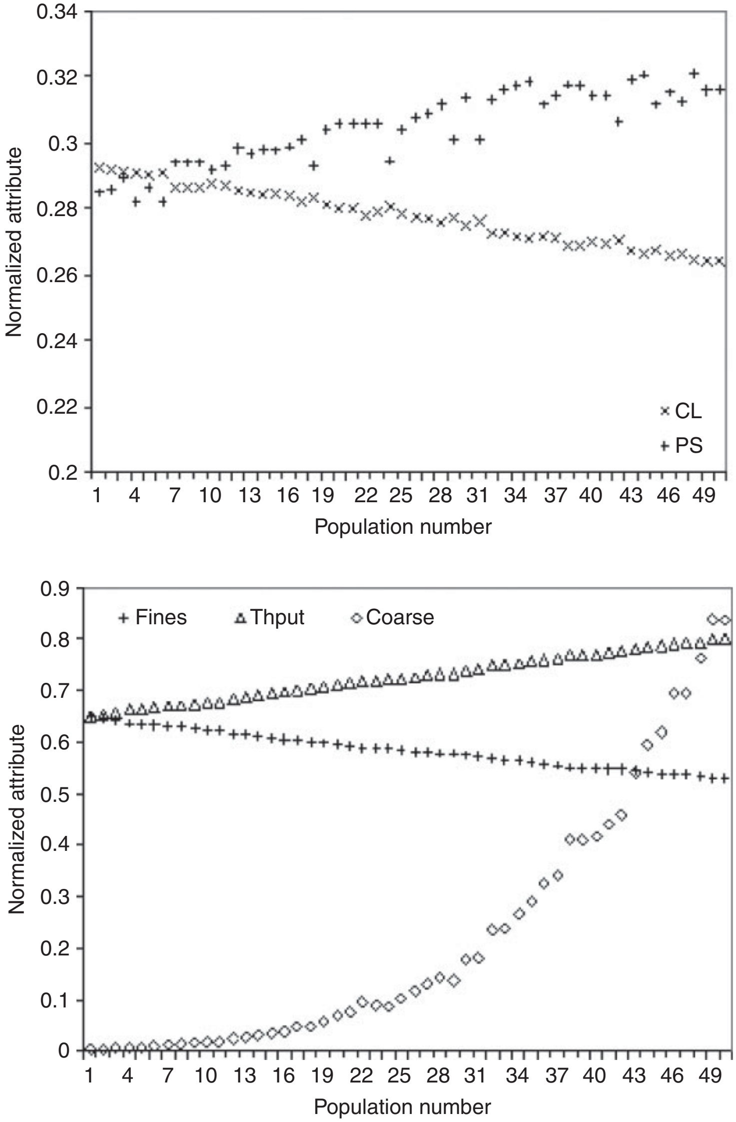

Figure 7.10 *Control variable trends corresponding to PO points for probability value 0.4 in Figure 7.4.*

(PCO), primary cyclone underflow (PCU), secondary cyclone overflow (SCO), secondary cyclone underflow (SCU). The entire Pareto front for probability value 0.9 in Figure 7.4 is divided into three regions: lower (0.65–0.7 on a normalized scale), medium (0.7–0.75 in normalized scale) and upper throughput region (0.75–0.8 on a normalized scale). A representative PO point from each of these regions is chosen and the corresponding size distributions for the 0.9 and 0.4 probability streams mentioned above are presented in

Figures 7.11, and 7.12, respectively. These figures show the change in extent of grinding (coarser or finer) in the process under different conditions. Considering the distribution of SCO (secondary Cyclone overflow) in Figure 7.11(a), (b) and (c), it is clear that the ground particle in Figure 7.11(a) is coarser as compared to that in Figure 7.11(c). As we move from lower to upper throughput regions, a greater percentage passing value for different size classes is reported (see Figure 7.11). A similar trend is also visible as we move towards higher probability values (from 0.4 to 0.9) for higher and medium throughput ranges; however, the trend reverses for the lower throughput range (see Figures 7.11 and 7.12).

