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Robust Targeting of Resource Requirement in a Continuous Water Network

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In this paper, a robust formulation is proposed to calculate the target of freshwater requirement as a resource for continuous processes in industries. The proposed robust counterpart linear programming formulation includes resource minimization constraints and has been applied to optimize the external resource, to satisfy unmet demands in source-sink water allocation problems, with deterministic flows and deterministic quality. Compared to the traditional-scenario-based stochastic programming method, a robust counterpart optimization method has a unique advantage. The scale of the corresponding optimization problem does not increase exponentially with the number of uncertain parameters. Robust optimization applicability has been applied to resource management networks with uncertain qualities and flows for the application of individual sources and demands with the desired reliability. The resultant formulation preserves the linearity of the mathematical model and can control the degree of conservatism for every constraint and guarantees feasibility for the problem. Decision-makers can also make a trade-off between uncertainty level and an upper probability of constraint violation. This model will assist the planner to decide the water requirement under uncertain conditions and to do the necessary preparation accordingly and immunes the process against uncertainties to satisfy demands.

1. Introduction

Water is one of the major resources in process industries. Water resource consumption has recently been identified as one of the important global environmental issues of the 21st Century. Significant research efforts in conserving various resources (such as energy, fresh water, cooling water, hydrogen, raw materials, etc.) in chemical process industries have been directed toward continuous processes. Various linear programming and graphical methodologies have been proposed to minimize the resource requirement for continuous processes. These methodologies are limited for the deterministic case. Uncertainty is a very important concern in real plants to satisfy a fixed demand while targeting minimum resource utilization.

Methodologies have been developed for targeting minimum freshwater requirement with uncertainties in parameters. In an important work, Al-Redhwan et al. (2005) developed an approach based on sensitivity analysis and stochastic programming to develop flexible and resilient process water networks. Further, Zhang et al. (2008) proposed new numerical indices to quantify the resilience of water network designs. Arya et al. (2018) proposed a stochastic Pinch Analysis approach to optimize resource allocation to deal with uncertainties related to source qualities and flows. Tan (2011) presented a fuzzy mathematical programming model for the synthesis of water networks when the model parameters exhibit fuzzy uncertainties.

As an alternative to the scenario-based and fuzzy formulation, the robust counterpart optimization has been proposed. The major advantage of robust counterpart optimization compared to scenario-based stochastic programming is that it doesn't require assumptions regarding the underlying probability distribution of the uncertain data. Previously robust optimization was applied to industrial applications, Bakosova et al. (2013) proposed robust model predictive control of heat exchanger network. Wei et al. (2017) optimized the hydrogen network using the worst case conditional value at risk concept. The proposed framework of the robust formulation (Bertismas and Theile, 2006) is based on solving the robust counterpart optimization problem for

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the uncertain source-sink problem. Bertsimas and Sim (2004) proposed a robust counterpart optimization and that work included sophisticated solution techniques with nontrivial uncertainty sets that described the data. In this paper a formulation for calculating the robust target of resource requirement in a water allocation network (WAN). The developed model utilizes the concept of robustness developed by Bertsimas and Sim (2004). The proposed model is linear and guarantees the optimality. The proposed model enables to decide the robust freshwater requirement based on budget parameters and uncertainty levels. An example is also presented which provides the set of optimal/feasible solutions, given the magnitude of the uncertain data and a reliability level. This solution set provides flexibility to the decision-maker to trade-off between the price of robustness and reliability level. The results are compared with the worst boundary values (Soyester, 1973).