This kind of problem of optimization under uncertainty can be solved at the top level of decision making where the higher level decision makers can decide the operating PO front based on the risk appetite in prevailing market conditions. We should remember here that the study of optimization under uncertainty provided us with several PO fronts with different solution reliability level. Once a PO front gets identified, the next target is to identify one solution out of several alternatives that can be treated as a target given to a model-based predictive control (MPC) algorithm to control the plant around it. The identification of a single solution is generally carried out based on the operational constraints at a particular situation. For example, in case of the grinding problem, the selection of the point of operation from the plethora of alternative solutions can be narrowed down by defining various thresholds of values for throughput or mid-size fraction beyond which either the operation is not cost effective or the quality is unacceptable. Here our target is to increase productivity after meeting quality standards. The plant can, therefore, be operated at higher productivity by slightly compromising the quality for some time and vice versa based on slightly stringent / lenient quality requirements of different vendors based on the end applications. This basically involves working with different alternative solutions at different times. In fact, information like the source of ore, the impact of which is very difficult to quantify inside the model, can also determine the operating point because sometimes a particular region of a mine can lead to inferior ore type (with difficult kinetics of ore liberation) for which even excellent plant operation can produce only a limited benefit. In these cases, increasing throughput and compromising quality has no meaning whereas the same principle makes perfect sense when the handled ore is very easy to liberate in the following flotation unit and therefore pushing for more throughput and compromising on mid size cumulative percent passing is a good strategy. The operating target for MPC in this case, therefore, can be a set of alternative solutions instead of a single solution for different operating regimes.

7.5 Conclusions

This chapter presented the fundamentals of chance-constrained programming, a preventive uncertainty-handling technique. First the treatment of linear constraints with uncertain terms separable from decision variables was examined, and this was extended to the case when uncertain and decision variables are inherently embedded with each other. These concepts were demonstrated with a simple example taken from the literature. A simulation-based chance-constrained programming approach was then presented for handling uncertainty for constraints that have a nonlinear relationship with the associated uncertain parameters