2. Problem Statement and Mathematical Formulation

A set of N_s internal sources is available, and each internal source produces an uncertain at an uncertain quality in a bounded interval with a known deviation from its nominal value. N_d internal demands to be satisfied are also known such that each demand accepts a flow with a quality that is less than a predetermined maximum quality. The unutilized flow from the internal sources is sent to an external demand, called waste, without any maximum quality or flow limits. The objective is to minimize the resource requirement R in a fixed resource allocation network for the desired reliability of each demand as well as each source.
Let $f_{i,j}$ and $f_{r,j}$ represent the flow from i^{th} source and resource to j^{th} demand, and let the flow from i^{th} source to waste be denoted by $f_{i,w}$.F_i^s and F_j^d represents total flow from internal sources and demands. The deterministic optimization problem (Eq(1) as objective) is to minimize resource subject to constraints in Eqs(2)-(4):

$$minimize\ R = \sum_{j=1}^{N_d} f_{r,j}\ ,\ s.t. \tag{1}$$

$$\sum_{j=1}^{N_d} f_{i,j} + f_{i,w} = F_i^s \quad \forall i \tag{2}$$

$$\sum_{j=1}^{N_s} f_{i,j} + f_{r,j} = F_j^d \quad \forall j \tag{3}$$

$$\sum_{i=1}^{N_s} f_{i,j} c_i^s + f_{r,j} c_r \le F_j^d c_j^d \quad \forall j \tag{4}$$

Where, c_i^s, c_r, c_j^d are the concentrations of i^{th} source, resource and j^{th} demand.
The main tools of robust optimization are uncertainty sets and a robust counterpart problem. The uncertainty in the internal source parameters(eg. concentration, flow) is described through uncertainty set. Let there be a matrix A (nonempty uncertainty set Eq(7) and Eq(8)), contains all possible values that may be realized for parametric uncertainties of internal sources. Uncertainty is considered to affect only the constraint coefficient a_α, where every element of the vector a_α i.e. $a_{\alpha\beta}, \beta \in \{1,2,\dots.\mathrm{n}\}$ is uncertain; here α is the index for constraint under uncertainty and β is the index of uncertain parameter. The decision-maker knows range forecasts for all the uncertain parameters, specifically; parameter $a_{\alpha\beta}$ belongs to the interval $[\,\overline{a}_{\alpha\beta} - \hat{a}_{\alpha\beta}, \overline{a}_{\alpha\beta} + \hat{a}_{\alpha\beta}]$. The interval is centred at a nominal value $\overline{a}_{\alpha\beta}$, while $\hat{a}_{\alpha\beta}$ measures the deviation magnitude. The scaled deviation $v_{\alpha\beta}$ of the parameter $a_{\alpha\beta}$ from its nominal value can be defined as in Eq(5) and belongs to [−1, 1].

$$v_{\alpha\beta} = \frac{a_{\alpha\beta} - \overline{a}_{\alpha\beta}}{\hat{a}_{\alpha\beta}} \tag{5}$$

The aggregate scaled deviation for constraint α, $\sum_{\beta=1}^{n} |v_{\alpha\beta}|$, which is more accurate than individual ones, can take any value between 0 and *n*; however, it is improbable that all the coefficients take their worst cases simultaneously. Consequently, the true value of $\sum_{\beta=1}^{n} |v_{\alpha\beta}|$ can be assumed to be a narrower range (Eq(6)), i.e.

$$\sum_{\beta=1}^{n} |v_{\alpha\beta}| \le \Gamma_\alpha \tag{6}$$

Where $\Gamma_\alpha \in [0, n]$ referred to as the budget of the uncertainty of constraint α, is used to adjust the robustness against the level of conservatism of the solution. $\Gamma_\alpha = 0$ Indicates no protection against uncertainty and $\Gamma_\alpha = n$ yields a very conservative solution since it can be interpreted as all the uncertain parameters, taking the worst case values at the same time. For any values between 0 and n, the decision-maker makes a trade-off between the protection level of the constraint and the degree of conservatism of the solution.