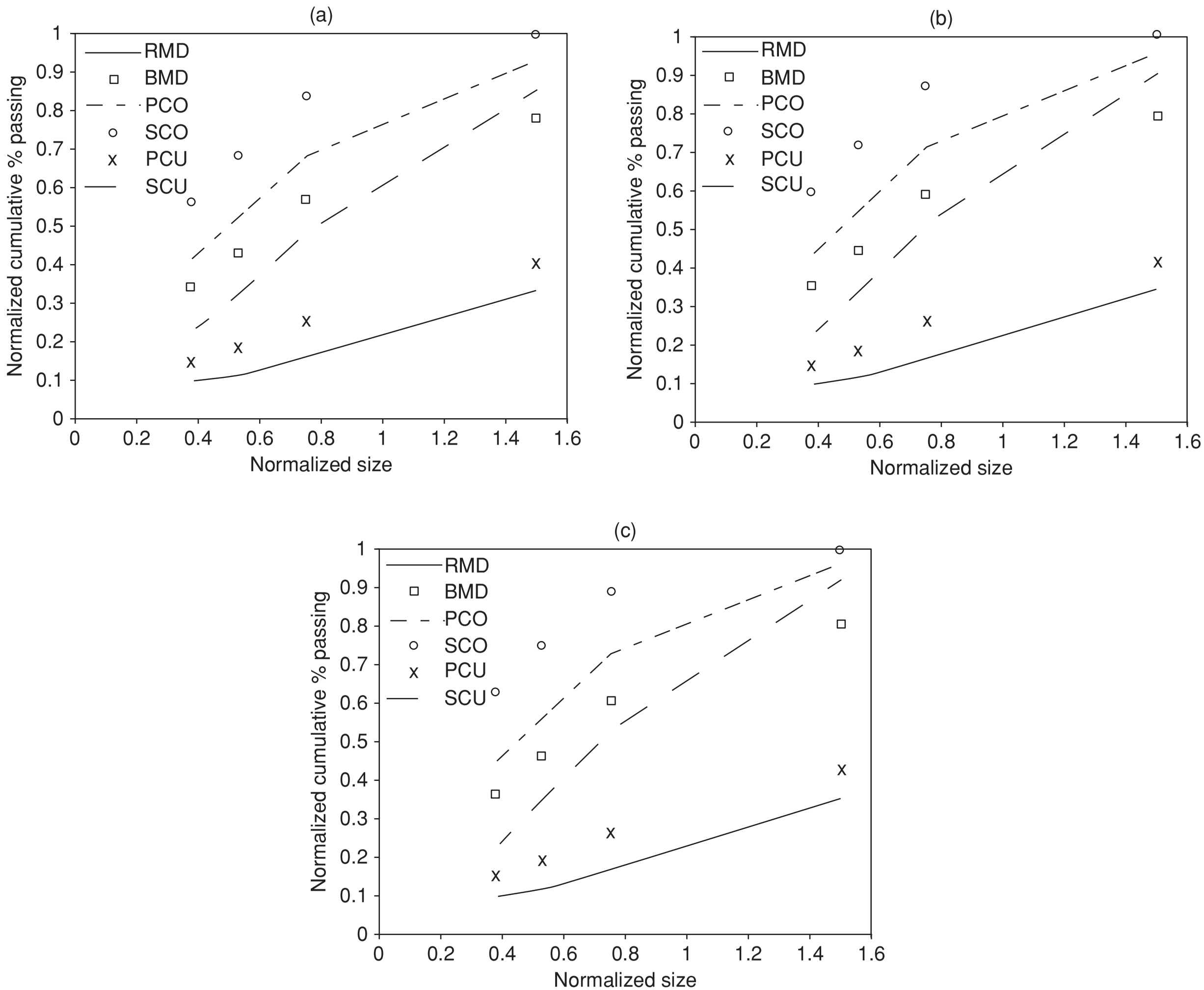

Figure 7.11 *Cumulative percentage passing values for different streams across varied size classes for a representative PO point for probability value 0.9 in Figure 7.4 ((a) high, (b) medium, and (c) low throughput region).*