The uncertainty set A is:

$$A = \{(a_{\alpha\beta})|a_{\alpha\beta} = \overline{a}_{\alpha\beta} + \hat{a}_{\alpha\beta}v_{\alpha\beta}, \quad \forall\, \alpha, \beta, v_{\alpha\beta} \in V_\alpha\} \tag{7}$$

Where V_α is the set of uncertain parameters in constraint α is defined as :

$$V_\alpha = \{v_\alpha = [v_{\alpha 1}, v_{\alpha 2}, \dots \dots v_{\alpha\beta}] \mid |v_{\alpha\beta}| \le 1, \ \forall v, \ \textstyle\sum_{\beta=1}^{n}|v_{\alpha\beta}| \le \Gamma_\beta\} \tag{8}$$

A robust optimal solution can now be obtained by modifying the deterministic constraint. A general robust counterpart constrained is as follows:

$$a_\alpha x + \min_{v_\alpha \in V_\alpha} \sum_{\beta=1}^{n} \hat{a}_{\alpha\beta}\, x_\beta v_{\alpha\beta} \ge 0\ , \quad \forall\, \alpha \tag{9}$$

Through the application of strong duality, the equivalent model to the problem is:

$$a_\alpha x - \Gamma_\alpha p_\alpha - \sum_{v \in V_\alpha} q_{\alpha\beta} \ge 0, \quad \forall\, \alpha \tag{10}$$

$$z_\alpha + q_{\alpha\beta} \ge \hat{a}_{\alpha\beta} u_\beta, \ \ \forall\, \alpha \tag{11}$$

$$z_\alpha \ge 0, q_{\alpha\beta} \ge 0, \forall\, \alpha \tag{12}$$

Variables $z_\alpha, q_{\alpha\beta}$, and u_β are additional variables introduced by duality theorem for each constraint (Eqs(10)-(12)) of the robust problem. Probability violation methodology can be adapted from Bertsimas and Sim (2004).

3. Robust Mathematical Model for WAN

Based on the formulation stated in Section 2, the mathematical model is described using two cases in order to obtain a robust WAN. Case 1 treats uncertainties only in source flow rates and case 2 treats uncertainties only in the concentration of source flows.

Case 1 - Flow uncertainty: Let us consider that the flow generated by each internal sources is uncertain and can vary in the region $F_i^s \in [\overline{F_\iota^s} - \widehat{F_\iota^s},\ \overline{F_\iota^s} + \widehat{F_\iota^s}]$. The following constraint Eqs(13)-(15) are then modified, analogous to Eqs(10)-(12) into the robust formulation instead of Eq(2) for problem Eq(1) as objective.

$$F_i^s - \textstyle\sum_{j=1}^{N_d} f_{i,j} - f_{i,w} - \Gamma^f z^f - q^f = 0, \quad \forall\, i,j \tag{13}$$

$$z^f + q^f \ge \widehat{F_\iota^s}, \qquad \forall\, i \tag{14}$$

$$z^f \ge 0, q^f \ge 0 \tag{15}$$

Case 2 - Concentration uncertainty: Similarly, quality q_i of each source i can also be uncertain and can vary between the region $[\overline{q_i} - \widehat{q_\iota},\ \overline{q_i} + \widehat{q_\iota}]$. Then the Eq(4) is reformulated as the following constraints:

$$\textstyle\sum_{i=1}^{N_s} f_{i,j} q_i^s + f_{r,j} q_r - F_j^d q_j^d + \Gamma^q z^q + \sum_i^{N_s} q_{i,j} \ \le 0, \quad \forall\, i,j \tag{16}$$