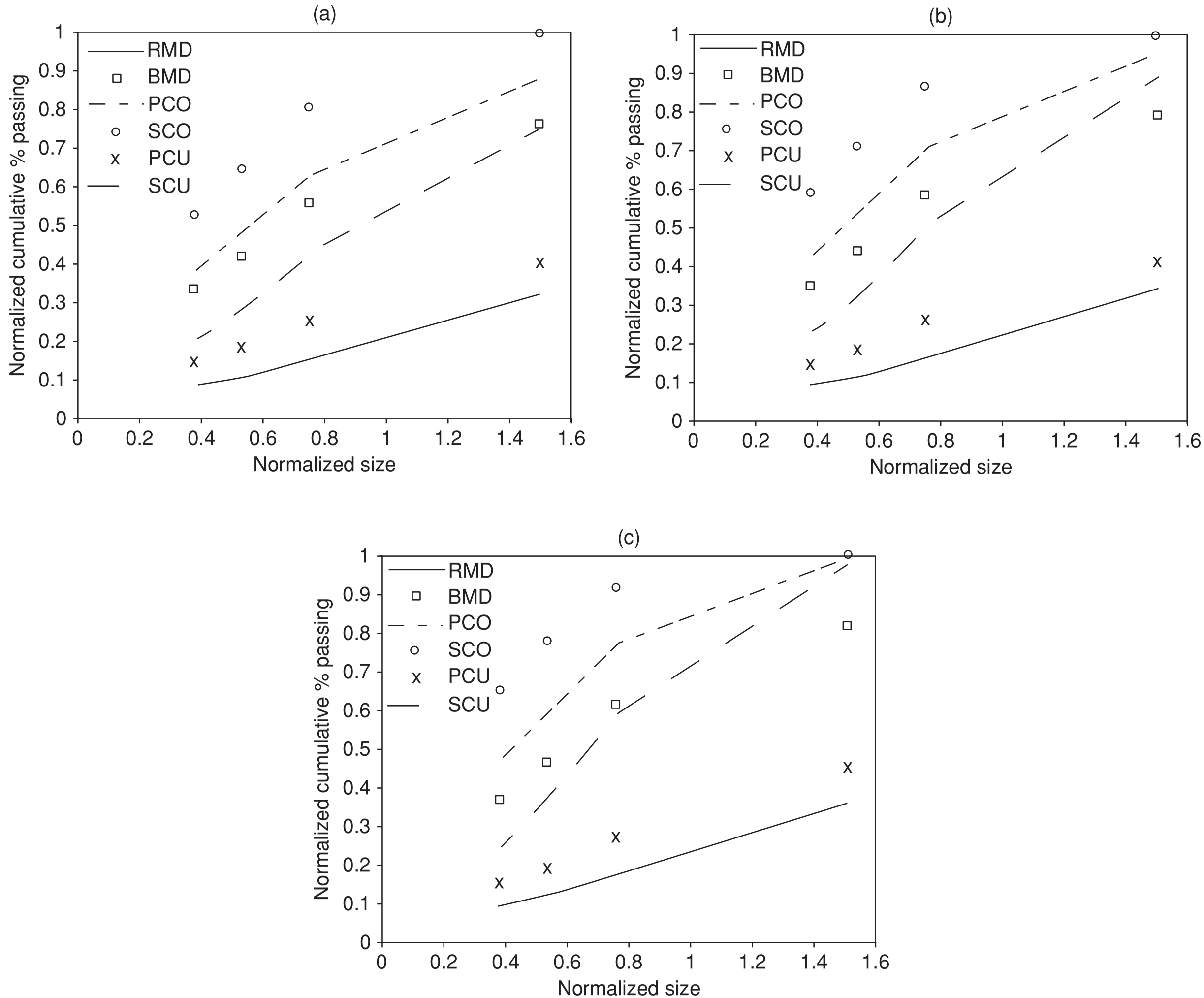

Figure 7.12 *Cumulative percentage passing values for different streams across varied size classes for a representative PO point for probability value 0.4 in Figure 7.4 ((a) high, (b) medium, and (c) low throughput region).*

because the deterministic equivalents of these complicated constraints are not as straightforward as their linear counterparts. The case study considered for this was taken from a real-world example of an industrial grinding operation where uncertainty was considered in parameters (e.g. grindability indices of rod mill and ball mill, sharpness indices of primary and secondary cyclones) that were derived from experiments as well as curve-fitting exercises leading to uncertainty (related to experimental and regression errors) present in obtaining their values. Uncertainty was also considered for parameters that are used as bounds to the constraints and parameters present in objective functions. The flavor of single and multi-objective optimization under uncertainty was demonstrated through various examples in this chapter, which can be solved using appropriate optimization solvers. The probability measure used in uncertainty formulation uses solution reliability as an additional dimension for this problem and this information can be utilized to show the tradeoff between optimality and reliability of solutions. This chapter also demonstrated how an effective postanalysis of multi-objective optimization under uncertainty can lead to intelligent plant operating rules as an outcome of Pareto characterization, which otherwise can be learnt only through extensive and elaborate operational experience on the shop floor over a very long time. A way of identifying solutions of interest from a plethora of alternatives from the chosen PO front has also been discussed.