$$z^q + q_{i,j} \ge \widehat{q_\iota} f_{i,j}, \qquad \forall\, i,j \tag{17}$$

$$z^q \ge 0, q_{i,j} \ge 0, \ \forall\, i,j \tag{18}$$

In Eq(13) and Eq(16), the parameter Γ^f and Γ^q are introduced that controlled the degree of conservatism and budget of uncertainty for uncertainty in source flow and quality. The flow chart in Figure 1 shows a resource targeting methodology with uncertain source parameters for optimal reliability of sources. First, the proposed mathematical model is solved using given data by assigning the budget parameter (Γ^f, Γ^q), this will result in attaining minimum target value for the assigned level of uncertainty. Further, calculate the upper bound probability violation for the assigned budget parameter. If the values are satisfactory for the decision-maker then the procedure may end by designing a network using the calculated effective flows, which can guarantee the desired reliability constraints. If the decision-maker is not satisfied then the whole procedure should be repeated with the new value of the budget parameter until the decision-maker can make an appropriate trade-off between the surplus requirement and calculated probability violation value.

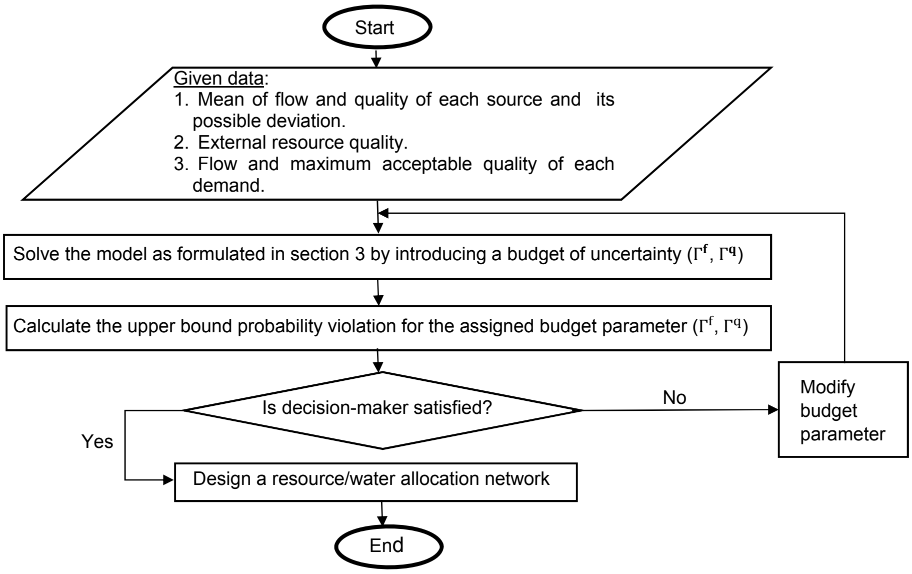

Figure 1: Flowchart for the methodology of targeting resource requirement with parametric uncertainty

4. Illustrative Example

Table 1 gives the source and demand data for the example. The resource is available with a contaminant concentration of 5 ppm. First, the problem (Eq(1) as objective) is solved for the deterministic case (i.e., without any uncertainty) using Eqs(2)-(4) as constraints and the minimum resource requirement is calculated to be 375.27 t/h and 185.27 t/h as waste. Figure 2 shows the WAN for the deterministic case, values in bracket represent the required quality and values outside bracket represent required flows. The network's solid lines represent designed flow allocation from sources to demands and waste.

Table 1: Source and demand data set

Source		**Demand**	
Flow (t/h)	**Contaminant concentration (ppm)**	**Flow (t/h)**	**Contaminant concentration (ppm)**
150 ± 20	80 ± 8	200	20
200 ± 20	60 ± 6	300	70
100 ± 20	55 ± 5.5	100	15
140 ± 20	75 ± 7.5	180	12