Nomenclature

ρ = ore density.
δ_i, β_i = premeditated confidence levels to the respective constraints.
ρ_w = water density.
$\bar{f}$ = auxiliary variable for handling uncertainty in objective function f.
$\tilde{S}_M$ = auxiliary variable for handling uncertainty in objective function $\hat{S}_M$.
F^L_{RM}, F^U_{RM} = upper and lower bounds for throughput to the grinding circuit.
W^L_{PS}, W^U_{PS} = upper and lower bounds for water flowrate at primary sump.
W^L_{SS}, W^U_{SS} = upper and lower bounds for water flowrate at secondary sump.
S^U_C = upper bound for percentage passing for the coarse size class.
S^U_F = upper bound for percentage passing for the fine size class.
P^U_S = upper bound for percentage solids of the final ground product.
C^U_L = upper bound for recirculation load of the grinding circuit.
C = solids per unit volume (slurry).
C_L = recirculation load of the grinding circuit.
d(i) = size (in microns) of i^{th} size class.
F = mass fraction of solids in slurry.
f = objective function in optimization problem.
F_{RM} = solid mass flowrate for rod mill.
G_{BM} = grindability index for ball mill.
g_i = i^{th} constraint in optimization problem.
G_{RM} = grindability index for rod mill.
H, H(i) = solids holdup, solids holdup in i^{th} size class.
M = mass flowrate (solids).
m(i) = mass fraction of i^{th} size class in a stream.

N_{max} = maximum number of generations in NSGA II.
N_{pop} = population size in NSGA II.
N_{samp} = sampling size in CCP simulation.
P = probability measure.
p_c = crossover probability in NSGA II.
p_m = mutation probability in NSGA II.
P_S = percent solids of the final ground product.
Q = volume flowrate (slurry).
S_C = percentage passing for the coarse size class.
S_F = percentage passing for the fine size class.
S_M = percentage passing for the mid size class.
S_{PS} = sharpness index for primary hydrocyclone.
S_{SS} = sharpness index for secondary hydrocyclone.
T = grinding circuit product throughput.
V = slurry volume.
W = volume flowrate (water).
W_{PS} = water flowrate at primary sump.
W_{SS} = water flowrate at secondary sump.
x = decision variable set.
ξ = set of uncertain parameters.

Subscripts

ff fresh feed to the unit.
m mill.
mf mill feed (ore + recycle).
mp mill product.
of overflow of a unit.
s sump.
sf sump feed.
sp sump product.
uf underflow of a unit.

Appendices

A.1 CCP for Normally Distributed Uncertain Parameters

In this subsection, we describe how to transform a linear chance constraint into its deterministic equivalent. To illustrate this, we consider the following chance constraint:

$$P\left[\sum_{i}^{n} a_i f_i(x) \leq 0\right] \geq \alpha \tag{7.A1}$$

Here a_i represents the uncertain parameters (normal) and $f_i(x)$ are a set of functions of the deterministic variables x. Denoting $\mu(a_i)$, $\mathrm{Var}(a_i) = E[a_i - \mu(a_i)]^2$, and $\mathrm{Cov}(a_i, a_{i'}) =$

$E[a_i-\mu(a_i)][a_{i'}-\mu(a_{i'})]$ as the mean, variance and covariance of the uncertain parameter a_i, the chance constraint in equation 7.A1 can be written as:

$$P\left[\frac{\sum_i^n a_i f_i(x) - \mu\left[\sum_i^n a_i f_i(x)\right]}{\left\{\mathrm{Var}\left[\sum_i^n a_i f_i(x)\right]\right\}^{1/2}} \le \frac{-\mu\left[\sum_i^n a_i f_i(x)\right]}{\left\{\mathrm{Var}\left[\sum_i^n a_i f_i(x)\right]\right\}^{1/2}}\right] \ge \alpha \tag{7.A2}$$