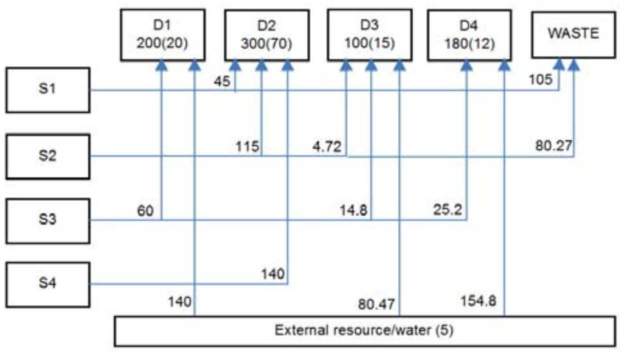

Figure 2: WAN assuming nominal values of the uncertain parameters

Flow uncertainty: In this case, bounded and symmetric uncertainty of flow availability from the source side is given. The availability of flow parameters has ± 20 t/h variability levels for each flow. Here budget parameter takes a value between [0, 1], its variation with objective value is calculated using Eqs(13)-(15) and observed to be linear (Figure 3b). For the worst case ($\Gamma^f = 1$) objective value is 377.09 t/h, producing aggregate waste from all sources at the rate of 107.1 t/h. A detailed comparison of objective value, budget parameter and maximum probability violation is shown in Table 2.

Concertation uncertainty: The variability level in each concentration is given to be 10 % from nominal values shown in Table 1. The resulting minimum resource requirement using Eqs(16)-(18) for worst-case by sticking on the upper bound of contaminant interval i.e. + 10 % for each source is calculated to be 389.55 t/h. Here to the trade-off between uncertainty level and optimum value, budget parameter takes a value between [0, 4]. The trend can be observed in Figure 3b.

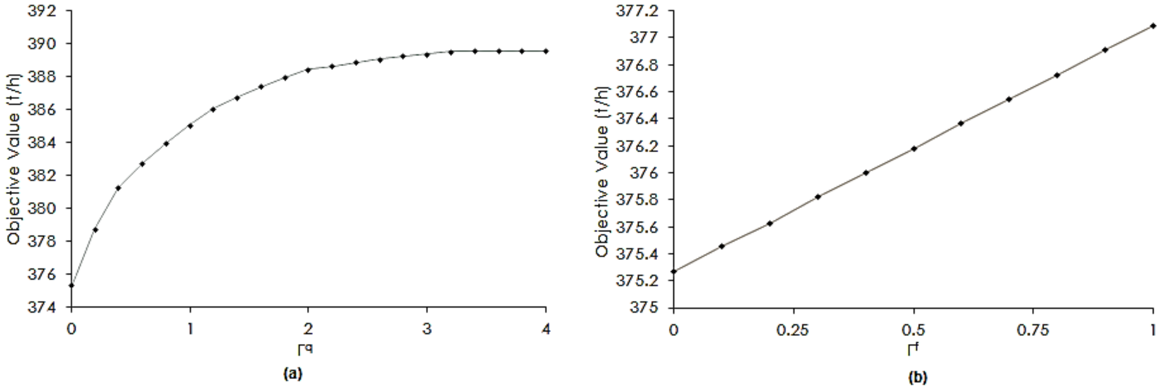

Figure 3: Impact on the objective value with variation in the budget parameter of (a) concentration,(b) flow

Table 2 comprises the set of the result of objective values along with maximum probability violation with respect to the budget parameter. Under full protection against uncertainty, worst case objective value is calculated 389.55 t/h, producing aggregate waste from all sources at the rate of 199.55 t/h. It can also be observed that increasing the protection level above $\Gamma^q = 3.4$ has a negligible impact on objective value.

Table 2. Solution data of example

Flow Uncertainty	**Budget parameter (Γ^f)**	**0**	**0.25**	**0.5**	**0.75**	**1**
	Objective (t/h)	375.27	375.72	376.18	376.63	377.09
	Probability of constrain violation	0.75	0.687	0.625	0.562	0.5
Concentration Uncertainty	**Budget parameter (Γ^q)**	**0**	**1**	**2**	**3**	**4**
	Objective (t/h)	375.27	385.02	388.4	389.35	389.55
	Probability of constraint violation	0.71	0.452	0.295	0.13	0.062
Flow and Concentration Uncertainty	**Budget parameter (Γ^f, Γ^q)**	**(0,0)**	**(0.25,1)**	**(0.5,2)**	**(0.75,3)**	**(1,4)**
	Objective (t/h)	375.27	386.65	392.36	396.59	399.51

Flow and concentration uncertainty: Finally, both uncertain parameters simultaneously including flow with the variability of 20 t/h and concentration with variability level of 10 % for each flow is considered. Several combinations of different budget parameters are used to solve the problem. The results are summarized in Table 2, it shows the relationship between the objective and budget parameter with an upper probability of constraint violation; higher budget parameter results in a more conservative solution with larger feasibility but with higher resource requirement. A simple WAN is shown as an example in Figure 4, for the budget parameters to be $\Gamma^f = 0.5$, $\Gamma^q = 2$, which consequently means the corresponding flow and concentration constraints may be violated with the maximum probability of 62.5 % and 29.5 %, with a minimum resource requirement of 392.36 t/h i.e. 4.5 % more than the requirement for the deterministic case and waste of 162.37 t/h. Optimization considering two different types of uncertainties is studied using the proposed formulation. If this example is solved considering all parameters to take their worst boundary values i.e. lower bound for flow rates and upper bound of contamination level using (Soyester, 1973), the resource requirement is calculated to be 399.51 t/h, which increase the resource requirement by 6.45 % from the deterministic case and with maximum protection against uncertainty. However, this value can be considered as overestimated if the uncertainties in the parametric coefficients lie in the narrower range. The proposed model offers an improvement. It will provide a feasible solution for a relative magnitude of uncertain data and assist decision-maker to trade-off between the feasibility tolerance and a reliability level. The applicability of the proposed mathematical model is demonstrated using an example. The models were solved by the GAMS/ XPRESS solver on the computer (Intel(R) Core(TM) i5 (3 GHz) and 4 GB RAM).

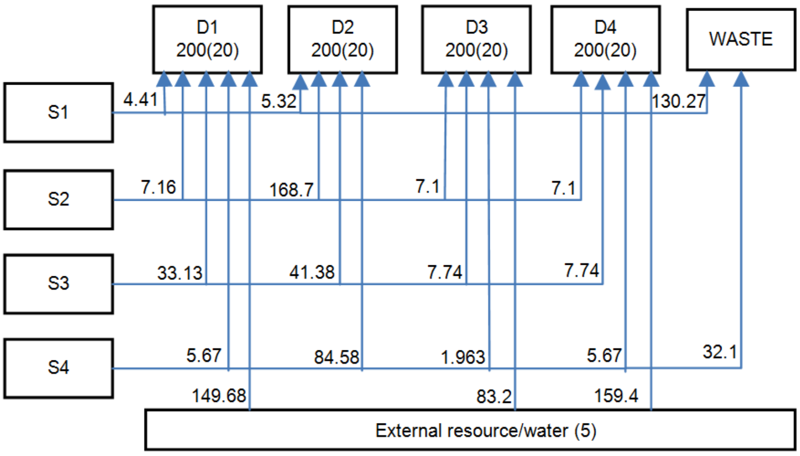

Figure 4. WAN for illustrative example (Γ^f=0.5, Γ^q=2)

5. Conclusions

While targeting minimum resource requirements in real process industries, it is necessary to address different parametric uncertainties related to it. This study examines the optimal use of water resources for WAN problems, considering the issue of parameter uncertainty. A robust optimization approach with the capability of adjusting the level of risk is applied to derive a robust optimal solution for WAN. It can also be observed from the illustrated example that with a certain risk from a full conservative solution, 7.5 t/h water or 180 t/d can be saved. This formulation does not increase the problem size significantly, maintains linearity, and it can control the degree of conservatism for every constraint and guarantee the feasibility for the robust optimization problem with the use of a budget parameter. In future work, the model formulation may be readily expanded to other similar industrial processes and multiperiod aspects.

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