As the uncertain parameter follows a normal distribution, the expression

$$\frac{\sum_i^n a_i f_i(x) - \mu\left[\sum_i^n a_i f_i(x)\right]}{\left\{\mathrm{Var}\left[\sum_i^n a_i f_i(x)\right]\right\}^{1/2}} \tag{7.A3}$$

is the standardized form of a normally distributed random variable with a mean of zero and a variance of unity. Denoting Φ as the standardized normal cumulative density distribution, equation 7.A2 can be written as:

$$\Phi\left(\frac{-\mu\left[\sum_i^n a_i f_i(x)\right]}{\left\{\mathrm{Var}\left[\sum_i^n a_i f_i(x)\right]\right\}^{1/2}}\right) \ge \alpha \tag{7.A4}$$

Application of inverse on both sides changes equation 7.A4 into

$$\frac{-\mu\left[\sum_i^n a_i f_i(x)\right]}{\left\{\mathrm{Var}\left[\sum_i^n a_i f_i(x)\right]\right\}^{1/2}} \ge \Phi^{-1}(\alpha) \tag{7.A5}$$

Rearranging terms yields

$$\mu\left[\sum_i^n a_i f_i(x)\right] + \Phi^{-1}(\alpha)\left\{\mathrm{Var}\left[\sum_i^n a_i f_i(x)\right]\right\}^{1/2} \le 0 \tag{7.A6}$$

where

$$\mu\left[\sum_i^n a_i f_i(x)\right] = \sum_i^n \mu(a_i) f_i(x) \tag{7.A7}$$

and

$$\mathrm{Var}\left[\sum_i^n a_i f_i(x)\right] = \sum_{i=1}^n \mathrm{Var}(a_i) f_i(x)^2 + 2\sum_{i=1}^n \sum_{i'=i+1}^n f_i(x)\,\mathrm{Cov}(a_i, a_{i'}) f_{i'}(x) \tag{7.A8}$$

Deterministic equivalent, therefore, consists of the mean term augmented by quantile times standard deviation value of the uncertain parameter. For α greater than 0.5, $\Phi^{-1}(\alpha) \ge 0$ in which case the standard deviation term penalizes the deterministic constraint.

A.2 Calculation of Mean and Variance for General Function

In this subsection, we will present certain known results that can be useful in understanding the material presented in this chapter.

Approximate mean and variance of a function of several random variables ($Y = g(X_1, X_2, \ldots, X_n)$, where $X_1, X_2, \ldots, X_n$ are random variables) can be obtained by expanding the function g following Taylor series about the mean values of the random variables:

$$Y = g\left(\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_n\right) + \sum_{i=1}^{n} (X_i - \bar{X}_i) \frac{\partial g}{\partial X_i} + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (X_i - \bar{X}_i)(X_j - \bar{X}_j) \frac{\partial^2 g}{\partial X_i \partial Y_i} + \ldots.. \quad (7.A9)$$

Here the derivatives are to be evaluated at $\left(\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_n\right)$. Considering only the linear terms, we can obtain the following

$$E(Y) = g\left(\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_n\right)$$

$$\mathrm{Var}(Y) = \sum_{i=1}^{n} c_i^2 \mathrm{Var}(X_i) + \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \mathrm{Cov}\left(X_i, X_j\right) \qquad i \neq j \qquad (7.A10)$$

where c_i, c_j terms represent the partial derivatives $\frac{\partial g}{\partial X_i}, \frac{\partial g}{\partial X_j}$ respectively evaluated at $\left(\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_n\right)$. Assuming Y as a linear function of several random variables $\left(Y = \sum_{i=1}^{n} a_i X_i\right)$, the following can be written:

$$E(Y) = \sum_{i=1}^{n} a_i E(X_i)$$

$$\mathrm{Var}(Y) = \sum_{i=1}^{n} a_i^2 \mathrm{Var}(X_i) + \sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j \mathrm{Cov}\left(X_i, X_j\right) \qquad i \neq j \qquad (7.A11)$$

When random variables are independent of each other, the covariance term equals zero.

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